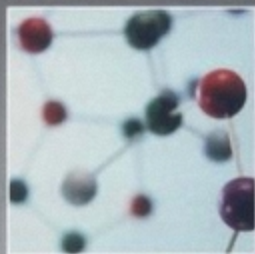


McGraw-Hill **HANDBOOKS**

DEAN'S HANDBOOK OF ORGANIC CHEMISTRY

SECOND EDITION



- Organic and inorganic compounds
- Spectroscopy
- Laboratory manipulations
- Thermodynamic properties

GEORGE W. GOKEL

DEAN'S HANDBOOK OF ORGANIC CHEMISTRY

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Second Edition

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PREFACE

The first edition of the *Handbook of Organic Chemistry* was edited by Professor John A. Dean. It appeared in 1987 and has served as a widely used and convenient reference work for more than 15 years. When Professor Dean asked if I would work with him to develop a second edition, I was pleased to do so. I felt that as valuable as the first edition was, it would be more broadly useful if it contained discussions of the data, the means by which the data were acquired, and perhaps even how the data are applied in modern science. We thus began the revision with enhanced usability as the foremost goal. Sadly, just as we were beginning the effort, Professor Dean passed away. He will be sorely missed.

In following the original plan, many figures, structures, discussions of the methods, and illustrations of the data have been incorporated. Some tables have been reorganized. In some cases tables have been printed twice; although they contain the same data, they are arranged by different criteria. The intent is to make the data easier for the researcher to access and use. Some Internet addresses that can serve as a supplementary resource are included. Despite the numerous additions, the volume remains compact and accessible.

As Professor Dean was not involved in producing this edition, I take responsibility for errors of fact or omission. I hope the volume is error-free, but I would appreciate being informed of any mistakes that are found. Finally, I wish to express my thanks to Mrs. Jolanta Pajewska, who helped in improving the manuscript and the proofreading.

GEORGE W. GOKEL

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SECTION 1

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NOMENCLATURE OF ORGANIC COMPOUNDS

The following synopsis of rules for naming organic compounds and the examples given in explanation are not intended to cover all the possible cases. For a more comprehensive and detailed description, see J. Rigaudy and S. P. Klesney, *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H, Pergamon Press, Oxford, 1979. This publication contains the recommendations of the Commission on Nomenclature of Organic Chemistry and was prepared under the auspices of the International Union of Pure and Applied Chemistry (IUPAC).

Hydrocarbons and Heterocycles

Alkanes. The saturated open-chain (acyclic) hydrocarbons (C_nH_{2n+2}) have names ending in -ane. The first four members have the trivial names *methane* (CH_4), *ethane* (CH_3CH_3 or C_2H_6), *propane* (C_3H_8), and *butane* (C_4H_{10}). For the remainder of the alkanes, the first portion of the name is derived from the Greek prefix (see Table 11.4) that cites the number of carbons in the alkane followed by -ane with elision of the terminal -a from the prefix, as shown in Table 1.1.

TABLE 1.1 Names of Straight-Chain Alkanes

n^*	Name	n^*	Name	n^*	Name	n^*	Name
1	Methane	11	Undecane‡	21	Henicosane	60	Hexacontane
2	Ethane	12	Dodecane	22	Docosane	70	Heptacontane
3	Propane	13	Tridecane	23	Tricosane	80	Octacontane
4	Butane	14	Tetradecane			90	Nonacontane
5	Pentane	15	Pentadecane	30	Triacontane	100	Hectane
6	Hexane	16	Hexadecane	31	Hentriacontane	110	Decahectane
7	Heptane	17	Heptadecane	32	Dotriacontane	120	Icosahectane
8	Octane	18	Octadecane			121	Henicosahectane
9	Nonane†	19	Nonadecane	40	Tetracontane		
10	Decane	20	Icosane§	50	Pentacontane		

* n = total number of carbon atoms.

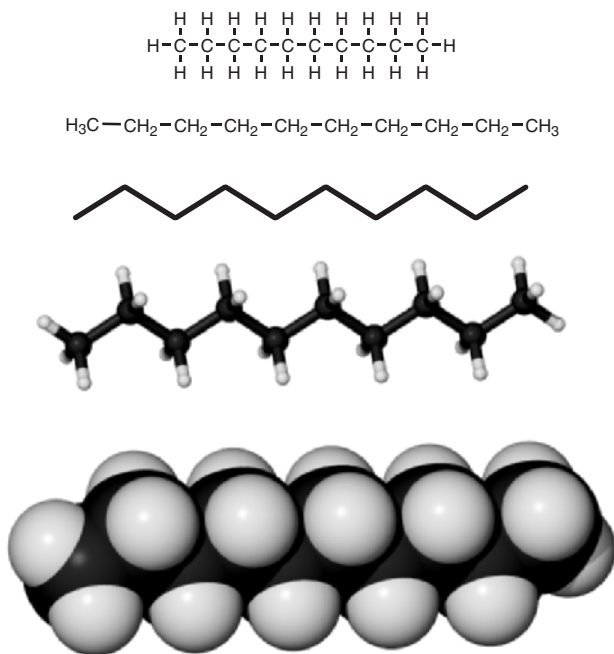
† Formerly called enneane.

‡ Formerly called hendecane.

§ Formerly called eicosane.

For branching compounds, the parent structure is the longest continuous chain present in the compound. Consider the compound to have been derived from this structure by replacement of hydrogen by various alkyl groups. Arabic number prefixes indicate the carbon to which the alkyl group is attached. Start numbering at whichever end of the parent structure that results in the lowest-numbered locants. The arabic prefixes are listed in numerical sequence, separated from each other by commas and from the remainder of the name by a hyphen.

If the same alkyl group occurs more than once as a side chain, this is indicated by the prefixes di-, tri-, tetra-, etc. Side chains are cited in alphabetical order (before insertion of any multiplying prefix). The name of a complex radical (side chain) is considered to begin with the first letter of its complete name. Where names of complex radicals are composed of identical words, priority for citation is given to that radical which contains the lowest-numbered locant at the first cited point of difference in the radical. If two or more side chains are in equivalent positions, the one to be assigned the lowest-numbered locant is that cited first in the name. The complete expression for the side chain may be enclosed in parentheses for clarity or the carbon atoms in side chains may be indicated by primed locants.

FIGURE 1.1 Projections for *n*-decane

If hydrocarbon chains of equal length are competing for selection as the parent, the choice goes in descending order to (1) the chain that has the greatest number of side chains, (2) the chain whose side chains have the lowest-numbered locants, (3) the chain having the greatest number of carbon atoms in the smaller side chains, or (4) the chain having the least-branched side chains.

These trivial names may be used for the unsubstituted hydrocarbons only:

Isobutane $(\text{CH}_3)_2\text{CHCH}_3$

Neopentane $(\text{CH}_3)_4\text{C}$

Isopentane $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$

Isohexane $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3$

Univalent radicals derived from saturated unbranched alkanes by removal of hydrogen from a terminal carbon atom are named by adding -yl in place of -ane to the stem name. Thus the alkane *ethane* becomes the radical *ethyl*. These exceptions are permitted for unsubstituted radicals only:

Isopropyl $(\text{CH}_3)_2\text{CH}-$

Isoptenyl $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2-$

Isobutyl $(\text{CH}_3)_2\text{CHCH}_2-$

Neopentyl $(\text{CH}_3)_3\text{CCH}_2-$

sec-Butyl $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)-$

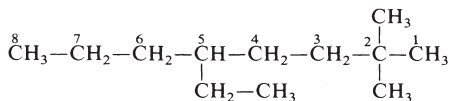
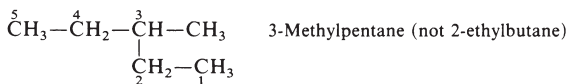
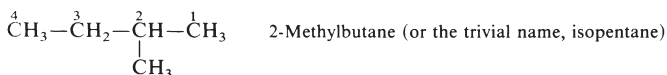
tert-Pentyl $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2-$

tert-Butyl $(\text{CH}_3)_3\text{C}-$

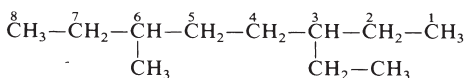
Isohexyl $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_2-$

Note the usage of the prefixes *iso*-, *neo*-, *sec*-, and *tert*-, and note when italics are employed. Italicized prefixes are never involved in alphabetization, except among themselves; thus *sec*-butyl would precede isobutyl, isohexyl would precede isopropyl, and *sec*-butyl would precede *tert*-butyl.

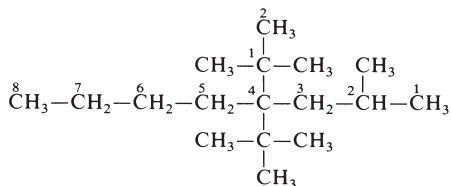
Examples of alkane nomenclature are



5-Ethyl-2,2-dimethyloctane (note cited order)



3-Ethyl-6-methyloctane (note locants reversed)



4,4-Bis(1,1-dimethylethyl)-2-methyloctane

4,4-Bis-1',1'-dimethylethyl-2-methyloctane

4,4-Bis(*tert*-butyl)-2-methyloctane

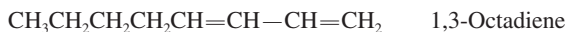
Bivalent radicals derived from saturated unbranched alkanes by removal of two hydrogen atoms are named as follows: (1) If both free bonds are on the same carbon atom, the ending -ane of the hydrocarbon is replaced with -ylidene. However, for the first member of the alkanes it is methylene rather than methyldiene. Isopropylidene, *sec*-butylidene, and neopentylidene may be used for the unsubstituted group only. (2) If the two free bonds are on different carbon atoms, the straight-chain group terminating in these two carbon atoms is named by citing the number of methylene groups comprising the chain. Other carbons groups are named as substituents. Ethylene is used rather than dimethylene for the first member of the series, and propylene is retained for $\text{CH}_3 - \text{CH} = \text{CH}_2 -$ (but trimethylene is $-\text{CH}_2 - \text{CH}_2 - \text{CH}_2 -$).

Trivalent groups derived by the removal of three hydrogen atoms from the same carbon are named by replacing the ending -ane of the parent hydrocarbon with -ylidyne.

Alkenes and Alkynes. Each name of the corresponding saturated hydrocarbon is converted to the corresponding alkene by changing the ending -ane to -ene. For alkynes the ending is -yne. With more than one double (or triple) bond, the endings are -adiene, -atriene, etc. (or -adiyne, -atriyne, etc.). The position of the double (or triple) bond in the parent chain is indicated by a locant obtained by numbering from the end of the chain nearest the double (or triple) bond; thus $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$ is 1-butene and $\text{CH}_3\text{C}\equiv\text{CCH}_3$ is 2-butyne.

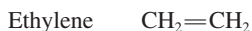
For multiple unsaturated bonds, the chain is so numbered as to give the lowest possible locants to the unsaturated bonds. When there is a choice in numbering, the double

bonds are given the lowest locants, and the alkene is cited before the alkyne where both occur in the name. Examples:

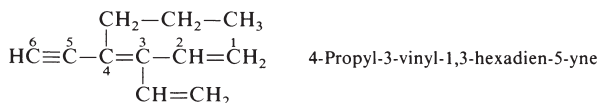


Unsaturated branched acyclic hydrocarbons are named as derivatives of the chain that contains the maximum number of double and/or triple bonds. When a choice exists, priority goes in sequence to (1) the chain with the greatest number of carbon atoms and (2) the chain containing the maximum number of double bonds.

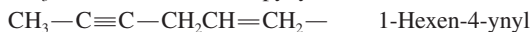
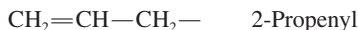
These nonsystematic names are retained:



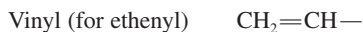
An example of nomenclature for alkenes and alkynes is



Univalent radicals have the endings -enyl, -ynyl, -dienyl, -diynyl, etc. When necessary, the positions of the double and triple bonds are indicated by locants, with the carbon atom with the free valence numbered as 1. Examples:



These names are retained:



Should there be a choice for the fundamental straight chain of a radical, that chain is selected which contains (1) the maximum number of double and triple bonds, (2) the largest number of carbon atoms, and (3) the largest number of double bonds. These are in descending priority.

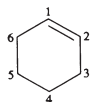
Bivalent radicals derived from unbranched alkenes, alkadienes, and alkynes by removing a hydrogen atom from each of the terminal carbon atoms are named by replacing the endings -ene, -diene, and -yne by -enylene, -dienylene, and -ynylene, respectively. Positions of double and triple bonds are indicated by numbers when necessary. The name *vinylene* instead of ethenylene is retained for $-\text{CH}=\text{CH}-$.

Monocyclic Aliphatic Hydrocarbons. Monocyclic aliphatic hydrocarbons (with no side chains) are named by prefixing cyclo- to the name of the corresponding open-chain hydrocarbon having the same number of carbon atoms as the ring. Radicals are formed as with the alkanes, alkenes, and alkynes. Examples:



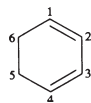
Cyclohexane

Cyclohexyl- (for the radical)



Cyclohexene

1-Cyclohexenyl- (for the radical with the free valence at carbon 1)

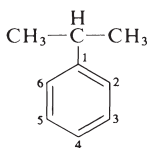


1,3-Cyclohexadiene

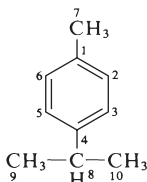
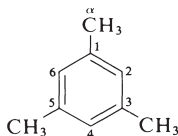
Cyclohexadienyl- (the unsaturated carbons are given numbers as low as possible, numbering from the carbon atom with the free valence given the number 1)

For convenience, aliphatic rings are often represented by simple geometric figures: a triangle for cyclopropane, a square for cyclobutane, a pentagon for cyclopentane, a hexagon (as illustrated) for cyclohexane, etc. It is understood that two hydrogen atoms are located at each corner of the figure unless some other group is indicated for one or both.

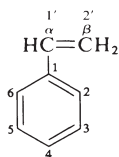
Monocyclic Aromatic Compounds. Except for six retained names, all monocyclic substituted aromatic hydrocarbons are named systematically as derivatives of benzene. Moreover, if the substituent introduced into a compound with a retained trivial name is identical with one already present in that compound, the compound is named as a derivative of benzene. These names are retained:



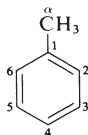
Cumene

Cymene (all three forms; *para*- shown)

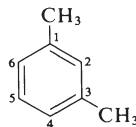
Mesitylene



Styrene



Toluene

Xylene (all three forms; *meta*- shown)

The position of substituents is indicated by numbers, with the lowest locant possible given to substituents. When a name is based on a recognized trivial name, priority for lowest-numbered locants is given to substituents implied by the trivial name. When only two substituents are present on a benzene ring, their position may be indicated by *o*- (*ortho*-), *m*- (*meta*-), and *p*- (*para*-) (and alphabetized in the order given) used in place of 1,2-, 1,3-, and 1,4-, respectively.

Radicals derived from monocyclic substituted aromatic hydrocarbons and having the free valence at a ring atom (numbered 1) are named phenyl (for benzene as parent, since benzyl is used for the radical $\text{C}_6\text{H}_5\text{CH}_2-$), cumenyl, mesityl, tolyl, and xylyl. All other radicals are named as substituted phenyl radicals. For radicals having a single free valence in the side chain, these trivial names are retained:

Benzyl $\text{C}_6\text{H}_5\text{CH}_2-$	Phenethyl $\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2-$
Benzhydryl (alternative to diphenylmethyl) $(\text{C}_6\text{H}_5)_2\text{CH}-$	Styryl $\text{C}_6\text{H}_5\text{CH}=\text{CH}-$
Cinnamyl $\text{C}_6\text{H}_5\text{CH}=\text{CH}-\text{CH}_2-$	Trityl $(\text{C}_6\text{H}_5)_3\text{C}-$

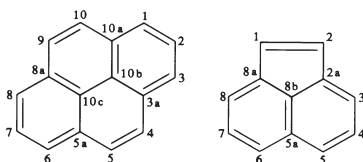
Otherwise, radicals having the free valence(s) in the side chain are named in accordance with the rules for alkanes, alkenes, or alkynes.

The name *phenylene* (*o*-, *m*-, or *p*-) is retained for the radical $-\text{C}_6\text{H}_4-$. Bivalent radicals formed from substituted benzene derivatives and having the free valences at ring atoms are named as substituted phenylene radicals, with the carbon atoms having the free valences being numbered 1,2-, 1,3-, or 1,4-, as appropriate.

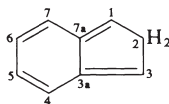
Radicals having three or more free valences are named by adding the suffixes -triyl, -tetrayl, etc. to the systematic name of the corresponding hydrocarbon.

Fused Polycyclic Hydrocarbons. The names of polycyclic hydrocarbons containing the maximum number of conjugated double bonds end in -ene. Here the ending does not denote one double bond. Names of hydrocarbons containing five or more fixed benzene rings in a linear arrangement are formed from a numerical prefix (see Table 11.4) followed by -acene. A partial list of the names of polycyclic hydrocarbons is given in Table 1.2. Many names are trivial.

Numbering of each ring system is fixed, as shown in Table 1.2, but it follows a systematic pattern. The individual rings of each system are oriented so that the greatest number of rings are (1) in a horizontal row and (2) the maximum number of rings are above and to the right (upper-right quadrant) of the horizontal row. When two orientations meet these requirements, the one is chosen that has the fewest rings in the lower-left quadrant. Numbering proceeds in a clockwise direction, commencing with the carbon atom not engaged in ring fusion that lies in the most counterclockwise position of the uppermost ring (upper-right quadrant); omit atoms common to two or more rings. Atoms common to two or more rings are designated by adding lowercase roman letters to the number of the position immediately preceding. Interior atoms follow the highest number, taking a clockwise sequence wherever there is a choice. Anthracene and phenanthrene are two exceptions to the rule on numbering. Two examples of numbering follow:



When a ring system with the maximum number of conjugated double bonds can exist in two or more forms differing only in the position of an "extra" hydrogen atom, the name can be made specific by indicating the position of the extra hydrogen(s). The compound name is modified with a locant followed by an italic capital *H* for each of these hydrogen atoms. Carbon atoms that carry an indicated hydrogen atom are numbered as low as possible. For example, 1*H*-indene is illustrated in Table 1.2; 2*H*-indene would be



Names of polycyclic hydrocarbons with less than the maximum number of noncumulative double bonds are formed from a prefix dihydro-, tetrahydro-, etc., followed by the

name of the corresponding unreduced hydrocarbon. The prefix perhydro- signifies full hydrogenation. For example, 1,2-dihydronaphthalene is

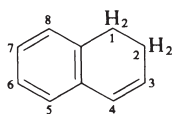
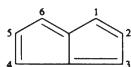


TABLE 1.2 Fused Polycyclic Hydrocarbons

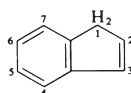
Listed in order of increasing priority for selection as parent compound

Asterisk after a compound denotes exception to systematic numbering.

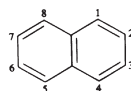
1. Pentalene



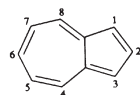
2. Indene



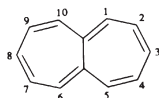
3. Naphthalene



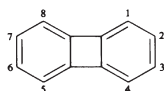
4. Azulene



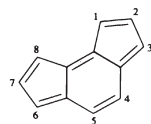
5. Heptalene



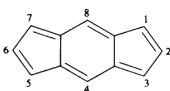
6. Biphenylene



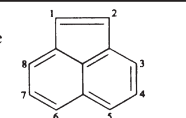
7. *asym*-Indacene



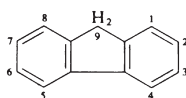
8. *sym*-Indacene



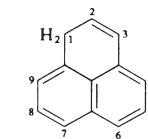
9. Acenaphthylene



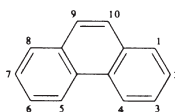
10. Fluorene



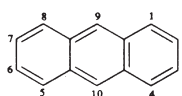
11. Phenalene



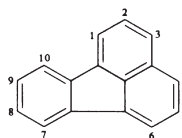
12. Phenanthrene*



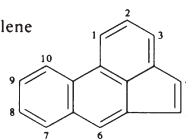
13. Anthracene*



14. Fluoranthene



15. Acephenanthrylene



16. Aceanthrylene

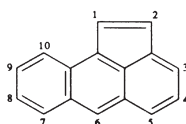
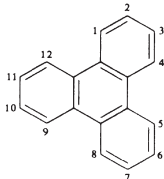
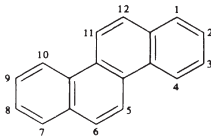
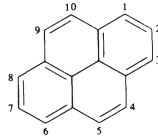
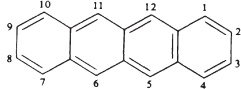
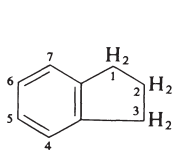


TABLE 1.2 Fused Polycyclic Hydrocarbons (*continued*)*Listed in order of increasing priority for selection as parent compound*

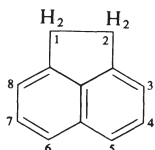
Asterisk after a compound denotes exception to systematic numbering.

<p>17. Triphenylene</p> 	<p>19. Chrysene</p> 
<p>18. Pyrene</p> 	<p>20. Naphthacene</p> 

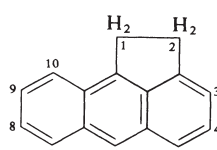
Examples of retained names and their structures are as follows:



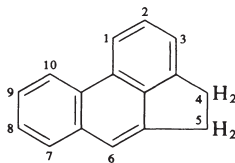
Indan



Acenaphthene



Aceanthrene



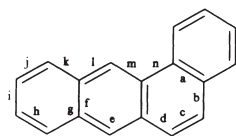
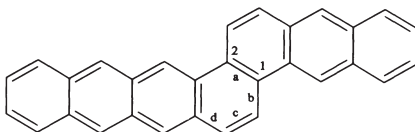
Polycyclic compounds in which two rings have two atoms in common or in which one ring contains two atoms in common with each of two or more rings of a contiguous series of rings and which contain at least two rings of five or more members with the maximum number of noncumulative double bonds and which have no accepted trivial name (Table 1.2) are named by prefixing to the name of the parent ring or ring system designations of the other components. The parent name should contain as many rings as possible (provided it has a trivial name) and should occur as far as possible from the beginning of the list in Table 1.2. Furthermore, the attached component(s) should be as simple as possible. For example, one writes dibenzo phenanthrene and not naphthophenanthrene because the attached component benzo- is simpler than naphtho-. Prefixes designating attached components are formed by changing the ending -ene into -eno-; for example, indeno- from

indene. Multiple prefixes are arranged in alphabetical order. Several abbreviated prefixes are recognized; the parent is given in parentheses:

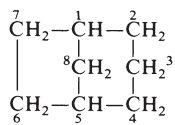
Acenaphtho-	(acenaphthylene)	Naphtho-	(naphthalene)
Anthra-	(anthracene)	Perylo-	(perylene)
Benzo-	(benzene)	Phenanthro-	(phenanthrene)

For monocyclic prefixes other than benzo-, the following names are recognized, each to represent the form with the maximum number of noncumulative double bonds: cyclopenta-, cyclohepta-, cycloocta-, etc.

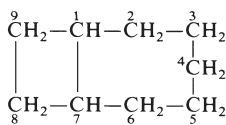
Isomers are distinguished by lettering the peripheral sides of the parent beginning with *a* for the side 1,2-, and so on, lettering every side around the periphery. If necessary for clarity, the numbers of the attached position (1,2-, for example) of the substituent ring are also denoted. The prefixes are cited in alphabetical order. The numbers and letters are enclosed in square brackets and placed immediately after the designation of the attached component. Examples are

Benz[α]anthraceneAnthra[2,1- α]naphthacene

Bridged Hydrocarbons. Saturated alicyclic hydrocarbon systems consisting of two rings that have two or more atoms in common take the name of the open-chain hydrocarbon containing the same total number of carbon atoms and are preceded by the prefix bicyclo-. The system is numbered commencing with one of the bridgeheads, numbering proceeding by the longest possible path to the second bridgehead. Numbering is then continued from this atom by the longer remaining unnumbered path back to the first bridgehead and is completed by the shortest path from the atom next to the first bridgehead. When a choice in numbering exists, unsaturation is given the lowest numbers. The number of carbon atoms in each of the bridges connecting the bridgeheads is indicated in brackets in descending order. Examples are



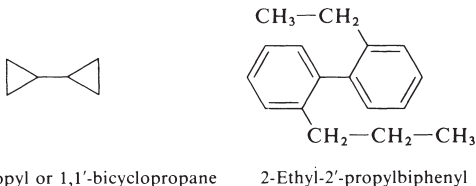
Bicyclo[3.2.1]octane



Bicyclo[5.2.0]nonane

Hydrocarbon Ring Assemblies. Assemblies are two or more cyclic systems, either single rings or fused systems, that are joined directly to each other by double or single bonds. For identical systems naming may proceed (1) by placing the prefix bi- before the name of the corresponding radical or (2) for systems joined through a single bond, by placing the prefix bi- before the name of the corresponding hydrocarbon. In each case, the numbering of the assembly is that of the corresponding radical or hydrocarbon, one system being assigned unprimed numbers and the other primed numbers. The points of attachment

are indicated by placing the appropriate locants before the name; an unprimed number is considered lower than the same number primed. The name *biphenyl* is used for the assembly consisting of two benzene rings. Examples are



1,1'-Bicyclopropyl or 1,1'-bicyclopropane

2-Ethyl-2'-propylbiphenyl

For nonidentical ring systems, one ring system is selected as the parent and the other systems are considered as substituents and are arranged in alphabetical order. The parent ring system is assigned unprimed numbers. The parent is chosen by considering the following characteristics in turn until a decision is reached: (1) the system containing the larger number of rings, (2) the system containing the larger ring, (3) the system in the lowest state of hydrogenation, and (4) the highest-order number of ring systems set forth in Table 1.2. Examples are given, with the deciding priority given in parentheses preceding the name:

- (1) 2-Phenylnaphthalene
- (2) and (4) 2-(2'-Naphthyl)azulene
- (3) Cyclohexylbenzene

Radicals from Ring Systems. Univalent substituent groups derived from polycyclic hydrocarbons are named by changing the final *e* of the hydrocarbon name to -yl. The carbon atoms having free valences are given locants as low as possible consistent with the fixed numbering of the hydrocarbon. Exceptions are naphthyl (instead of naphthalenyl), anthryl (for anthracenyl), and phenanthryl (for phenanthrenyl). However, these abbreviated forms are used only for the simple ring systems. Substituting groups derived from fused derivatives of these ring systems are named systematically. Substituting groups having two or more free bonds are named as described in Monocyclic Aliphatic Hydrocarbons on p. 1.5.

Cyclic Hydrocarbons with Side Chains. Hydrocarbons composed of cyclic and aliphatic chains are named in a manner that is the simplest permissible or the most appropriate for the chemical intent. Hydrocarbons containing several chains attached to one cyclic nucleus are generally named as derivatives of the cyclic compound, and compounds containing several side chains and/or cyclic radicals attached to one chain are named as derivatives of the acyclic compound. Examples are

- | | |
|-----------------------------|--------------------------------|
| 2-Ethyl-1-methylnaphthalene | Diphenylmethane |
| 1,5-Diphenylpentane | 2,3-Dimethyl-1-phenyl-1-hexene |

Recognized trivial names for composite radicals are used if they lead to simplifications in naming. Examples are

- 1-Benzyl-naphthalene 1,2,4-Tris(3-*p*-tolylpropyl)benzene

Fulvene, for methylenecyclopentadiene, and stilbene, for 1,2-diphenylethylene, are trival names that are retained.

Heterocyclic Systems. Heterocyclic compounds can be named by relating them to the corresponding carbocyclic ring systems by using replacement nomenclature. Heteroatoms are denoted by prefixes ending in *-a*, as shown in Table 1.3. If two or more replacement prefixes are required in a single name, they are cited in the order of their listing in the table. The lowest possible numbers consistent with the numbering of the corresponding carbocyclic system are assigned to the heteroatoms and then to carbon atoms bearing double

TABLE 1.3 Specialist Nomenclature for Heterocyclic Systems

Heterocyclic atoms are listed in decreasing order of priority

Element	Valence	Prefix	Element	Valence	Prefix
Oxygen	2	Oxa-	Antimony	3	Stiba-*
Sulfur	2	Thia-	Bismuth	3	Bisma-
Selenium	2	Selena-	Silicon	4	Sila-
Tellurium	2	Tellura-	Germanium	4	Germa-
Nitrogen	3	Aza-	Tin	4	Stanna-
Phosphorus	3	Phospha-*	Lead	4	Plumba-
Arsenic	3	Arsa-*	Boron	3	Bora-
			Mercury	2	Mercura-

* When immediately followed by *-in* or *-ine*, *phospha-* should be replaced by *phosphor-*, *arsa-* by *arsen-*, and *stiba-* by *antimon-*. The saturated six-membered rings corresponding to phosphorin and arsenin are named *phosphorinane* and *arsenane*. A further exception is the replacement of borin by borinane.

TABLE 1.4 Suffixes for Specialist Nomenclature of Heterocyclic Systems

Number of ring members	Rings containing nitrogen		Rings containing no nitrogen	
	Unsaturation*	Saturation	Unsaturation*	Saturation
3	-irine	-iridine	-irene	-irane
4	-ete	-etidine	-ete	-etane
5	-ole	-olidine	-ole	-olane
6	-ine†	‡	-in	-ane§
7	-epine	‡	-epin	-epane
8	-ocene	‡	-ocin	-ocane
9	-onine	‡	-onin	-onane
10	-ecine	‡	-ecin	-ecane

* Unsaturation corresponding to the maximum number of noncumulative double bonds. Heteroatoms have the normal valences given in Table 1.3.

† For phosphorus, arsenic, antimony, and boron, see the special provisions in Table 1.3.

‡ Expressed by prefixing *perhydro-* to the name of the corresponding unsaturated compound.

§ Not applicable to silicon, germanium, tin, and lead; *perhydro-* is prefixed to the name of the corresponding unsaturated compound.

TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names*Listed in order of increasing priority as senior ring system*

Asterisk after a compound denotes exception to systematic numbering.



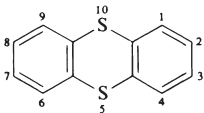



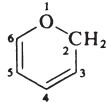

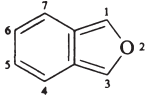

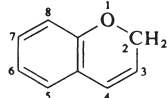

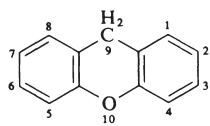

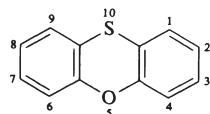
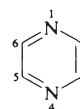
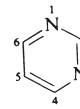

Structure	Parent name	Radical name	Structure	Parent name	Radical name
	Thiophene	Thienyl		2H-Pyrrole	2H-Pyrrolyl
	Thianthrene	Thianthrenyl		Pyrrole	Pyrrolyl
	Furan	Furyl		Imidazole	Imidazolyl
	Pyran (2H-shown)	Pyranyl		Pyrazole	Pyrazolyl
	Isobenzofuran	Isobenzofuranyl		Isothiazole	Isothiazolyl
	Chromene (2H-shown)	Chromenyl		Isoxazole	Isoxazolyl
	Xanthene*	Xanthenyl		Pyridine	Pyridyl
	Phenoxathiin	Phenoxathiinyl		Pyrazine	Pyrazinyl
				Pyrimidine	Pyrimidinyl
				Pyridazine	Pyridazinyl

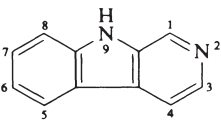
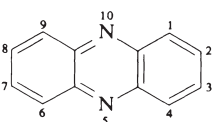
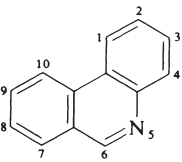
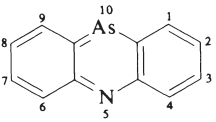
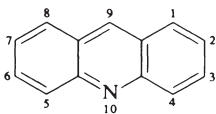
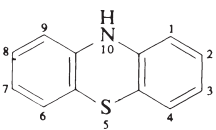
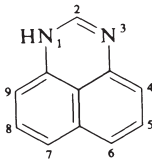

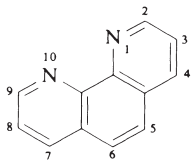
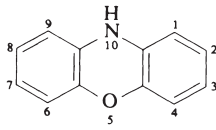
TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names (*continued*)
Listed in order of increasing priority as senior ring system

Asterisk after a compound denotes exception to systematic numbering.

Structure	Parent name	Radical name	Structure	Parent name	Radical name
	Indolizine	IndolizinyI		Phthalazine	PhthalazinyI
	Isoindole	IsoindolyI		Naphthyridine (1,8-shown)	NaphthyridinyI
	3 <i>H</i> -Indole	3 <i>H</i> -IndolyI		Quinoxaline	QuinoxalinyI
	Indole	IndolyI		Quinazoline	QuinazolinyI
	1 <i>H</i> -Indazole	1 <i>H</i> -Indazolyl		Cinnoline	CinnolinyI
	Purine*	PurinyI		Pteridine	PteridinyI
	4 <i>H</i> -Quinolizine	4 <i>H</i> -QuinolizinyI		4 <i>aH</i> -Carbazole*	4 <i>aH</i> -Carbazolyl
	Isoquinoline	IsoquinolyI		Carbazole*	Carbazolyl
	Quinoline	QuinolyI			

TABLE 1.5 Trivial Names of Heterocyclic Systems Suitable for Use in Fusion Names (*continued*)
 Listed in order of increasing priority as senior ring system

Asterisk after a compound denotes exception to systematic numbering.

Structure	Parent name	Radical name	Structure	Parent name	Radical name
	β -Carboline	β -Carbolinyl		Phenazine	Phenazinyl
	Phenanthri- dine	Phenanthri- dinyl		Phenarsazine	Phenarsazinyl
	Acridine*	Acridinyl		Phenothiazine	Phenothiazinyl
	Perimidine	Perimidinyl		Furazan	Furazanyl
	Phenanthroline (1,10-shown)	Phenanthrolinyl		Phenoxazine	Penoxazinyl

or triple bonds. Locants are cited immediately preceding the prefixes or suffixes to which they refer. Multiplicity of the same heteroatom is indicated by the appropriate prefix in the series: di-, tri-, tetra-, penta-, hexa-, etc.

If the corresponding carbocyclic system is partially or completely hydrogenated, the additional hydrogen is cited using the appropriate *H*- or hydro- prefixes. A trivial name from Tables 1.5 and 1.6, if available, along with the state of hydrogenation may be used. In the specialist nomenclature for heterocyclic systems, the prefix or prefixes from

TABLE 1.6 Trivial Names for Heterocyclic Systems that are Not Recommended for Use in Fusion Names*Listed in order of increasing priority*

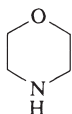
Structure	Parent name	Radical name	Structure	Parent name	Radical name
	Isochroman	Isochromanyl		Pyrazoline (3-shown*)	Pyrazolynyl
	Chroman	Chromanyl		Piperidine	Piperidyl†
	Pyrrolidine	Pyrrolidinyl		Piperazine	Piperazinyl
	Pyrroline (2-shown*)	Pyrrolinyl		Indoline	Indolynyl
	Imidazolidine	Imidazolidinyl		Isoindoline	Isoindolynyl
	Imidazoline (2-shown*)	Imidazolynyl		Quinuclidine	Quinuclidinyl
	Pyrazolidine	Pyrazolidinyl		Morpholine	Morpholynyl‡

* Denotes position of double bond.

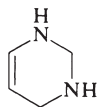
† For 1-piperidyl, use piperidino.

‡ For 4-morpholynyl, use morpholino.

Table 1.3 are combined with the appropriate stem from Table 1.4, eliding an *-a* where necessary. Examples of acceptable usage, including (1) replacement and (2) specialist nomenclature, are



- (1) 1-Oxa-4-azacyclohexane
(2) 1,4-Oxazoline
Morpholine



- (1) 1,3-Diazacyclohex-5-ene
(2) 1,2,3,4-Tetrahydro-1,3-diazine



- (1) Thiacyclopropane
(2) Thiirane
Ethylene sulfide

Radicals derived from heterocyclic compounds by removal of hydrogen from a ring are named by adding *-yl* to the names of the parent compounds (with elision of the final *e*, if present). These exceptions are retained:

Furyl (from furan)	Furfuryl (for 2-furylmethyl)
Pyridyl (from pyridine)	Furfurylidene (for 2-furylmethylene)
Piperidyl (from piperidine)	Thienyl (from thiophene)
Quinolyl (from quinoline)	Thenylidyne (for thienylmethyldiyne)
Isoquinolyl	Furfuryldiyne (for 2-furylmethyldiyne)
Thenylidene (for thienylmethylene)	Thenyl (for thienylmethyl)

Also, piperidino- and morpholino- are preferred to 1-piperidyl- and 4-morpholinyl-, respectively.

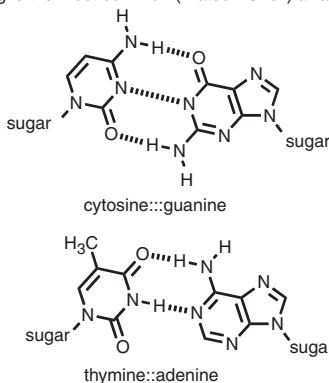
If there is a choice among heterocyclic systems, the parent compound is decided in the following order of preference:

1. A nitrogen-containing component
2. A component containing a heteroatom, in the absence of nitrogen, as high as possible in Table 1.3
3. A component containing the greatest number of rings
4. A component containing the largest possible individual ring
5. A component containing the greatest number of heteroatoms of any kind
6. A component containing the greatest variety of heteroatoms
7. A component containing the greatest number of heteroatoms first listed in Table 1.3

If there is a choice between components of the same size containing the same number and kind of heteroatoms, choose as the base component that one with the lower numbers for the heteroatoms before fusion. When a fusion position is occupied by a heteroatom, the names of the component rings to be fused are selected to contain the heteroatom.

Common Names of Heterocycles Used Broadly in Biology. The naming of heterocycles by systematic methods is important but cumbersome for designating some of the most commonly occurring heterocycles. In particular, the bases that occur in ribonucleic acids (RNA) and deoxyribonucleic acids (DNA) have specific substitution patterns. Because they occur so commonly, they have been given trivial names that are invariably used when discussed or named in the biological literature.

Base pairing is the most common (Watson-Crick) arrangement.



The individual elements of RNA and DNA chains.

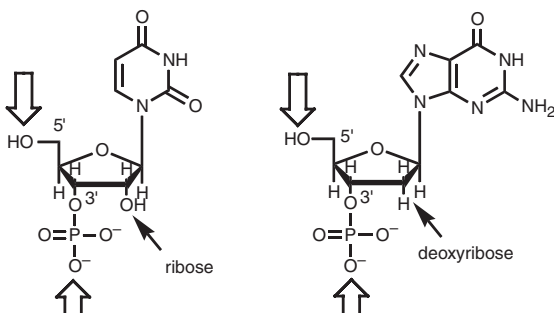


FIGURE 1.2 Base pairing in the most common (Watson-Crick) arrangement. The individual elements of RNA and DNA chains are shown in the lower panel of the figure. Hollow arrows indicate the points at which the 5'-hydroxyl group is esterified to the 3'-phosphate group to form the so-called "sugar-phosphate" backbone. Note the hydroxyl group (arrow) that is present on ribose but missing in deoxyribose.

The structural frameworks of DNA and RNA are organized by hydrogen bond formation between pairs of purine and pyrimidine bases. The pyrimidines are shown near the end of Table 1.5. Cytosine (C) and thymine (T) occur in DNA and form hydrogen-bonded pairs with the purines guanine (G) and adenine (A), respectively. The base pairs are abbreviated AT and GC, sometimes with dotted lines connecting them. The AT pair is held together by two hydrogen bonds and may be represented in shorthand as A::T. Three H-bonds hold together guanine and cytosine, giving G::C. The so-called Watson-Crick base pairing is shown in Figure 1.2. In RNA, uracil replaces thymine but pairing still occurs with adenine to give A::U.

An alternative form of hydrogen bonding between base pairs is designated "Hoogsteen." This type of bonding cannot readily occur in nature because the purine and pyrimidine bases are constrained to long chains that must interact at numerous points.

Functionalized Compounds

There are several types of nomenclature systems that are recognized. Which type to use is sometimes obvious from the nature of the compound. Substitutive nomenclature, in general, is preferred because of its broad applicability, but radicofunctional, additive, and replacement nomenclature systems are convenient in certain situations.

Substitutive Nomenclature. The first step is to determine the kind of characteristic (functional) group for use as the principal group of the parent compound. A characteristic group is a recognized combination of atoms that confers characteristic chemical properties on the molecule in which it occurs. Carbon-to-carbon unsaturation and heteroatoms in rings are considered nonfunctional for nomenclature purposes.

Substitution means the replacement of one or more hydrogen atoms in a given compound by some other kind of atom or group of atoms, functional or nonfunctional. In substitutive nomenclature, each substituent is cited as either a prefix or a suffix to the name of the parent (or substituting radical) to which it is attached; the latter is denoted the parent compound (or parent group if a radical).

In Table 1.7 are listed the general classes of compounds in descending order of preference for citation as suffixes, that is, as the parent or characteristic compound. When oxygen is

TABLE 1.7 Characteristic Groups for Substitutive Nomenclature

Listed in order of decreasing priority for citation as principal group or parent name

Class	Formula*	Prefix	Suffix
1. Cations	H_4N^+ H_3O^+ H_3S^+ H_3Se^+ H_2Cl^+ H_2Br^+ H_2I^+	-onio- Ammonio- Oxonio- Sulfonio- Selenonio- Chloronio- Bromonio- Iodonio-	-onium -ammonium -oxonium -sulfonium -selenonium -chloronium -bromonium -iodonium
2. Acids			
Carboxylic	$-\text{COOH}$ $-(\text{C})\text{OOH}$ $-\text{C}(=\text{O})\text{OOH}$	Carboxy-	-carboxylic acid -oic acid -peroxy...carboxylic acid -peroxy...oic acid
Sulfonic	$-(\text{C}=\text{O})\text{OOH}$		-peroxy...oic acid
Sulfinic	$-\text{SO}_3\text{H}$	Sulfo-	-sulfonic acid
Sulfenic	$-\text{SO}_2\text{H}$	Sulfinio-	-sulfinic acid
Salts	$-\text{SOH}$	Sulfeno-	-sulfenic acid
	$-\text{COOM}$		Metal...carboxylate
	$-(\text{C})\text{OOM}$		Metal...oate
	$-\text{SO}_3\text{M}$		Metal...sulfonate
	$-\text{SO}_2\text{M}$		Metal...sulfinate
	$-\text{SOM}$		Metal...sulfenate
3. Derivatives of acids			
Anhydrides	$-\text{C}(=\text{O})\text{OC}(=\text{O})-$ $-(\text{C}=\text{O})\text{O}(\text{C}=\text{O})-$		-carboxylic anhydride -oic anhydride
Esters	$-\text{COOR}$ $-\text{C}(\text{OOR})$	R-oxycarbonyl-	R...carboxylate R...oate
Acid halides	$-\text{CO}-\text{halogen}$	Haloformyl	-carbonyl halide
Amides	$-\text{CO}-\text{NH}_2$ $(\text{C})\text{O}-\text{NH}_2$	Carbamoyl-	-carboxamide -amide

TABLE 1.7 Characteristic Groups for Substitutive Nomenclature (*continued*)*Listed in order of decreasing priority for citation as principal group or parent name*

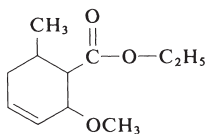
Class	Formula*	Prefix	Suffix
Hydrazides	—CO—NHNH ₂ —(CO)—NHNH ₂	Carbonyl-hydrazino-	-carbohydrazide -ohydrazide
Imides	—CO—NH—CO—	R-imido-	-carboximide
Amidines	—C(=NH)—NH ₂ —(C=NH)—NH ₂	Amidino-	-carboxamidine -amidine
4. Nitrile (cyanide)	—CN —(C)N	Cyano-	-carbonitrile -nitrile
5. Aldehydes	—CHO —(C=O)H (then their analogs and derivatives)	Formyl- Oxo-	-carbaldehyde -al
6. Ketones	>(C=O) (then their analogs and derivatives)	Oxo-	-one
7. Alcohols (and phenols)	—OH	Hydroxy-	-ol
Thiols	—SH	Mercapto-	-thiol
8. Hydroperoxides	—O—OH	Hydroperoxy-	
9. Amines	—NH ₂	Amino-	-amine
Imines	=NH	Imino-	-imine
Hydrazines	—NHNH ₂	Hydrazino-	-hydrazine
10. Ethers	—OR	R-oxy-	
Sulfides	—SR	R-thio-	
11. Peroxides	—O—OR	R-dioxy-	

* Carbon atoms enclosed in parentheses are included in the name of the parent compound and not in the suffix or prefix.

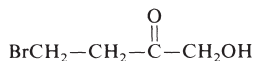
replaced by sulfur, selenium, or tellurium, the priority for these elements is in the descending order listed. The higher valence states of each element are listed before considering the successive lower valence states. Derivative groups have priority for citation as principal group after the respective parents of their general class.

In Table 1.8 are listed characteristic groups that are cited only as prefixes (never as suffixes) in substitutive nomenclature. The order of listing has no significance for nomenclature purposes.

Systematic names formed by applying the principles of substitutive nomenclature are single words except for compounds named as acids. First one selects the parent compound, and thus the suffix, from the characteristic group listed earliest in Table 1.7. All remaining functional groups are handled as prefixes that precede, in alphabetical order, the parent name. Two examples may be helpful:



Structure 1



Structure 2

TABLE 1.8 Characteristic Groups Cited Only as Prefixes in Substitutive Nomenclature

Characteristic group	Prefix	Characteristic group	Prefix
—Br	Bromo-	—IX ₂	X may be halogen or a radical; dihalogenoiodo- or diacetoxyiodo-, e.g., —ICl ₂ is dichloroiodo-
—Cl	Chloro-	$=N^{\oplus}=N^{\ominus}$	Diazo-
—ClO	Chlorosyl-	—N ₃ , —N=N ⁺ =N [−]	Azido-
—ClO ₂	Chloryl-	—N=O	Nitroso-
—ClO ₃	Perchloryl-	—NO ₂ , —N ⁺ ≡O	Nitro-
—F	Fluoro-	$=N^{\oplus} \begin{array}{l} \text{OH} \\ \diagup \\ \text{O}^{\ominus} \end{array}$	<i>aci</i> -Nitro-
—I	Iodo-	—OR	R-oxy-; alkoxy- or aryloxy-
—IO	Iodosyl-	—SR	R-thio-; alkylthio- or arylthio-
—IO ₂	Iodyl*	—SeR (—TeR)	R-seleno- (R-telluro-)
—I(OH) ₂	Dihydroxyiodo-		

* Formerly iodoxy-.

Structure 1 contains an ester group and an ether group. Since the ester group has higher priority, the name is ethyl 2-methoxy-6-methyl-3-cyclohexene-1-carboxylate. Structure 2 contains a carbonyl group, an hydroxy group, and a bromo group. The latter is never a suffix. Between the other two, the carbonyl group has higher priority, the parent has -one as suffix, and the name is 4-bromo-1-hydroxy-2-butanone.

Selection of the principal alicyclic chain or ring system is governed by the following selection rules:

1. For purely alicyclic compounds, the selection process proceeds successively until a decision is reached: (a) the maximum number of substituents corresponding to the characteristic group cited earliest in Table 1.7, (b) the maximum number of double and triple bonds considered together, (c) the maximum length of the chain, and (d) the maximum number of double bonds. Additional criteria, if needed for complicated compounds, are given in the IUPAC nomenclature rules.
2. If the characteristic group occurs only in a chain that carries a cyclic substituent, the compound is named as an aliphatic compound into which the cyclic component is substituted; a radical prefix is used to denote the cyclic component. This chain need not be the longest chain.
3. If the characteristic group occurs in more than one carbon chain and the chains are not directly attached to one another, then the chain chosen as parent should carry the largest number of the characteristic group. If necessary, the selection is continued as in rule 1.
4. If the characteristic group occurs only in one cyclic system, that system is chosen as the parent.
5. If the characteristic group occurs in more than one cyclic system, that system is chosen as parent which (a) carries the largest number of the principal group or, failing to reach a decision, (b) is the senior ring system.
6. If the characteristic group occurs both in a chain and in a cyclic system, the parent is that portion in which the principal group occurs in largest number. If the numbers are the same, that portion is chosen which is considered to be the most important or is the senior ring system.

7. When a substituent is itself substituted, all the subsidiary substituents are named as prefixes and the entire assembly is regarded as a parent radical.
8. The seniority of ring systems is ascertained by applying the following rules successively until a decision is reached: (a) all heterocycles are senior to all carbocycles, (b) for heterocycles, the preference follows the decision process described under "Heterocyclic Systems," page 1–12, (c) the largest number of rings, (d) the largest individual ring at the first point of difference, (e) the largest number of atoms in common among rings, (f) the lowest letters in the expression for ring functions, (g) the lowest numbers at the first point of difference in the expression for ring junctions, (h) the lowest state of hydrogenation, (i) the lowest-numbered locant for indicated hydrogen, (j) the lowest-numbered locant for point of attachment (if a radical), (k) the lowest-numbered locant for an attached group expressed as a suffix, (l) the maximum number of substituents cited as prefixes, (m) the lowest-numbered locant for substituents named as prefixes, hydro prefixes, -ene, and -yne, all considered together in one series in ascending numerical order independent of their nature, and (n) the lowest-numbered locant for the substituent named as prefix which is cited first in the name.

Numbering of Compounds. If the rules for aliphatic chains and ring systems leave a choice, the starting point and direction of numbering of a compound are chosen so as to give lowest-numbered locants to these structural factors, if present, considered successively in the order listed below until a decision is reached. Characteristic groups take precedence over multiple bonds.

1. Indicated hydrogen, whether cited in the name or omitted as being conventional.
2. Characteristic groups named as suffix following the ranking order of Table 1.7.
3. Multiple bonds in acyclic compounds; in bicycloalkanes, tricycloalkanes, and polycycloalkanes, double bonds having priority over triple bonds; and in heterocyclic systems whose names end in -etine, -oline, or -olene.
4. The lowest-numbered locant for substituents named as prefixes, hydro prefixes, -ene, and -yne, all considered together in one series in ascending numerical order.
5. The lowest locant for that substituent named as prefix which is cited first in the name.

For cyclic radicals, indicated hydrogen and thereafter the point of attachment (free valency) have priority for the lowest available number.

Prefixes and Affixes. Prefixes are arranged alphabetically and placed before the parent name; multiplying affixes, if necessary, are inserted and *do not* alter the alphabetical order already attained. The parent name includes any syllables denoting a change of ring member or relating to the structure of a carbon chain. Nondetachable parts of parent names include

1. Forming rings: cyclo-, bicyclo-, spiro-;
2. Fusing two or more rings: benzo-, naphtho-, imidazo-;
3. Substituting one ring or chain member atom for another: oxa-, aza-, thia-;
4. Changing positions of ring or chain members: iso-, *sec*-, *tert*-, neo-;
5. Showing indicated hydrogen;
6. Forming bridges: ethano-, epoxy- and;
7. Hydro-.

Prefixes that represent complete terminal characteristic groups are preferred to those representing only a portion of a given group. For example, for the group —C(=O)CH_3 , the prefix (formylmethyl-) is preferred to (oxoethyl-).

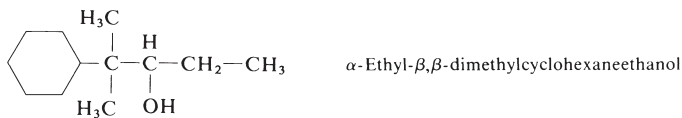
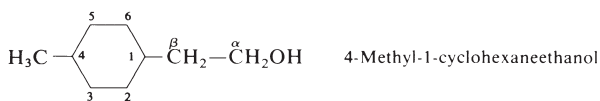
The multiplying affixes di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, deca-, undeca-, and so on are used to indicate a set of *identical* unsubstituted radicals or parent compounds. The forms bis-, tris-, tetrakis-, pentakis-, and so on are used to indicate a set of identical radicals or parent compounds *each substituted in the same way*. The affixes bi-, ter-, quater-, quinque-, sexi-, septi-, octi-, novi-, deci-, and so on are used to indicate the number of identical rings joined together by a single or double bond.

Although multiplying affixes may be omitted for very common compounds when no ambiguity is caused thereby, such affixes are generally included throughout this handbook in alphabetical listings. An example would be ethyl ether for diethyl ether.

Conjunctive Nomenclature. Conjunctive nomenclature may be applied when a principal group is attached to an acyclic component that is directly attached by a carbon-carbon bond to a cyclic component. The name of the cyclic component is attached directly in front of the name of the acyclic component carrying the principal group. This nomenclature is not used when an unsaturated side chain is named systematically. When necessary, the position of the side chain is indicated by a locant placed before the name of the cyclic component. For substituents on the acyclic chain, carbon atoms of the side chain are indicated by Greek letters proceeding from the principal group to the cyclic component. The terminal carbon atom of acids, aldehydes, and nitriles is omitted when allocating Greek positional letters. Conjunctive nomenclature is not used when the side chain carries more than one of the principal group, except in the case of malonic and succinic acids.

The side chain is considered to extend only from the principal group to the cyclic component. Any other chain members are named as substituents, with appropriate prefixes placed before the name of the cyclic component.

When a cyclic component carries more than one identical side chain, the name of the cyclic component is followed by di-, tri-, etc., and then by the name of the acyclic component, and it is preceded by the locants for the side chains. Examples are



When side chains of two or more different kinds are attached to a cyclic component, only the senior side chain is named by the conjunctive method. The remaining side chains are named as prefixes. Likewise, when there is a choice of cyclic component, the senior is chosen. Benzene derivatives may be named by the conjunctive method only when two or more identical side chains are present. Trivial names for oxo carboxylic acids may be used for the acyclic component. If the cyclic and acyclic components are joined by a double bond, the locants of this bond are placed as superscripts to a Greek capital delta that is

inserted between the two names. The locant for the cyclic component precedes that for the acyclic component, e.g., indene- $\Delta^{1,\alpha}$ -acetic acid.

Radicofunctional Nomenclature. The procedures of radicofunctional nomenclature are identical with those of substitutive nomenclature except that suffixes are never used. Instead, the functional class name (Table 1.9) of the compound is expressed as one word and the remainder of the molecule as another that precedes the class name. When the functional class name refers to a characteristic group that is bivalent, the two radicals attached to it are each named, and when different, they are written as separate words arranged in alphabetical order. When a compound contains more than one kind of group listed in Table 1.9, that kind is cited as the functional group or class name that occurs higher in the table, all others being expressed as prefixes.

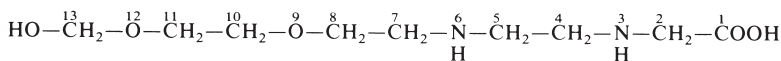
Radicofunctional nomenclature finds some use in naming ethers, sulfides, sulfoxides, sulfones, selenium analogs of the preceding three sulfur compounds, and azides.

TABLE 1.9 Functional Class Names Used in Radicofunctional Nomenclature

Groups are listed in order of decreasing priority

Group	Functional class names
X in acid derivatives	Name of X (in priority order: fluoride, chloride, bromide, iodide; cyanide, azide; then the sulfur and selenium analogs)
—CN, —NC	Cyanide, isocyanide
>CO	Ketone; then S and Se analogs
—OH	Alcohol; then S and Se analogs
—O—OH	Hydroperoxide
>O	Ether or oxide
>S, >SO, >SO ₂	Sulfide, sulfoxide, sulfone
>Se, >SeO, >SeO ₂	Selenide, selenoxide, selenone
—F, —Cl, —Br, —I	Fluoride, chloride, bromide, iodide
—N ₃	Azide

Replacement Nomenclature. Replacement nomenclature is intended for use only when other nomenclature systems are difficult to apply in the naming of chains containing heteroatoms. When no group is present that can be named as a principal group, the longest chain of carbon and heteroatoms terminating with carbon is chosen and named as though the entire chain were that of an acyclic hydrocarbon. The heteroatoms within this chain are identified by means of prefixes aza-, oxa-, thia-, etc., in the order of priority stated in Table 1.3. Locants indicate the positions of the heteroatoms in the chain. Lowest-numbered locants are assigned to the principal group when such is present. Otherwise, lowest-numbered locants are assigned to the heteroatoms considered together and, if there is a choice, to the heteroatoms cited earliest in Table 1.3. An example is



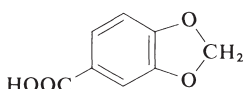
13-Hydroxy-9,12-dioxa-3,6-diazatridecanoic acid

Specific Functional Groups

Characteristic groups will now be treated briefly in order to expand the terse outline of substitutive nomenclature presented in Table 1.7. Alternative nomenclature will be indicated whenever desirable.

Acetals and Acylals. Acetals, which contain the group $>\text{C}(\text{OR})_2$, where R may be different, are named (1) as dialkoxy compounds or (2) by the name of the corresponding aldehyde or ketone followed by the name of the hydrocarbon radical(s) followed by the word *acetal*. For example, $\text{CH}_3-\text{CH}(\text{OCH}_3)_2$ is named either (1) 1,1-dimethoxyethane or (2) acetaldehyde dimethyl acetal.

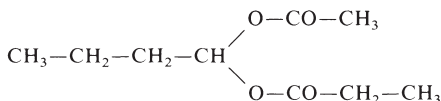
A cyclic acetal in which the two acetal oxygen atoms form part of a ring may be named (1) as a heterocyclic compound or (2) by use of the prefix methylenedioxy for the group $-\text{O}-\text{CH}_2-\text{O}-$ as a substituent in the remainder of the molecule. For example,



(1) 1,3-Benzo[*d*]dioxole-5-carboxylic acid

(2) 3,4-Methylenedioxybenzoic acid

Acylals, $\text{R}^1\text{R}^2\text{C}(\text{OCOR}^3)_2$, are named as acid esters:

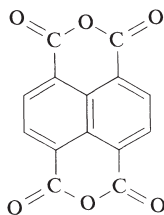


Butylidene acetate
propionate

α -Hydroxy ketones, formerly called acyloins, had been named by changing the ending -ic acid or -oic acid of the corresponding acid to -oin. They are preferably named by substitutive nomenclature. For example,



Acid Anhydrides. Symmetrical anhydrides of monocarboxylic acids, when unsubstituted, are named by replacing the word *acid* by *anhydride*. Anhydrides of substituted monocarboxylic acids, if symmetrically substituted, are named by prefixing bis- to the name of the acid and replacing the word *acid* by *anhydride*. Mixed anhydrides are named by giving in alphabetical order the first part of the names of the two acids followed by the word *anhydride*, e.g., acetic propionic anhydride or acetic propanoic anhydride. Cyclic anhydrides of polycarboxylic acids, although possessing a heterocyclic structure, are preferably named as acid anhydrides. For example,



1,8;4,5-Naphthalenetetracarboxylic dianhydride. (Note the use of a semicolon to distinguish the pairs of locants.)

Acyl Halides. Acyl halides, in which the hydroxyl portion of a carboxyl group is replaced by a halogen, are named by placing the name of the corresponding halide after that of the acyl radical. When another group is present that has priority for citation as principal group or when the acyl halide is attached to a side chain, the prefix haloformyl- is used as, for example, in fluoroformyl-.

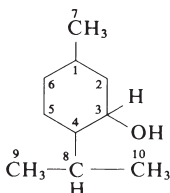
Alcohols and Phenols. The hydroxyl group is indicated by a suffix -ol when it is the principal group attached to the parent compound and by the prefix hydroxy- when another group with higher priority for citation is present or when the hydroxy group is present in a side chain. When confusion may arise in employing the suffix -ol, the hydroxy group is indicated as a prefix; this terminology is also used when the hydroxyl group is attached to a heterocycle, as, for example, in the name 3-hydroxythiophene to avoid confusion with thiophenol ($\text{C}_6\text{H}_5\text{SH}$). Designations such as isopropanol, *sec*-butanol, and *tert*-butanol are incorrect because no hydrocarbon exists to which the suffix can be added. Many trivial names are retained. These structures are shown in Table 1.10. The radicals ($\text{RO}-$) are named by adding -oxy as a suffix to the name of the R radical, e.g., pentyloxy for $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{O}-$. These contractions are exceptions: methoxy ($\text{CH}_3\text{O}-$), ethoxy ($\text{C}_2\text{H}_5\text{O}-$), propoxy ($\text{C}_3\text{H}_7\text{O}-$), butoxy ($\text{C}_4\text{H}_9\text{O}-$), and phenoxy ($\text{C}_6\text{H}_5\text{O}-$). For unsubstituted radicals only, one may use isopropoxy [$(\text{CH}_3)_2\text{CH}-\text{O}-$], isobutoxy [$(\text{CH}_3)_2\text{CH}_2\text{CH}-\text{O}-$], *sec*-butoxy [$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)-\text{O}-$], and *tert*-butoxy [$(\text{CH}_3)_3\text{C}-\text{O}-$].

TABLE 1.10 Retained Trivial Names of Alcohols and Phenols with Structures

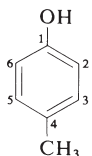
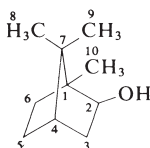
Allyl alcohol	$\text{CH}_2=\text{CHCH}_2\text{OH}$
<i>tert</i> -Butyl alcohol	$(\text{CH}_3)_3\text{COH}$
Benzyl alcohol	$\text{C}_6\text{H}_5\text{CH}_2\text{OH}$
Phenethyl alcohol	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{OH}$
Ethylene glycol	$\text{HOCH}_2\text{CH}_2\text{OH}$
1,2-Propylene glycol	$\text{CH}_3\text{CHOHCH}_2\text{OH}$
Glycerol	$\text{HOCH}_2\text{CHOHCH}_2\text{OH}$
Pentaerythritol	$\text{C}(\text{CH}_2\text{OH})_4$
Pinacol	$(\text{CH}_3)_2\text{COHCOH}(\text{CH}_3)_2$
Phenol	$\text{C}_6\text{H}_5\text{OH}$
Xylitol	$\begin{array}{c} \text{OH} \\ \\ \text{HOCH}_2\text{CH}-\text{CH}-\text{CH}-\text{CH}_2\text{OH} \\ \quad \quad \\ \text{OH} \quad \quad \text{OH} \end{array}$
Geraniol	$\begin{array}{c} (\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_2\text{C}=\text{CHCH}_2\text{OH} \\ \\ \text{CH}_3 \end{array}$
Phytol	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_2\text{CH}_2\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2 \\ \quad \quad \quad \\ \text{CH}_2\text{CHCH}_2\text{CH}_2\text{CH}_2\text{C}=\text{CHCH}_2\text{OH} \\ \quad \quad \quad \\ \text{CH}_3 \quad \quad \quad \text{CH}_3 \end{array}$

TABLE 1.10 Retained Trivial Names of Alcohols and Phenols with Structures (*continued*)

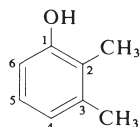
Menthyl



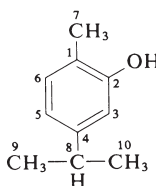
Borneol



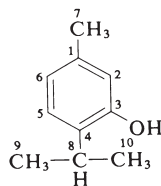
Cresol (1,4-isomer shown)



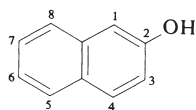
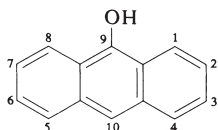
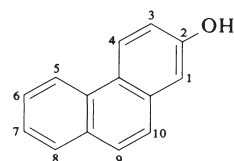
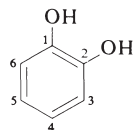
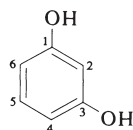
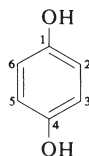
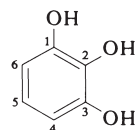
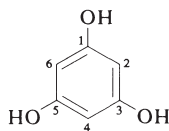
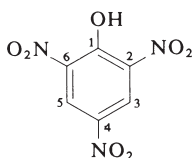
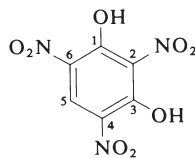
Xylenol (2,3-isomer shown)



Carvacrol



Thymol

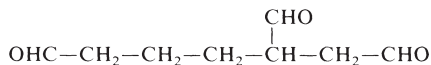
Naphthol (2-isomer shown)
2-HydroxynaphthaleneAnthrol (9-isomer shown)
9-HydroxyanthracenePhenanthrol (2-isomer shown)
2-HydroxyphenanthrenePyrocatechol
1,2-DihydroxybenzeneResorcinol
1,3-DihydroxybenzeneHydroquinone
1,4-DihydroxybenzenePyrogallol
1,2,3-TrihydroxybenzenePhloroglucinol
1,3,5-TrihydroxybenzenePicric acid
2,4,6-TrinitrophenolStyphnic acid
1,3-Dihydroxy-2,4,6-trinitrobenzene

Bivalent radicals of the form $\text{O}-\text{Y}-\text{O}$ are named by adding -dioxy to the name of the bivalent radicals except when forming part of a ring system. Examples are $\text{O}-\text{CH}_2-\text{O}-$ (methylenedioxy), $\text{O}-\text{CO}-\text{O}-$ (carbonyldioxy), and $\text{O}-\text{SO}_2-\text{O}-$ (sulfonyldioxy). Anions derived from alcohols or phenols are named by changing the final -ol to -olate.

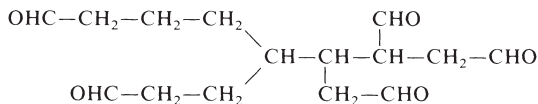
Salts composed of an anion, $\text{RO}-$, and a cation, usually a metal, can be named by citing first the cation and then the RO anion (with its ending changed to -yl oxide), e.g., sodium benzyl oxide for $\text{C}_6\text{H}_5\text{CH}_2\text{ONa}$. However, when the radical has an abbreviated name, such as methoxy, the ending -oxy is changed to -oxide. For example, CH_3ONa is named sodium methoxide (not sodium methylate).

Aldehydes. When the group $-\text{C}(=\text{O})\text{H}$, usually written $-\text{CHO}$, is attached to carbon at one (or both) end(s) of a linear acyclic chain the name is formed by adding the suffix -al (or -dial) to the name of the hydrocarbon containing the same number of carbon atoms. Examples are butanal for $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$ and propanedial for OHCCH_2CHO .

Naming an acyclic polyaldehyde can be handled in two ways. (1) When more than two aldehyde groups are attached to an unbranched chain, the proper affix is added to -carbaldehyde, which becomes the suffix to the name of the longest chain carrying the maximum number of aldehyde groups. The name and numbering of the main chain do not include the carbon atoms of the aldehyde groups. (2) The name is formed by adding the prefix formyl- to the name of the -dial that incorporates the principal chain. Any other chains carrying aldehyde groups are named by the use of formylalkyl- prefixes. Examples are



- (1) 1,2,5-Pentanetricarbaldehyde
(2) 3-Formylheptanedial



- (1) 4-(2-Formylethyl)-3-(formylmethyl)-1,2,7-heptanetricarbaldehyde
(2) 3-Formyl-5-(2-formylethyl)-4-(formylmethyl)nonanedial

When the aldehyde group is directly attached to a carbon atom of a ring system, the suffix -carbaldehyde is added to the name of the ring system, e.g., 2-naphthalenecarbaldehyde. When the aldehyde group is separated from the ring by a chain of carbon atoms, the compound is named (1) as a derivative of the acyclic system or (2) by conjunctive nomenclature, for example, (1) (2-naphthyl)propionaldehyde or (2) 2-naphthalenepropionaldehyde.

An aldehyde group is denoted by the prefix formyl- when it is attached to a nitrogen atom in a ring system or when a group having priority for citation as principal group is present and part of a cyclic system.

When the corresponding monobasic acid has a trivial name, the name of the aldehyde may be formed by changing the ending -ic acid or -oic acid to -aldehyde. Examples are

Formaldehyde	Acrylaldehyde (not acrolein)
Acetaldehyde	Benzaldehyde
Propionaldehyde	Cinnamaldehyde
Butyraldehyde	2-Furaldehyde (not furfural)

The same is true for polybasic acids, with the proviso that all the carboxyl groups must be changed to aldehyde; then it is not necessary to introduce affixes. Examples are

Glyceraldehyde	Succinaldehyde
Glycolaldehyde	Phthalaldehyde (<i>o</i> -, <i>m</i> -, <i>p</i> -)
Malonaldehyde	

These trivial names may be retained: citral (3,7-dimethyl-2,6-octadienal), vanillin (4-hydroxy-3-methoxybenzaldehyde), and piperonal (3,4-methylenedioxybenzaldehyde).

Amides. For primary amides the suffix -amide is added to the systematic name of the parent acid. For example, $\text{CH}_3\text{—CO—NH}_2$ is acetamide. Oxamide is retained for $\text{H}_2\text{N—CO—CO—NH}_2$. The name -carboxylic acid is replaced by -carboxamide.

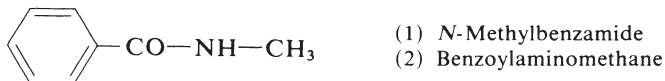
For amino acids having trivial names ending in -ine, the suffix -amide is added after the name of the acid (with elision of -e for monoamides). For example, $\text{H}_2\text{N—CH}_2\text{—CO—NH}_2$ is glycineamide.

In naming the radical R—CO—NH— , either (1) the -yl ending of RCO— is changed to -amido or (2) the radicals are named as acylamino radicals. For example,



The latter nomenclature is always used for amino acids with trivial names.

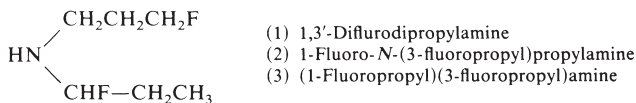
N-substituted primary amides are named either (1) by citing the substituents as *N* prefixes or (2) by naming the acyl group as an *N* substituent of the parent compound. For example,



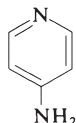
Amines. Amines are preferably named by adding the suffix -amine (and any multiplying affix) to the name of the parent radical. Examples are

$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$	Pentylamine
$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$	1,5-Pentyl diamine or pentamethylenediamine

Locants of substituents of symmetrically substituted derivatives of symmetrical amines are distinguished by primes or else the names of the complete substituted radicals are enclosed in parentheses. Unsymmetrically substituted derivatives are named similarly or as *N*-substituted products of a primary amine (after choosing the most senior of the radicals to be the parent amine). For example,



Complex cyclic compounds may be named by adding the suffix -amine or the prefix amino- (or aminoalkyl-) to the name of the parent compound. Thus three names are permissible for



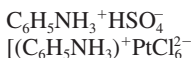
- (1) 4-Pyridylamine
- (2) 4-Pyridinamine
- (3) 4-Aminopyridine

Complex linear polyamines are best designated by replacement nomenclature. These trivial names are retained: aniline, benzidine, phenetidine, toluidine, and xylydine.

The bivalent radical —NH— linked to two identical radicals can be denoted by the prefix imino-, as well as when it forms a bridge between two carbon ring atoms. A trivalent nitrogen atom linked to three identical radicals is denoted by the prefix nitrilo-. Thus ethylenedi- aminetetraacetic acid (an allowed exception) should be named ethylenedinitrilotetraacetic acid.

Ammonium Compounds. Salts and hydroxides containing quadricovalent nitrogen are named as a substituted ammonium salt or hydroxide. The names of the substituting radicals precede the word *ammonium*, and then the name of the anion is added as a separate word. For example, $(\text{CH}_3)_4\text{N}^+\text{I}^-$ is tetramethylammonium iodide.

When the compound can be considered as derived from a base whose name does not end in -amine, its quaternary nature is denoted by adding -ium to the name of that base (with elision of -e), substituent groups are cited as prefixes, and the name of the anion is added separately at the end. Examples are



Anilinium hydrogen sulfate
Dianilinium hexachloroplatinate

The names *choline* and *betaine* are retained for unsubstituted compounds.

In complex cases, the prefixes amino- and imino- may be changed to ammonio- and iminio- and are followed by the name of the molecule representing the most complex group attached to this nitrogen atom and are preceded by the names of the other radicals attached to this nitrogen. Finally the name of the anion is added separately. For example, the name might be 1-trimethylammonioacridine chloride or 1-acridinyltrimethylammonium chloride.

When the preceding rules lead to inconvenient names, then (1) the unaltered name of the base may be used followed by the name of the anion or (2) for salts of hydrohalogen acids only the unaltered name of the base is used followed by the name of the hydrohalide. An example of the latter would be 2-ethyl-*p*-phenylenediamine monohydrochloride.

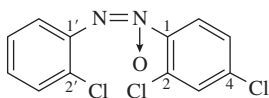
Azo Compounds. When the azo group (—N=N—) connects radicals derived from identical unsubstituted molecules, the name is formed by adding the prefix azo- to the name of the parent unsubstituted molecules. Substituents are denoted by prefixes and suffixes. The azo group has priority for lowest-numbered locant. Examples are azobenzene for $\text{C}_6\text{H}_5\text{—N=N—C}_6\text{H}_5$, azobenzene-4- sulfonic acid for $\text{C}_6\text{H}_5\text{—N=N—C}_6\text{H}_4\text{SO}_3\text{H}$, and 2',4-dichloroazobenzene-4'-sulfonic acid for $\text{ClC}_6\text{H}_4\text{—N=N—C}_6\text{H}_3\text{ClSO}_3\text{H}$.

When the parent molecules connected by the azo group are different, azo is placed between the complete names of the parent molecules, substituted or unsubstituted. Locants

are placed between the affix azo and the names of the molecules to which each refers. Preference is given to the more complex parent molecule for citation as the first component, e.g., 2-aminonaphthalene-1-azo-(4'-chloro-2'-methylbenzene).

In an alternative method, the senior component is regarded as substituted by $RN=N-$, this group R being named as a radical. Thus 2-(7-phenylazo-2-naphthylazo)anthracene is the name by this alternative method for the compound named anthracene-2-azo-2'-naphthalene-7'-azobenzene.

Azoxy Compounds. Where the position of the azoxy oxygen atom is unknown or immaterial, the compound is named in accordance with azo rules, with the affix azo replaced by azoxy. When the position of the azoxy oxygen atom in an unsymmetrical compound is designated, a prefix *NNO-* or *ONN-* is used. When both the groups attached to the azoxy radical are cited in the name of the compound, the prefix *NNO-* specifies that the second of these two groups is attached directly to $-N(O)-$; the prefix *ONN-* specifies that the first of these two groups is attached directly to $-N(O)-$. When only one parent compound is cited in the name, the prefixed *ONN-* and *NNO-* specify that the group carrying the primed and unprimed substituents is connected, respectively, to the $-N(O)-$ group. The prefix *NON-* signifies that the position of the oxygen atom is unknown; the azoxy group is then written as $-N_2O-$. For example,



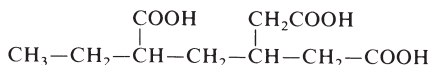
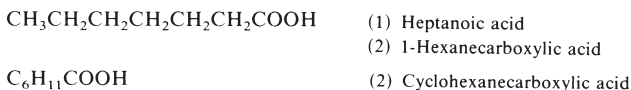
2,2',4-Trichloro-*NNO*-azoxybenzene

Boron Compounds. Molecular hydrides of boron are called boranes. They are named by using a multiplying affix to designate the number of boron atoms and adding an Arabic numeral within parentheses as a suffix to denote the number of hydrogen atoms present. Examples are pentaborane(9) for B_5H_9 and pentaborane(11) for B_5H_{11} .

Organic ring systems are named by replacement nomenclature. Three- to ten-membered monocyclic ring systems containing uncharged boron atoms may be named by the specialist nomenclature for heterocyclic systems. Organic derivatives are named as outlined for substitutive nomenclature. The complexity of boron nomenclature precludes additional details; the text by Rigaudy and Klesney should be consulted.

Carboxylic Acids. Carboxylic acids may be named in several ways. (1) $-COOH$ groups replacing CH_3- at the end of the main chain of an acyclic hydrocarbon are denoted by adding -oic acid to the name of the hydrocarbon. (2) When the $-COOH$ group is the principal group, the suffix -carboxylic acid can be added to the name of the parent chain whose name and chain numbering *does not include* the carbon atom of the $-COOH$ group. The former nomenclature is preferred unless use of the ending -carboxylic acid leads to citation of a larger number of carboxyl groups as suffix. (3) Carboxyl groups are designated by the prefix carboxy- when attached to a group named as a substituent or when another group is present that has higher priority for citation as principal group. In all cases, the

principal chain should be linked to as many carboxyl groups as possible even though it might not be the longest chain present. Examples are



(3) 2-(Carboxymethyl)-1,4-hexanedicarboxylic acid

Removal of the OH from the $-\text{COOH}$ group to form the acyl radical results in changing the ending -oic acid to -oyl or the ending -carboxylic acid to -carbonyl. Thus the radical $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$ is named either pentanoyl or butanecarbonyl. When the hydroxyl has not been removed from all carboxyl groups present in an acid, the remaining carboxyl groups are denoted by the prefix carboxy-. For example, $\text{HOOCCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$ is named 6-carboxyhexanoyl.

Many trivial names exist for acids: these are listed in Table 1.11. Generally, radicals are formed by replacing -ic acid by -oyl.* When a trivial name is given to an acyclic monoacid or diacid, the numeral 1 is always given as locant to the carbon atom of a carboxyl group in the acid or to the carbon atom with a free valence in the radical $\text{RCO}-$.

Ethers ($\text{R}^1-\text{O}-\text{R}^2$). In substitutive nomenclature, one of the possible radicals, $\text{R}-\text{O}-$, is stated as the prefix to the parent compound that is senior from among R^1 or R^2 . Examples are methoxyethane for $\text{CH}_3\text{OCH}_2\text{CH}_3$ and butoxyethanol for $\text{C}_4\text{H}_9\text{OCH}_2\text{CH}_2\text{OH}$.

When another principal group has precedence and oxygen is linking two identical parent compounds, the prefix oxy- may be used, as with 2,2'-oxydiethanol for $\text{HOCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{OH}$.

Compounds of the type $\text{RO}-\text{Y}-\text{OR}$, where the two parent compounds are identical and contain a group having priority over ethers for citation as suffix, are named as assemblies of identical units. For example, $\text{HOOC}-\text{CH}_2-\text{O}-\text{CH}_2\text{CH}_2-\text{O}-\text{CH}_2-\text{COOH}$ is named 2,2'-(ethylenedioxy)diacetic acid.

Linear polyethers derived from three or more molecules of aliphatic dihydroxy compounds, particularly when the chain length exceeds ten units, are most conveniently named by open-chain replacement nomenclature. For example, $\text{CH}_3\text{CH}_2-\text{O}-\text{CH}_2\text{CH}_2-\text{O}-\text{CH}_2\text{CH}_3$ could be 3,6-dioxaoctane or (2-ethoxy)ethoxyethane.

An oxygen atom directly attached to two carbon atoms already forming part of a ring system or to two carbon atoms of a chain may be indicated by the prefix epoxy-. For example, $\text{CH}_2-\text{CH}-\text{CH}_2\text{Cl}$ is named 1-chloro-2,3-epoxypropane.

Symmetrical linear polyethers may be named (1) in terms of the central oxygen atom when there is an odd number of ether oxygen atoms or (2) in terms of the central hydrocarbon group when there is an even number of ether oxygen atoms. For example, $\text{C}_2\text{H}_5-\text{O}-\text{C}_4\text{H}_8-\text{O}-\text{C}_4\text{H}_8-\text{O}-\text{C}_2\text{H}_5$ is bis-(4-ethoxybutyl)ether, and 3,6-dioxaoctane (earlier example) could be named 1,2-bis(ethoxy)ethane.

Polyethers and Cyclic Polyethers. During the past several decades, linear and cyclic polyethers have gained considerable prominence. This is largely due to their remarkable ability to complex metallic and organic cations. The linear polyethers of the polyethylene

*Exceptions: formyl, acetyl, propionyl, butyryl, isobutyryl, valeryl, isovaleryl, oxalyl, malonyl, succinyl, glutaryl, furoyl, and thenoyl.

TABLE 1.11 Names of Some Carboxylic Acids

Systematic name	Trivial name	Systematic name	Trivial name
Methanoic	Formic	<i>trans</i> -Methylbutenedioic	Mesaconic*
Ethanoic	Acetic		
Propanoic	Propionic	1,2,2-Trimethyl-1,3-cyclopentanedicarboxylic acid	Camphoric
Butanoic	Butyric		
2-Methylpropanoic	Isobutyric*	Benzenecarboxylic	Benzoic
Pentanoic	Valeric	1,2-Benzenedicarboxylic	Phthalic
3-Methylbutanoic	Isovaleric*	1,3-Benzenedicarboxylic	Isophthalic
2,2-Dimethylpropanoic	Pivalic*	1,4-Benzenedicarboxylic	Terephthalic
Hexanoic	(Caproic)	Naphthalenecarboxylic	Naphthoic
Heptanoic	(Enanthic)	Methylbenzenecarboxylic	Toluic
Octanoic	(Caprylic)	2-Phenylpropanoic	Hydratropic
Decanoic	(Capric)	2-Phenylpropenoic	Atropic
Dodecanoic	Lauric*	<i>trans</i> -3-Phenylpropenoic	Cinnamic
Tetradecanoic	Myristic*	Furancarboxylic	Furoic
Hexadecanoic	Palmitic*	Thiophenecarboxylic	Thenoic
Octadecanoic	Stearic*	3-Pyridinecarboxylic	Nicotinic
		4-Pyridinecarboxylic	Isonicotinic
Ethanedioic	Oxalic		
Propanedioic	Malonic	Hydroxyethanoic	Glycolic
Butanedioic	Succinic	2-Hydroxypropanoic	Lactic
Pentanedioic	Glutaric	2,3-Dihydroxypropanoic	Glyceric
Hexanedioic	Adipic	Hydroxypropanedioic	Tartronic
Heptanedioic	Pimelic*	Hydroxybutanedioic	Malic
Octanedioic	Suberic*	2,3-Dihydroxybutanedioic	Tartaric
Nonanedioic	Azelaic*	3-Hydroxy-2-phenylpropanoic	Tropic
Decanedioic	Sebacic*	2-Hydroxy-2,2-diphenylethanoic	Benzilic
Propenoic	Acrylic	2-Hydroxybenzoic	Salicylic
Propynoic	Propiolic	Methoxybenzoic	Anisic
2-Methylpropenoic	Methacrylic	4-Hydroxy-3-methoxybenzoic	Vanillic
<i>trans</i> -2-Butenoic	Crotonic		
<i>cis</i> -2-Butenoic	Isocrotonic	3,4-Dimethoxybenzoic	Veratric
<i>cis</i> -9-Octadecenoic	Oleic	3,4-Methylenedioxybenzoic	Piperonylic
<i>trans</i> -9-Octadecenoic	Elaidic	3,4-Dihydroxybenzoic	Protocatechuic
<i>cis</i> -Butenedioic	Maleic	3,4,5-Trihydroxybenzoic	Gallic
<i>trans</i> -Butenedioic	Fumaric		
<i>cis</i> -Methylbutenedioic	Citraconic*		

The names in parentheses are abandoned but are listed for reference to older literature.

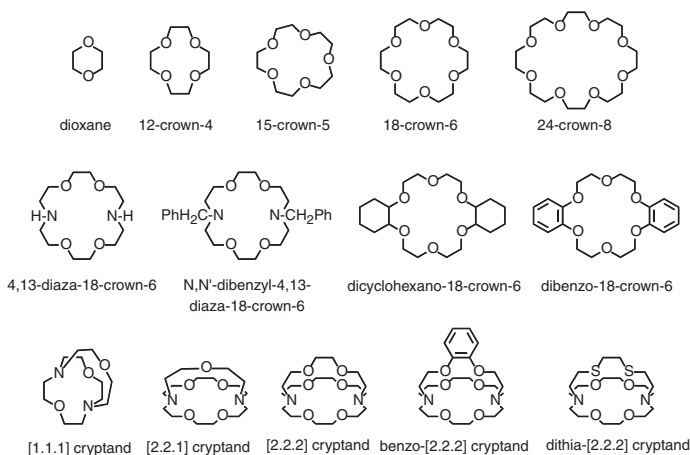
* Systematic names should be used in derivatives formed by substitution on a carbon atom.

glycol type are discussed in Section 10. The cyclic polyethers are called crown ethers if they are monocyclic and cryptands if they are di- or multi-cyclic compounds.

Crown ethers are typically complicated structures and their names have evolved from the convenient, semi-systematic nomenclature developed by the pioneers in the field. The name “crown” was suggested because the cyclic polyethers “crown a cation” when they complex it. The most general naming system consists in identifying the largest cycle and then denoting the number and type of heteroatoms present. The most common repeating unit is ethyleneoxy or $\text{—CH}_2\text{CH}_2\text{O—}$, normally in the form 1,2-ethylenedioxy and this is

presumed to be present unless otherwise noted. Ethylene oxide (oxirane) is the smallest cyclic compound containing this unit. Dioxane is formally its dimer. The trimer, called 9-crown-3, is known but the smallest compound normally considered to be a crown ether is 12-crown-4. 18-Crown-6 has six repeating ethyleneoxy units and is systematically named 1,4,7,10,13,16-hexaoxacyclooctadecane.

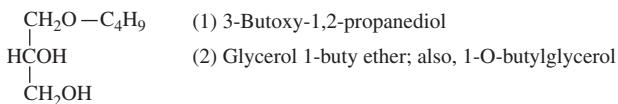
Examples of various crown ethers and cryptands are shown here. The top line of compounds may be named readily enough although the problem with this semi-systematic approach is obvious. If two methylenes were added to 18-crown-6, the compound could correctly be called 20-crown-6 but in the absence of unequivocal descriptors, the positions of the 3-carbon bridges would be unclear. The more cumbersome name 1,4,7,11,13,17-hexaoxacycloicosane tells clearly that the longer bridges are adjacent to each other. A similar problem is apparent in the last two entries of the second line. The designations dicyclohexano and dibenzo are clear as to the substituents but not their positions. The semi-systematic nomenclature is widely used, however, because it is so much less cumbersome for most purposes.



An additional nuance in the nomenclature of these compounds concerns their complexes. The open-chained compounds are often referred to as podands and their complexes as podates. The cyclic ethers may also be called coronands and their complexes are therefore coronates. Complexed cryptands are cryptates. The even more complicated structures known as spherands, cavitands, or carcerands are called spherates, cavitates, or carcerates, respectively, when complexed. The combination of a macrocycle (crown ether or coronand) and a sidechain (podand) is typically called a lariat ether.

An alternate nomenclature system based upon IUPAC principles polymer systems has also been developed but it has not been adopted broadly. Using this method, 15-crown-5 would be called cyclo[pentakis(oxyethylene)] instead of 1,4,7,10,13-pentaoxacyclooctadecane. In this case, substituents and other heteroatoms make the names more complex.

Partial ethers of polyhydroxy compounds may be named (1) by substitutive nomenclature or (2) by stating the name of the polyhydroxy compound followed by the name of the etherifying radical(s) followed by the word *ether*. For example,



Cyclic ethers are named either as heterocyclic compounds or by specialist rules of heterocyclic nomenclature. Radicofunctional names are formed by citing the names of the radicals R^1 and R^2 followed by the word *ether*. Thus methoxyethane becomes ethyl methyl ether and ethoxyethane becomes diethyl ether.

Halogen Derivatives. Using substitutive nomenclature, names are formed by adding prefixes listed in Table 1.8 to the name of the parent compound. The prefix perhalo- implies the replacement of all hydrogen atoms by the particular halogen atoms.

Cations of the type $R^1R^2X^+$ are given names derived from the halonium ion, H_2X^+ , by substitution, e.g., diethyliodonium chloride for $(C_2H_5)_2I^+Cl^-$.

These trivial names are retained: bromoform ($CHBr_3$), chloroform ($CHCl_3$), fluoroform (CHF_3), iodoform (CHI_3), phosgene ($COCl_2$), thiophosgene ($CSCl_2$), and dichlorocarbene radical ($\text{>}CCl_2$). Inorganic nomenclature leads to such names as carbonyl and thiocarbonyl halides (COX_2 and CSX_2) and carbon tetrahalides (CX_4).

Hydroxylamines and Oximes. For $RNH-OH$ compounds, prefix the name of the radical R to hydroxylamine. If another substituent has priority as principal group, attach the prefix hydroxyamino- to the parent name. For example, C_6H_5NHOH would be named *N*-phenylhydroxylamine, but HOC_6H_4NHOH would be (hydroxyamino)phenol, with the point of attachment indicated by a locant preceding the parentheses.

Compounds of the type R^1NH-OR_2 are named (1) as alkoxyamino derivatives of compound R^1H , (2) as *N,O*-substituted hydroxylamines, (3) as alkoxyamines (even if R^1 is hydrogen), or (4) by the prefix aminooxy- when another substituent has priority for parent name. Examples of each type are as follows:

1. 2-(Methoxyamino)-8-naphthalenecarboxylic acid for $CH_3ONH-C_{10}H_6COOH$
2. *O*-phenylhydroxylamine for $H_2N-O-C_6H_5$ or *N*-phenylhydroxylamine for C_6H_5NH-OH
3. Phenoxyamine for $H_2N-O-C_6H_5$ (not preferred to *O*-phenylhydroxylamine)
4. Ethyl (aminooxy)acetate for $H_2N-O-CH_2CO-OC_2H_5$

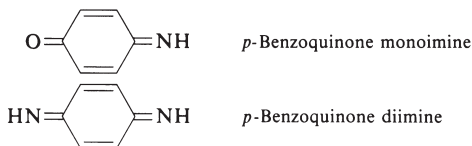
Acyl derivatives, $RCO-NH-OH$ and $H_2N-O-CO-R$, are named as *N*-hydroxy derivatives of amides and as *O*-acylhydroxylamines, respectively. The former may also be named as hydroxamic acids. Examples are *N*-hydroxyacetamide for $CH_3CO-NH-OH$ and *O*-acetylhydroxylamine for $H_2N-O-CO-CH_3$. Further substituents are denoted by prefixes with *O*- and/or *N*-locants. For example, $C_6H_5NH-O-C_2H_5$ would be *O*-ethyl-*N*-phenylhydroxylamine or *N*-ethoxylaniline.

For oximes, the word *oxime* is placed after the name of the aldehyde or ketone. If the carbonyl group is not the principal group, use the prefix hydroxyimino-. Compounds with the group $\text{>}N-OR$ are named by a prefix alkyloxyimino- as oxime *O*-ethers or as *O*-substituted oximes. Compounds with the group $\text{>}C=N(O)R$ are named by adding *N*-oxide after the name of the alkylideneamine compound. For amine oxides, add the word *oxide* after the name of the base, with locants. For example, C_5H_5N-O is named pyridine *N*-oxide or pyridine 1-oxide.

Imines. The group $\text{>}C=NH$ is named either by the suffix -imine or by citing the name of the bivalent radical $R^1R^2C\text{<}$ as a prefix to amine. For example, $CH_3CH_2CH_2CH=NH$

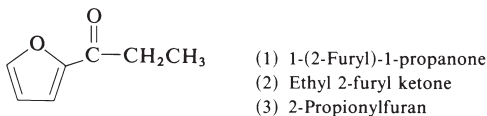
could be named 1-butanamine or butylideneamine. When the nitrogen is substituted, as in $\text{CH}_2=\text{N}-\text{CH}_2\text{CH}_3$, the name is *N*-(methylidene) ethylamine.

Quinones are exceptions. When one or more atoms of quinonoid oxygen have been replaced by $>\text{NH}$ or $>\text{NR}$, they are named by using the name of the quinone followed by the word *imine* (and preceded by proper affixes). Substituents on the nitrogen atom are named as prefixes. Examples are



Ketenes. Derivatives of the compound ketene, $\text{CH}_2=\text{C}=\text{O}$, are named by substitutive nomenclature. For example, $\text{C}_4\text{H}_9\text{CH}=\text{C}=\text{O}$ is butyl ketene. An acyl derivative, such as $\text{CH}_3\text{CH}_2-\text{CO}-\text{CH}_2\text{CH}=\text{C}=\text{O}$, may be named as a polyketone, 1-hexene-1,4-dione. Bis-ketene is used for two to avoid ambiguity with diketene (dimeric ketene).

Ketones. Acyclic ketones are named (1) by adding the suffix -one to the name of the hydrocarbon forming the principal chain or (2) by citing the names of the radicals R^1 and R^2 followed by the word *ketone*. In addition to the preceding nomenclature, acyclic monoacyl derivatives of cyclic compounds may be named (3) by prefixing the name of the acyl group to the name of the cyclic compound. For example,

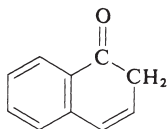


When the cyclic component is benzene or naphthalene, the -ic acid or -oic acid of the acid corresponding to the acyl group is changed to -ophenone or -onaphthone, respectively. For example, $\text{C}_6\text{H}_5-\text{CO}-\text{CH}_2\text{CH}_2\text{CH}_3$ can be named either butyrophenone (or butanophenone) or phenyl propyl ketone.

Radicalofunctional nomenclature can be used when a carbonyl group is attached directly to carbon atoms in two ring systems and no other substituent is present having priority for citation.

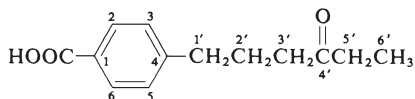
When the methylene group in polycarbocyclic and heterocyclic ketones is replaced by a keto group, the change may be denoted by attaching the suffix -one to the name of the ring system. However, when >CH in an unsaturated or aromatic system is replaced by a keto group, two alternative names become possible. (1) The maximum number of noncumulative double bonds is added after introduction of the carbonyl group(s), and any hydrogen that remains to be added is denoted as indicated hydrogen with the carbonyl group having priority over the indicated hydrogen for lower-numbered locant. (2) The prefix oxo- is used, with the hydrogenation indicated by hydro prefixes; hydrogenation is considered

to have occurred before the introduction of the carbonyl group. For example,

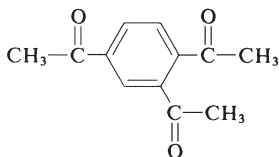


- (1) 1(2*H*)-Naphthalenone
(2) 1-Oxo-1,2-dihydronaphthalene

When another group having higher priority for citation as principal group is also present, the ketonic oxygen may be expressed by the prefix oxo-, or one can use the name of the carbonyl-containing radical, as, for example, acyl radicals and oxo-substituted radicals. Examples are



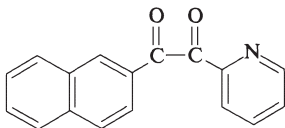
4-(4'-Oxo-hexyl)-1-benzoic acid



1,2,4-Triacetylbenzene

Diketones and tetraketones derived from aromatic compounds by conversion of two or four $\equiv\text{CH}$ groups into keto groups, with any necessary rearrangement of double bonds to a quinonoid structure, are named by adding the suffix -quinone and any necessary affixes.

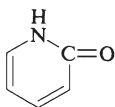
Polyketones in which two or more contiguous carbonyl groups have rings attached at each end may be named (1) by the radicofunctional method or (2) by substitutive nomenclature. For example,



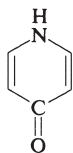
- (1) 2-Naphthyl 2-pyridyl diketone
(2) 1-(2-Naphthyl)-2-(2-pyridyl)ethanedione

Some trivial names are retained: acetone (2-propanone), biacetyl (2,3-butanedione), propiophenone ($\text{C}_6\text{H}_5-\text{CO}-\text{CH}_2\text{CH}_3$), chalcone ($\text{C}_6\text{H}_5-\text{CH}=\text{CH}-\text{CO}-\text{C}_6\text{H}_5$), and deoxybenzoin ($\text{C}_6\text{H}_5-\text{CH}_2-\text{CO}-\text{C}_6\text{H}_5$).

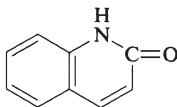
These contracted names of heterocyclic nitrogen compounds are retained as alternatives for systematic names, sometimes with indicated hydrogen. In addition, names of oxo derivatives of fully saturated nitrogen heterocycles that systematically end in -idinone are often contracted to end in -idone when no ambiguity might result. For example,



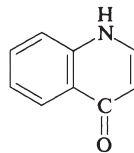
2-Pyridone
2(1*H*)-Pyridone



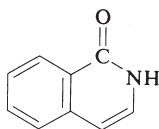
4-Pyridone
4(1*H*)-Pyridone



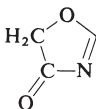
2-Quinolone
2(1*H*)-Quinolone



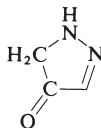
4-Quinolone
4(1*H*)-Quinolone



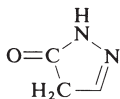
1-Isoquinolone
1(2*H*)-Isoquinolone



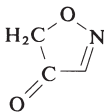
4-Oxazolone
4(5*H*)-Oxazolone



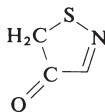
4-Pyrazolone
4(5*H*)-Pyrazolone



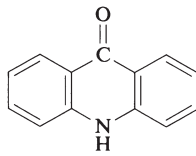
5-Pyrazolone
5(4*H*)-Pyrazolone



4-Isloxazoline
4(5*H*)-Isloxazoline



4-Thiazolone
4(5*H*)-Thiazolone



9-Acridone
9(10*H*)-Acridone

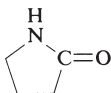
Lactones, Lactides, Lactams, and Lactims. When the hydroxy acid from which water may be considered to have been eliminated has a trivial name, the lactone is designated by substituting -olactone for -ic acid. Locants for a carbonyl group are numbered as low as possible, even before that of a hydroxyl group.

Lactones formed from aliphatic acids are named by adding -olide to the name of the nonhydroxylated hydrocarbon with the same number of carbon atoms. The suffix -olide signifies the change of $\text{>CH}\cdots\text{CH}_3$ into $\text{>C}\cdots\text{C}=\text{O}$

Structures in which one or more (but not all) rings of an aggregate are lactone rings are named by placing -carbolactone (denoting the —O—CO— bridge) after the names of the structures that remain when each bridge is replaced by two hydrogen atoms. The locant for —CO— is cited before that for the ester oxygen atom. An additional carbon atom is incorporated into this structure as compared to the -olide.

These trivial names are permitted: γ -butyrolactone, γ -valerolactone, and δ -valerolactone. Names based on heterocycles may be used for all lactones. Thus, γ -butyrolactone is also tetrahydro-2-furanone or dihydro-2(3*H*)-furanone.

Lactides, intermolecular cyclic esters, are named as heterocycles. **Lactams** and **lactims**, containing a —CO—NH— and —C(OH)=N— group, respectively, are named as heterocycles, but they may also be named with -lactam or -lactim in place of -olide. For example,



(1) 2-Pyrrolidinone
(2) 4-Butanellactam

Nitriles and Related Compounds. For acids whose systematic names end in -carboxylic acid, nitriles are named by adding the suffix -carbonitrile when the —CN group replaces the —COOH group. The carbon atom of the —CN group is excluded from the numbering of a chain to which it is attached. However, when the triple-bonded nitrogen atom is considered to replace three hydrogen atoms at the end of the main chain of an acyclic hydrocarbon, the suffix -nitrile is added to the name of the hydrocarbon. Numbering begins with the carbon attached to the nitrogen. For example, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CN}$ is named (1) pentanecarbonitrile or (2) hexanenitrile.

Trivial acid names are formed by changing the endings -oic acid or -ic acid to -onitrile. For example, CH_3CN is acetonitrile. When the $-\text{CN}$ group is not the highest priority group, the $-\text{CN}$ group is denoted by the prefix cyano-.

In order of decreasing priority for citation of a functional class name, and the prefix for substitutive nomenclature, are the following related compounds:

Functional group	Prefix	Radicofunctional ending
$-\text{NC}$	Isocyano-	Isocyanide
$-\text{OCN}$	Cyanato-	Cyanate
$-\text{NCO}$	Isocyanato-	Isocyanate
$-\text{ONC}$	—	Fulminate
$-\text{SCN}$	Thiocyanato-	Thiocyanate
$-\text{NCS}$	Isothiocyanato-	Isothiocyanate
$-\text{SeCN}$	Selenocyanato-	Selenocyanate
$-\text{NCSe}$	Isoselenocyanato-	Isoselenocyanate

Peroxides. Compounds of the type $\text{R}-\text{O}-\text{OH}$ are named (1) by placing the name of the radical R before the word *hydroperoxide* or (2) by use of the prefix *hydroperoxy-* when another parent name has higher priority. For example, $\text{C}_2\text{H}_5\text{OOH}$ is ethyl hydroperoxide.

Compounds of the type $\text{R}^1\text{O}-\text{OR}^2$ are named (1) by placing the names of the radicals in alphabetical order before the word *peroxide* when the group $-\text{O}-\text{O}-$ links two chains, two rings, or a ring and a chain, (2) by use of the affix *dioxy* to denote the bivalent group $-\text{O}-\text{O}-$ for naming assemblies of identical units or to form part of a prefix, or (3) by use of the prefix *epidioxy-* when the peroxide group forms a bridge between two carbon atoms, a ring, or a ring system. Examples are methyl propyl peroxide for $\text{CH}_3-\text{O}-\text{O}-\text{C}_3\text{H}_7$ and 2,2'-dioxidiacetic acid for $\text{HOOC}-\text{CH}_2-\text{O}-\text{O}-\text{CH}_2-\text{COOH}$.

Phosphorus Compounds. Acyclic phosphorus compounds containing only one phosphorus atom, as well as compounds in which only a single phosphorus atom is in each of several functional groups, are named as derivatives of the parent structures listed in Table 1.12. Often these are purely hypothetical parent structures. When hydrogen attached to phosphorus is replaced by a hydrocarbon group, the derivative is named by substitution nomenclature. When hydrogen of an $-\text{OH}$ group is replaced, the derivative is named by radicofunctional nomenclature. For example, $\text{C}_2\text{H}_5\text{PH}_2$ is ethylphosphine; $(\text{C}_2\text{H}_5)_2\text{PH}$, diethylphosphine; $\text{CH}_3\text{P}(\text{OH})_2$, dihydroxy-methyl-phosphine or methylphosphonous acid; $\text{C}_2\text{H}_5-\text{PO}(\text{Cl})(\text{OH})$, ethylchlorophosphonic acid or ethylphosphonochloridic acid or hydrogen chlorodioxoethylphosphate(V); $\text{CH}_3\text{CH}(\text{PH}_2)\text{COOH}$, 2-phosphinopropionic acid; $\text{HP}(\text{CH}_2\text{COOH})_2$, phosphinediylldiacetic acid; $(\text{CH}_3)_2\text{HP}(\text{O})\text{OH}$, methylphosphinic acid or hydrogen hydridomethyldioxophosphate(V); $(\text{CH}_3\text{O})_3\text{PO}$, trimethyl phosphate; and $(\text{CH}_3\text{O})_3\text{P}$, trimethyl phosphite.

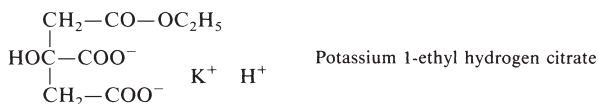
Salts and Esters of Acids. Neutral salts of acids are named by citing the cation(s) and then the anion, whose ending is changed from -oic to -oate or from -ic to -ate. When different acidic residues are present in one structure, prefixes are formed by changing the anion ending -ate to -ato- or -ide to -ido-. The prefix *carboxylato-* denotes the ionic group $-\text{COO}^-$. The phrase: (metal) salt of (the acid) is permissible when the carboxyl groups are not all named as affixes.

Acid salts include the word *hydrogen* (with affixes, if appropriate) inserted between the name of the cation and the name of the anion (or word *salt*).

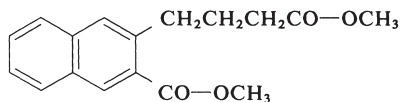
TABLE 1.12 Parent Structures of Phosphorus-containing Compounds

Formula	Parent name	Substitutive prefix	Radicalfunctional ending
H ₃ P	Phosphine	H ₂ P— Phosphino-	Phosphide
H ₃ P	Phosphorane	H ₄ P— Phosphoranyl-	—
		H ₃ P< Phosphoroanediyl-	—
		H ₂ P≡ Phosphoranetriyl-	—
H ₃ PO	Phosphine oxide	—	—
H ₃ PS	Phosphine sulfide	—	—
H ₃ PNH	Phosphine imide	—	—
P(OH) ₃	Phosphorous acid	—	Phosphite
HP(OH) ₂	Phosphonous acid	—	Phosphonite
H ₂ POH	Phosphinous acid	—	Phosphinite
P(O)(OH) ₃	Phosphoric acid	P(O)≡ Phosphoryl-	Phosphate(V)
HP(O)(OH) ₂	Phosphonic acid	HP(O)< Phosphonoyl-	Phosphonate
		—P(O)OH ₂ Phosphinoyl-	—
H ₂ P(O)OH	Phosphinic acid	H ₂ P(O)— Phosphinoyl-	Phosphinate
		>P(O)OH Phosphinoco-	—
		Phosphinato-	—

Esters are named similarly, with the name of the alkyl or aryl radical replacing the name of the cation. Acid esters of acids and their salts are named as neutral esters, but the components are cited in the order: cation, alkyl or aryl radical, hydrogen, and anion. Locants are added if necessary. For example,



Ester groups in R¹—CO—OR² compounds are named (1) by the prefix alkoxy carbonyl- or aryloxy carbonyl- for —CO—OR² when the radical R¹ contains a substituent with priority for citation as principal group or (2) by the prefix acyloxy- for R¹—CO—O— when the radical R² contains a substituent with priority for citation as principal group. Examples are



Methyl 3-methoxycarbonyl-2-naphthalenebutyrate



The trivial name *acetoxy* is retained for the CH₃—CO—O— group. Compounds of the type R²C(OR²)₃ are named as R² esters of the hypothetical ortho acids. For example, CH₃C(OCH₃)₃ is trimethyl orthoacetate.

Silicon Compounds. SiH_4 is called silane; its acyclic homologs are called disilane, trisilane, and so on, according to the number of silicon atoms present. The chain is numbered from one end to the other so as to give the lowest-numbered locant in radicals to the free valence or to substituents on a chain. The abbreviated form silyl is used for the radical SiH_3- . Numbering and citation of side chains proceed according to the principles set forth for hydrocarbon chains. Cyclic nonaromatic structures are designated by the prefix cyclo-.

When a chain or ring system is composed entirely of alternating silicon and oxygen atoms, the parent name *siloxane* is used with a multiplying affix to denote the number of silicon atoms present. The parent name *silazane* implies alternating silicon and nitrogen atoms; multiplying affixes denote the number of silicon atoms present.

The prefix *sila-* designates replacement of carbon by silicon in replacement nomenclature. Prefix names for radicals are formed analogously to those for the corresponding carbon-containing compounds. Thus silyl is used for SiH_3- , silylene for $-\text{SiH}_2-$, silyldiyne for $-\text{SiH}-$.

Sulfur Compounds

Bivalent Sulfur. The prefix thio-, placed before an affix that denotes the oxygen-containing group or an oxygen atom, implies the replacement of that oxygen by sulfur. Thus the suffix -thiol denotes $-\text{SH}$, -thione denotes $-(\text{C})=\text{S}$ and implies the presence of an $=\text{S}$ at a nonterminal carbon atom, -thioic acid denotes $[(\text{C})=\text{S}]\text{OH} \rightleftharpoons [(\text{C})=\text{O}]\text{SH}$ (that is, the *O*-substituted acid and the *S*-substituted acid, respectively), -dithioic acid denotes $[-\text{C}(\text{S})]\text{SH}$, and -thial denotes $-(\text{C})\text{HS}$ (or -carbothialdehyde denotes $-\text{CHS}$). When -carboxylic acid has been used for acids, the sulfur analog is named -carbothioic acid or -carbodithioic acid.

Prefixes for the groups $\text{HS}-$ and $\text{RS}-$ are mercapto- and alkylthio-, respectively; this latter name may require parentheses for distinction from the use of thio- for replacement of oxygen in a trivially named acid. Examples of this problem are $4-\text{C}_2\text{H}_5-\text{C}_6\text{H}_4-\text{CSOH}$ named *p*-ethyl(thio)benzoic acid and $4-\text{C}_2\text{H}_5-\text{S}-\text{C}_6\text{H}_4-\text{COOH}$ named *p*-(ethylthio)benzoic acid. When $-\text{SH}$ is not the principal group, the prefix mercapto- is placed before the name of the parent compound to denote an unsubstituted $-\text{SH}$ group.

The prefix thioxo- is used for naming $=\text{S}$ in a thioketone. Sulfur analogs of acetals are named as alkylthio- or arylthio-. For example, $\text{CH}_3\text{CH}(\text{SCH}_3)\text{OCH}_3$ is 1-methoxy-1-(methylthio)ethane. Prefix forms for -carbothioic acids are hydroxy(thiocarbonyl)- when referring to the *O*-substituted acid and mercapto(carbonyl)- for the *S*-substituted acid.

Salts are formed as with oxygen-containing compounds. For example, $\text{C}_2\text{H}_5-\text{S}-\text{Na}$ is named either sodium ethanethiolate or sodium ethyl sulfide. If mercapto- has been used as a prefix, the salt is named by use of the prefix sulfido- for $-\text{S}^-$.

Compounds of the type $\text{R}^1-\text{S}-\text{R}^2$ are named alkylthio- (or arylthio-) as a prefix to the name of R^1 or R^2 , whichever is the senior.

Sulfonium Compounds. Sulfonium compounds of the type $\text{R}^1\text{R}^2\text{R}^3\text{S}^+\text{X}^-$ are named by citing in alphabetical order the radical names followed by -sulfonium and the name of the anion. For heterocyclic compounds, -ium is added to the name of the ring system. Replacement of $>\text{CH}$ by sulfonium sulfur is denoted by the prefix thionia-, and the name of the anion is added at the end.

Organosulfur Halides. When sulfur is directly linked only to an organic radical and to a halogen atom, the radical name is attached to the word *sulfur* and the name(s) and number of the halide(s) are stated as a separate word. Alternatively, the name can be formed from $\text{R}-\text{SOH}$, a sulfenic acid whose radical prefix is sulphenyl-. For example, $\text{CH}_3\text{CH}_2-\text{S}-\text{Br}$ would be named either ethylsulfur monobromide or ethanesulphenyl bromide. When another principal group is present, a composite prefix is formed from the number and substitutive name(s) of the halogen atoms in front of the syllable thio. For example, $\text{BrS}-\text{COOH}$ is (bromothio)formic acid.

Sulfoxides. Sulfoxides, R^1-SO-R^2 , are named by placing the names of the radicals in alphabetical order before the word *sulfoxide*. Alternatively, the less senior radical is named followed by sulfinyl- and concluded by the name of the senior group. For example, $CH_3CH_2-SO-CH_2CH_2CH_3$ is named either ethyl propyl sulfoxide or 1-(ethylsulfinyl)-propane.

When an $\geq SO$ group is incorporated in a ring, the compound is named an oxide.

Sulfones. Sulfones, $R^1-SO_2-R^2$, are named in an analogous manner to sulfoxides, using the word *sulfone* in place of *sulfoxide*. In prefixes, the less senior radical is followed by -sulfonyl-. When the $\geq SO_2$ group is incorporated in a ring, the compound is named as a dioxide.

Sulfur Acids. Organic oxy acids of sulfur, that is, $-SO_3H$, $-SO_2H$, and $-SOH$, are named sulfonic acid, sulfinic acid, and sulfenic acid, respectively. In subordinate use, the respective prefixes are sulfo-, sulfino, and sulfeno-. The grouping $-SO_2-O-SO_2-$ or $-SO-O-SO-$ is named sulfonic or sulfinic anhydride, respectively.

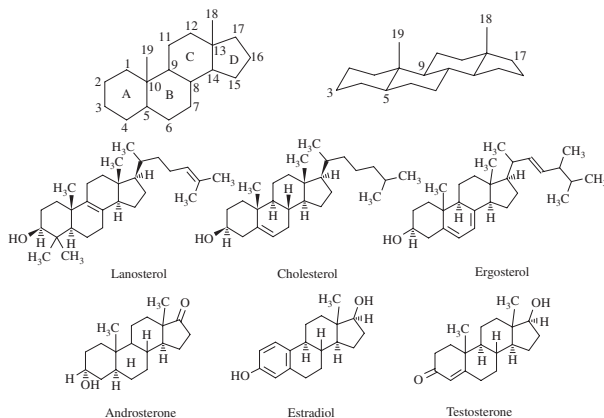
Inorganic nomenclature is employed in naming sulfur acids and their derivatives in which sulfur is linked only through oxygen to the organic radical. For example, $(C_2H_5O)_2SO_2$ is diethyl sulfate and $C_2H_5O-SO_2-OH$ is ethyl hydrogen sulfate. Prefixes *O*- and *S*- are used where necessary to denote attachment to oxygen and to sulfur, respectively, in sulfur replacement compounds. For example, CH_3-S-SO_2-ONa is sodium *S*-methyl thiosulfate.

When sulfur is linked only through nitrogen, or through nitrogen and oxygen, to the organic radical, naming is as follows: (1) *N*-substituted amides are designated as *N*-substituted derivatives of the sulfur amides and (2) compounds of the type $R-NH-SO_3H$ may be named as *N*-substituted sulfamic acids or by the prefix sulfoamino- to denote the group HO_3S-NH- . The groups $-N=SO$ and $-N=SO_2$ are named sulfinylamines and sulfonylamines, respectively.

Sultones and Sultams. Compounds containing the group $-SO_2-O-$ as part of the ring are called -sultone. The $-SO_2-$ group has priority over the $-O-$ group for lowest-numbered locant.

Similarly, the $-SO_2-N-$ group as part of a ring is named by adding -sultam to the name of the hydrocarbon with the same number of carbon atoms. The $-SO_2-$ has priority over $-N=$ for lowest-numbered locant.

Steroids. Steroids are important natural products that have a special nomenclature. They typically consist of three fused 6-membered rings and a four fused 5-membered ring. The

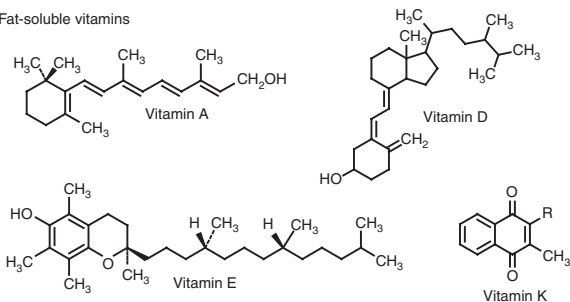


rings are designated A, B, C, and D as shown here. The most common, all *trans* ring fusion is illustrated in the right hand structure. Most steroids that occur naturally possess the two methyl groups ("bridgehead" or angular methyl groups) shown as carbons 18 and 19 at positions 10 and 13, respectively.

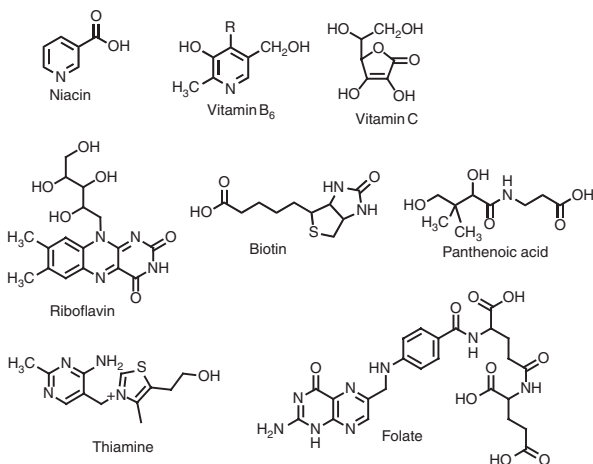
Cholesterol is the most common steroid of mammalian membranes. It is formed biologically from lanosterol, as shown. Ergosterol is the most common steroid of fungal membranes. It differs from cholesterol by the presence of two additional double bonds that affect its three dimensional structure. Also shown are three so-called steroid hormones, androsterone, estradiol, and testosterone. Note the presence of an aromatic A-ring in estradiol.

Vitamins. The vitamins are natural organic compounds of considerable diversity that occur widely. The name derives from the Latin *vita* (life) and "amin," a shortened form of amine. The name reflects the historical discovery of these substances, not all of which are amines. They are all of relatively low molecular weight, especially compared to peptides but in a range comparable to steroids. These substances are uniformly active and play various roles in biosynthesis and metabolism. The vitamins are too numerous to detail here but the most common examples are illustrated. They are classed using the common system, that is, water or fat soluble, depending on their approximate level of hydrophobicity or hydrophilicity. Their names are typically nonsystematic but the diversity of their structures requires that the trivial names be used.

Fat-soluble vitamins



Water-soluble vitamins



Biological Nomenclature

The names assigned to compounds by organic chemists and biologists sometimes differ. Moreover, biological structures are made up of repeating components and rapidly become large and complex molecules. Thus, special terminology has been developed to assist in describing these compounds.

Amino Acids. An amino acid is any organic compound that possesses both amine ($-\text{NH}_2$) and carboxyl ($-\text{COOH}$) groups within the same organic framework. When both functional groups are attached to the same carbon atom, they are designated α -amino acids. These are of special significance in biology as they form the diverse monomer set from which peptides and proteins are built.

Aminoacetic acid is the simplest example of an α -amino acid. Among the 20 biologically most important amino acids, its structure is unique in two ways. First, it possesses no “sidechain” attached to the methylene carbon. Second, the lack of any substituent (other than hydrogen) means that aminoacetic acid, more commonly called glycine, is achiral. The other 19 “essential” or “common” amino acids possess sidechains attached in a stereochemically identical fashion.

The other 19 common α -amino acids have side chains attached at the position represented by R. Among these 19, proline is unique because its sidechain is attached at the other end to the amino nitrogen, which is therefore secondary rather than primary.

The twenty common α -amino acids may be named systematically. For example, when R is methyl, the compound may be called 2-methylaminoacetic acid. It may also correctly be called 2-aminopropanoic acid. By far, however, it is most commonly called alanine.

TABLE 1.13

Common	IUPAC	IUB	$-\text{pK}_{\text{COOH}}$	$-\text{pK}_{\text{NH}_3^+}$	$\text{pK}_{\text{Side chain}}$	I_{pH}	
Alanine	Ala	A	2.34	9.69	—	6.01	
Arginine	Arg	R	2.17	9.04	12.84	10.76	
Asparagine	Asn	N	2.02	8.60	—	5.41	

TABLE 1.13 (*continued*)

Common	IUPAC	IUB	$-\text{pK}_{\text{COOH}}$	$-\text{pK}_{\text{NH}_3^+}$	$\text{pK}_{\text{Side chain}}$	I_{pH}	
Aspartic acid	Asp	D	1.88	9.60	3.65	2.77	
Cystine	Cys	C	1.71	8.18	10.28	5.02	
Glutamic acid	Glu	E	2.16	9.67	4.32	3.24	
Glutamine	Gln	Q	2.17	9.13	—	5.65	
Glycine	Gly	G	2.34	9.60	—	5.97	
Histidine	His	H	1.82	9.17	6.00	7.59	
Isoleucine	Ile	I	2.36	9.68	—	6.02	
Leucine	Leu	L	2.36	9.60	—	5.98	
Lysine	Lys	K	2.18	9.12	10.53	9.82	
Methionine	Met	M	2.28	9.21	—	5.74	
Phenylalanine	Phe	F	1.83	9.13	—	5.84	
Proline	Pro	P	1.99	10.6	—	6.30	
Serine	Ser	S	2.21	9.15	—	5.68	

TABLE 1.13 (continued)

Common	IUPAC	IUB	—pK _{COOH}	—pK _{NH₃⁺}	pK _{Side chain}	I _{pH}	
Threonine	Thr	T	2.71	9.62	—	6.16	
Tryptophan	Trp	W	2.38	9.39	—	5.89	
Tyrosine	Tyr	Y	2.20	9.11	10.07	5.66	
Valine	Val	V	2.32	9.62	—	5.96	

The names and structures of the twenty natural amino acids are given in Table 1.13. The International Union of Pure and Applied Chemistry (IUPAC) uses the three-letter abbreviations shown in the second column of Table 1.13 to describe amino acids. These are widely used in biological circles as well but are inappropriate when long peptide or protein sequences need to be described. For example, when proinsulin is cleaved, it forms the biologically important peptide insulin and another peptide usually called C-peptide. The human peptide consists of a linear chain of 31 amino acids that have the sequence, from amino to carboxyl, H₂N-Glu-Ala-Glu-Asp-Leu-Gln-Val-Glu-Gln-Glu-Leu-Gly-Gly-Pro-Gly-Ala-Gly-Ser-Leu-Gln-Pro-Leu-Ala-Leu-Glu-Gly-Ser-Leu-Gln-OH. This is readily comprehensible to most chemists because the abbreviations are typically the first three letters of the amino acid. Thus, alanine is Ala and arginine is Arg. Aspartic acid and asparagine cannot both be named Asp so the latter is distinguished as Asn.

Biologists often must compare peptides or proteins from different species. If the IUPAC nomenclature was used, the descriptor for this peptide would be about four-fold longer than if the International Union of Biology’s (IUB) single-letter codes are used. Where possible, the first letter of the amino acid’s name is used. As with the three-letter abbreviations, this is not always possible. Alanine is A and aspartic acid is arbitrarily assigned the letter D. Asparagine is called N. Glycine is G so glutamic acid is designated E. Although arbitrary, the name is logical for the homologue of aspartic acid. Glutamine is called Q. Arginine cannot use “A,” which is taken by alanine, but the letter “R” is suggestive and serves as a mnemonic.

When the single-letter abbreviations are used, the human C-peptide sequence reduces to EAEDLQVGQVELGGGPGAGSLQPLALEGSLQ, often written in groups of five letters as EAEDLQVGQVELGGG PGAGS LQPLA LEGSL Q so that the sequence can be more conveniently read and compared with other sequences.

Most of three-letter abbreviations are taken from the first three letters of the name of the corresponding amino acid and are pronounced as written (alanine—Ala, cysteine—Cys). The one-letter symbol for the amino acids is usually the first letter of the amino acid’s name and is often used when comparing the amino acids sequences of several similar proteins.

Note that the single-letter abbreviations permit a fast comparison of the sequences so that their differences and similarities can quickly be discerned. The sequences for C-peptides from humans and from rats are compared below (differences are highlighted):

EAEDI	QVGQV	ELGGG	PGAGS	LQPLA	LEGSL	Q (Human)
EVEDP	QVPQL	ELGGG	PEAGD	LQTLA	LEVAR	Q (Rat)

Ten of the amino acids in each sequence differ. Thus, 21 of the 31 amino acids are identical within the sequence. The sequence homology is said to be $(21/31 \times 100) = 68\%$. It would have been much more difficult to make this comparison using the longer three-letter abbreviations. For a protein having 200 or 300 amino acids, the problem becomes correspondingly greater.

Despite the greater economy of using single letter amino acid abbreviations, it is the three-letter abbreviations that have become shortened names for the essential amino acids. For example, practicing scientists would identify the sequence GPAGW as "Gly-Pro-Ala-Gly-Try." A sequence containing both aspartic acid and asparagine such as GAGE would be referred to in conversation as "Gly-Asp-Gly-Asparagine."

Formally, however, the amino acids contained either in peptides or proteins are named in a fashion related to that used for alkanes. The "-ine" suffix is replaced by "-yl" to give, for GAG, glycyl-alanyl-glycine. Peptide and protein sequences are always written and named from the N-terminus to the C-terminus. The C-terminal amino acid retains its full name.

Stereochemistry

Concepts in stereochemistry, that is, chemistry in three-dimensional space, are in the process of rapid expansion. This section will deal with only the main principles. The compounds discussed will be those that have identical molecular formulas but differ in the arrangement of their atoms in space. *Stereoisomers* is the name applied to these compounds.

Stereoisomers can be grouped into three categories: (1) Conformational isomers differ from each other only in the way their atoms are oriented in space, but can be converted into one another by rotation about sigma bonds. (2) Geometric isomers are compounds in which rotation about a double bond is restricted. (3) Configurational isomers differ from one another only in configuration about a chiral center, axis, or plane. In subsequent structural representations, a broken line denotes a bond projecting behind the plane of the paper and a wedge denotes a bond projecting in front of the plane of the paper. A line of normal thickness denotes a bond lying essentially in the plane of the paper.

Conformational Isomers. A molecule in a conformation into which its atoms return spontaneously after small displacements is termed a *conformer*. Different arrangements of atoms that can be converted into one another by rotation about single bonds are called *conformational isomers* (see Figure 1.3). A pair of conformational isomers can be but do not have to be mirror images of each other. When they are not mirror images, they are called *diastereomers*.

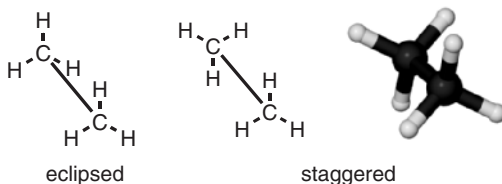


FIGURE 1.3 Eclipsed (left) and staggered (right) conformations of ethane. The ball and stick model is in the staggered conformation.

Acyclic Compounds. Different conformations of acyclic compounds are best viewed by construction of ball-and-stick molecules or by use of Newman projections. Both types of representations are shown for ethane. Atoms or groups that are attached at opposite ends of a single bond should be viewed along the bond axis. If two atoms or groups attached at opposite ends of the bond appear directly one behind the other, these atoms or groups are described as eclipsed. That portion of the molecule is described as being in the eclipsed conformation. If not eclipsed, the atoms or groups and the conformation may be described as staggered. Newman projections show these conformations clearly.

Certain physical properties show that rotation about the single bond is not quite free. For ethane there is an energy barrier of about $3\text{ kcal} \cdot \text{mol}^{-1}$ ($12\text{ kJ} \cdot \text{mol}^{-1}$). The potential energy of the molecule is at a minimum for the staggered conformation, increases with rotation, and reaches a maximum at the eclipsed conformation. The energy required to rotate the atoms or groups about the carbon-carbon bond is called *torsional energy*. Torsional strain is the cause of the relative instability of the eclipsed conformation or any intermediate skew conformations.

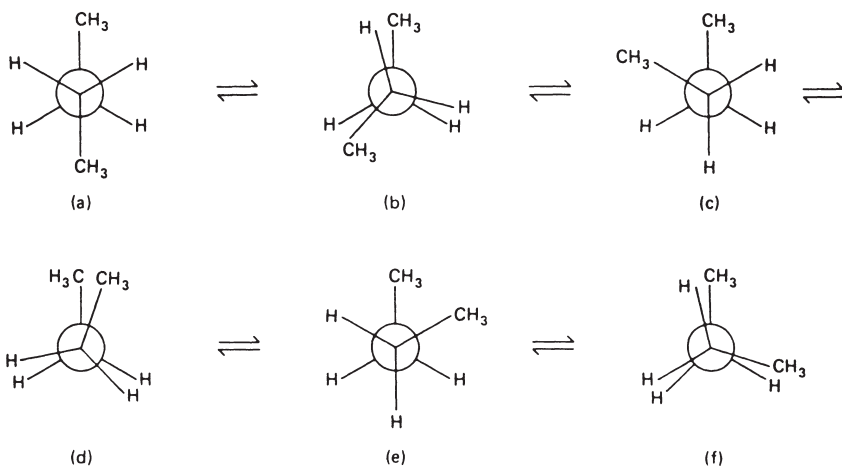


FIGURE 1.4 Conformations of butane. (a) *Anti*-staggered; (b) eclipsed; (c) *gauche*-staggered; (d) eclipsed; (e) *gauche*-staggered; (f) eclipsed. (Eclipsed conformations are slightly staggered for convenience in drawing; actually they are superimposed.)

In butane, with a methyl group replacing one hydrogen on each carbon of ethane, there are several different staggered conformations (see Figure 1.4). There is the *anti* conformation in which the methyl groups are as far apart as they can be (dihedral angle of 180°). There are two *gauche* conformations in which the methyl groups are only 60° apart; these are two nonsuperimposable mirror images of each other. The *anti* conformation is more stable than the *gauche* by about $0.9 \text{ kcal} \cdot \text{mol}^{-1}$ ($4 \text{ kJ} \cdot \text{mol}^{-1}$). Both are free of torsional strain. However, in a *gauche* conformation the methyl groups are closer together than the sum of their van der Waals' radii. Under these conditions van der Waals' forces are repulsive and raise the energy of conformation. This strain can affect not only the relative stabilities of various staggered conformations but also the heights of the energy barriers between them. The energy maximum (estimated at $4.8\text{--}6.1 \text{ kcal} \cdot \text{mol}^{-1}$ or $20\text{--}25 \text{ kJ} \cdot \text{mol}^{-1}$) is reached when two methyl groups swing past each other (the eclipsed conformation) rather than past hydrogen atoms.

Cyclic Compounds. Although cyclic aliphatic compounds are often drawn as if they were planar geometric figures (a triangle for cyclopropane, a square for cyclobutane, and so on), their structures are not that simple. Cyclopropane does possess the maximum angle strain if one considers the difference between a tetrahedral angle (109.5°) and the 60° angle of the cyclopropane structure. Nevertheless the cyclopropane structure is thermally quite stable. The highest electron density of the carbon–carbon bonds does not lie along the lines connecting the carbon atoms. Bonding electrons lie principally outside the triangular internuclear lines and result in what are known as *bent bonds* (see Figure 1.5).

Cyclobutane has less angle strain than cyclopropane (only 19.5°). It is also believed to have some bent-bond character associated with the carbon–carbon bonds. The molecule exists in a nonplanar conformation in order to minimize hydrogen–hydrogen eclipsing strain.

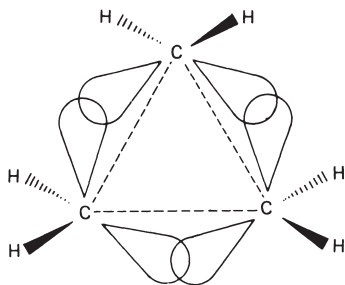


FIGURE 1.5 The bent bonds ("tear drops") of cyclopropane.



FIGURE 1.6 The conformations of cyclopentane.

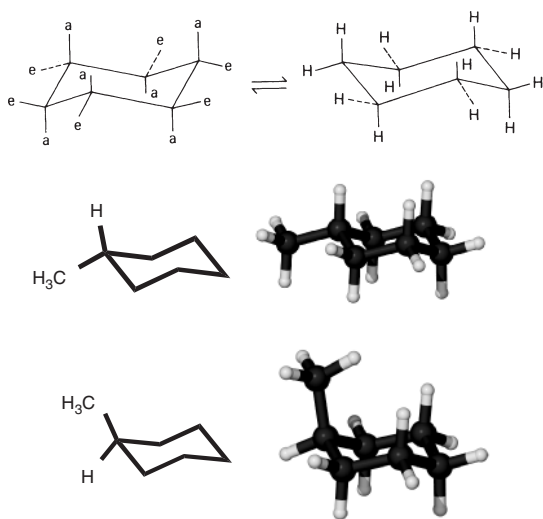


FIGURE 1.7 The two chair conformations of cyclohexane: *a* = axial hydrogen atom and *e* = equatorial hydrogen atom. The middle and bottom panels show methylcyclohexane in the chair form with the methyl group equatorial (middle) and axial (bottom).

Cyclopentane is nonplanar, with a structure that resembles an envelope (see Figure 1.6). Four of the carbon atoms are in one plane, and the fifth is out of that plane. The molecule is in continual motion so that the out-of-plane carbon moves rapidly around the ring.

The 12 hydrogen atoms of cyclohexane do not occupy equivalent positions. In the chair conformation six hydrogen atoms are perpendicular to the average plane of the molecule and six are directed outward from the ring, slightly above or below the molecular plane (see Figure 1.7). Bonds which are perpendicular to the molecular plane are known as *axial bonds*, and those which extend outward from the ring are known as *equatorial bonds*. The three axial bonds directed upward originate from alternate carbon atoms and are parallel with each other; a similar situation exists for the three axial bonds directed downward. Each equatorial bond is drawn so as to be parallel with the ring carbon–carbon bond once removed from the point of attachment to that equatorial bond. At room temperature, cyclohexane is interconverting rapidly between two chair conformations. As one chair form converts to the other, all the equatorial hydrogen atoms become axial and all the axial hydrogens become equatorial. The interconversion is so rapid that all hydrogen atoms on cyclohexane can be considered equivalent. Interconversion is believed to take place by movement of one side of the chair structure to produce the twist boat, and then movement of the other side of the twist boat to give the other chair form. The chair conformation is the most favored structure for cyclohexane. No angle strain is encountered since all bond angles remain tetrahedral. Torsional strain is minimal because all groups are staggered.

In the boat conformation of cyclohexane (Figure 1.8) eclipsing torsional strain is significant, although no angle strain is encountered. Nonbonded interaction between the two hydrogen atoms across the ring from each other (the “flagpole” hydrogens) is unfavorable. The boat conformation is about $6.5 \text{ kcal} \cdot \text{mol}^{-1}$ ($27 \text{ kJ} \cdot \text{mol}^{-1}$) higher in energy than the chair form at 25°C .

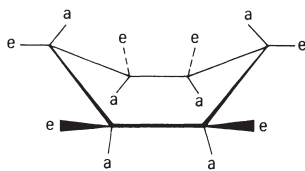


FIGURE 1.8 The boat conformation of cyclohexane. *a* = axial hydrogen atom and *e* = equatorial hydrogen atom.



FIGURE 1.9 Twist-boat conformation of cyclohexane.

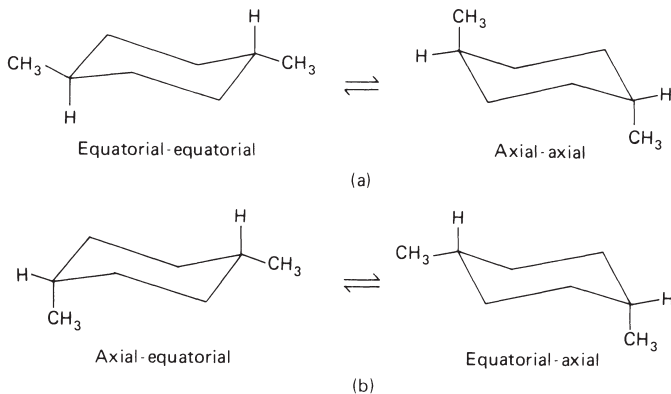


FIGURE 1.10 Two isomers of 1,4-dimethylcyclohexane. (a) *Trans* isomer; (b) *cis* isomer.

A modified boat conformation of cyclohexane, known as the twist boat (Figure 1.9), or skew boat, has been suggested to minimize torsional and nonbonded interactions. This particular conformation is estimated to be about $1.5 \text{ kcal} \cdot \text{mol}^{-1}$ (6 kJ mol^{-1}) lower in energy than the boat form at room temperature.

The medium-size rings (7–12 ring atoms) are relatively free of angle strain and can easily take a variety of spatial arrangements. They are not large enough to avoid all nonbonded interactions between atoms.

Disubstituted cyclohexanes can exist as *cis-trans* isomers as well as axial-equatorial conformers. Two isomers are predicted for 1,4-dimethylcyclohexane (see Figure 1.10). For the *trans* isomer the diequatorial conformer is the energetically favorable form. Only one *cis* isomer is observed, since the two conformers of the *cis* compound are identical. Interconversion takes place between the conformational (equatorial-axial) isomers but not configurational (*cis-trans*) isomers.

The bicyclic compound decahydronaphthalene, or bicyclo[4.4.0]decane, has two fused six-membered rings. It exists in *cis* and *trans* forms (see Figure 1.11), as determined by the configurations at the bridgehead carbon atoms. Both *cis*- and *trans*-decahydronaphthalene can be constructed with two chair conformations.

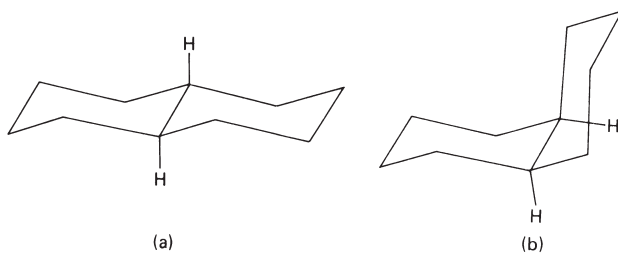


FIGURE 1.11 Two isomers of decahydronaphthalene, or bicyclo[4.4.0]decane. (a) *Trans* isomer; (b) *cis* isomer.

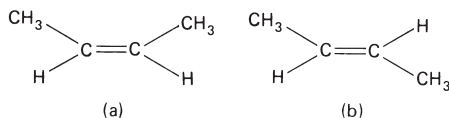


FIGURE 1.12 Two isomers of 2-butene. (a) *Cis* isomer, bp 3.8°C, mp -138.9°C, dipole moment 0.33 D; (b) *trans* isomer, bp 0.88°C, mp -105.6°C, dipole moment 0 D.

Geometrical Isomerism. Rotation about a carbon-carbon double bond is restricted because of interaction between the *p* orbitals which make up the pi bond. Isomerism due to such restricted rotation about a bond is known as *geometric isomerism*. Parallel overlap of the *p* orbitals of each carbon atom of the double bond forms the molecular orbital of the pi bond. The relatively large barrier to rotation about the pi bond is estimated to be nearly 63 kcal · mol⁻¹ (263 kJ · mol⁻¹).

When two different substituents are attached to each carbon atom of the double bond, *cis-trans* isomers can exist. In the case of *cis*-2-butene (Figure 1.12a), both methyl groups are on the same side of the double bond. The other isomer has the methyl groups on opposite sides and is designated as *trans*-2-butene (Figure 1.12b). Their physical properties are quite different. Geometric isomerism can also exist in ring systems; examples were cited in the previous discussion on conformational isomers.

For compounds containing only double-bonded atoms, the reference plane contains the double-bonded atoms and is perpendicular to the plane containing these atoms and those directly attached to them. It is customary to draw the formulas so that the reference plane is perpendicular to that of the paper. For cyclic compounds the reference plane is that in which the ring skeleton lies or to which it approximates. Cyclic structures are commonly drawn with the ring atoms in the plane of the paper.

Sequence Rules for Geometric Isomers and Chiral Compounds. Although *cis* and *trans* designations have been used for many years, this approach becomes useless in complex systems. To eliminate confusion when each carbon of a double bond or a chiral center is

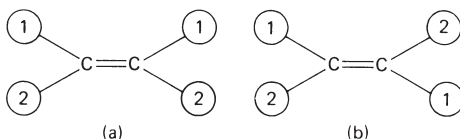
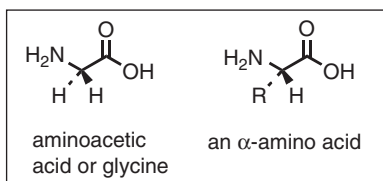


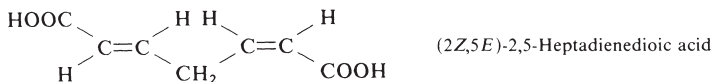
FIGURE 1.13 Configurations designated by priority groups. (a) *Z* (*cis*); (b) *E* (*trans*).

connected to different groups, the Cahn, Ingold, and Prelog system for designating configuration about a double bond or a chiral center has been adopted by IUPAC. Groups on each carbon atom of the double bond are assigned a first (1) or second (2) priority. Priority is then compared at one carbon relative to the other. When both first priority groups are on the *same side* of the double bond, the configuration is designated as *Z* (from the German *zusammen*, “together”), which was formerly *cis*. If the first priority groups are on *opposite sides* of the double bond, the designation is *E* (from the German *entgegen*, “in opposition to”), which was formerly *trans*. (See Figure 1.13.)

When a molecule contains more than one double bond, each *E* or *Z* prefix has associated with it the lower-numbered locant of the double bond concerned. Thus (see also the rules that follow)

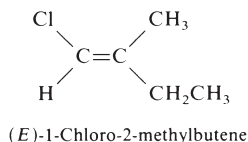
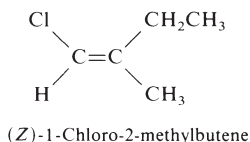


When the sequence rules permit alternatives, preference for lower-numbered locants and for inclusion in the principal chain is allotted as follows in the order stated: *Z* over *E* groups and *cis* over *trans* cyclic groups. If a choice is still not attained, then the lower-numbered locant for such a preferred group at the first point of difference is the determining factor. For example,



RULE 1. Priority is assigned to atoms on the basis of atomic number. Higher priority is assigned to atoms of higher atomic number. If two atoms are isotopes of the same element, the atom of higher mass number has the higher priority. For example, in 2-butene, the carbon atom of each methyl group receives first priority over the hydrogen atom connected to the same carbon atom. Around the asymmetric carbon atom in chloriodomethanesulfonic acid, the priority sequence is I, Cl, S, H. In 1-bromo-1-deuteroethane, the priority sequence is Cl, C, D, H.

RULE 2. When atoms attached directly to a double-bonded carbon have the same priority, the second atoms are considered and so on, if necessary, working outward once again from the double bond or chiral center. For example, in 1-chloro-2-methylbutene, in CH_3 the second atoms are H, H, H and in CH_2CH_3 they are C, H, H. Since carbon has a higher atomic number than hydrogen, the ethyl group has the next highest priority after the chlorine atom.



RULE 3. When groups under consideration have double or triple bonds, the multiple-bonded atom is replaced conceptually by two or three single bonds to that same kind of

atom. Thus, $=\text{A}$ is considered to be equivalent to two A's, or $\begin{array}{c} \text{A} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{A} \end{array}$ and $\equiv\text{A}$ equals $\begin{array}{c} \text{A} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{A} \end{array}$.

However, a real $\begin{array}{c} \text{A} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{A} \end{array}$ has priority over $=\text{A}$; likewise a real $\begin{array}{c} \text{A} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{A} \end{array}$ has priority over $\equiv\text{A}$.

Actually, both atoms of a multiple bond are duplicated, or triplicated, so that $\text{C}=\text{O}$ is

treated as $\begin{array}{c} \text{C}-\text{O} \\ | \quad | \\ \text{O} \quad \text{C} \end{array}$, that is $\begin{array}{c} \text{C}-\text{O} \\ | \\ (\text{O}) \end{array}$ and $\begin{array}{c} \text{O}-\text{C} \\ | \\ (\text{C}) \end{array}$, and $\text{C}\equiv\text{N}$ is treated as

$\begin{array}{c} \text{C} \quad \quad \text{N} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ (\text{N}) \quad (\text{N}) \quad (\text{C}) \quad (\text{C}) \end{array}$. A phenyl carbon becomes $\begin{array}{c} \text{CH} \\ \diagdown \quad \diagup \\ \text{C}-\text{C} \\ \diagup \quad \diagdown \\ \text{CH} \end{array}$. Only the double-bonded

atoms themselves are duplicated, not the atoms or groups attached to them. The duplicated atoms (or phantom atoms) may be considered as carrying atomic number zero. For example, among the groups OH, CHO, CH_2OH , and H, the OH group has the highest priority, and the C(O, O, H) of CHO takes priority over the C(O, H, H) of CH_2OH .

Chirality and Optical Activity. A compound is chiral (the term *dissymmetric* was formerly used) if it is not superimposable on its mirror image. A chiral compound does not have a plane of symmetry. Each chiral compound possesses one (or more) of three types of chiral element, namely, a chiral center, a chiral axis, or a chiral plane.

Chiral Center. The chiral center, which is the chiral element most commonly met, is exemplified by an asymmetric carbon with a tetrahedral arrangement of ligands about the carbon. The ligands comprise four different atoms or groups. One "ligand" may be a lone pair of electrons; another, a phantom atom of atomic number zero. This situation is encountered in sulfoxides or with a nitrogen atom. Lactic acid is an example of a molecule with an asymmetric (chiral) carbon. (See Figure 1.14.)

A simpler representation of molecules containing asymmetric carbon atoms is the Fischer projection, which is shown here for the same lactic acid configurations. A Fischer

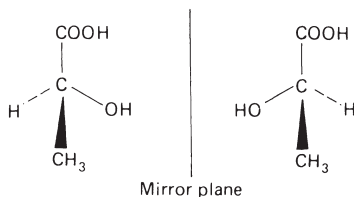


FIGURE 1.14A Stereo drawing of the lactic acid molecule.

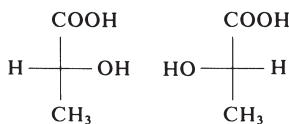


FIGURE 1.14B Fischer projection of the lactic acid molecule.

projection involves drawing a cross and attaching to the four ends the four groups that are attached to the asymmetric carbon atom. The asymmetric carbon atom is understood to be located where the lines cross. The horizontal lines are understood to represent bonds coming toward the viewer out of the plane of the paper. The vertical lines represent bonds going away from the viewer behind the plane of the paper as if the vertical line were the side of a circle. The principal chain is depicted in the vertical direction; the lowest-numbered (locant) chain member is placed at the top position. These formulas may be moved sideways or rotated through 180° in the plane of the paper, but they may not be removed from the plane of the paper (i.e., rotated through 90°). In the latter orientation it is essential to use thickened lines (for bonds coming toward the viewer) and dashed lines (for bonds receding from the viewer) to avoid confusion.

Enantiomers. Two nonsuperimposable structures that are mirror images of each other are known as *enantiomers*. Enantiomers are related to each other in the same way that a right hand is related to a left hand. Except for the direction in which they rotate the plane of polarized light, enantiomers are identical in all physical properties. Enantiomers have identical chemical properties except in their reactivity toward optically active reagents.

Enantiomers rotate the plane of polarized light in opposite directions but with equal magnitude. If the light is rotated in a clockwise direction, the sample is said to be dextro-rotatory and is designed as (+). When a sample rotates the plane of polarized light in a counterclockwise direction, it is said to be levorotatory and is designed as (−). Use of the designations *d* and *l* is discouraged.

Specific Rotation. Optical rotation is caused by individual molecules of the optically active compound. The amount of rotation depends upon how many molecules the light beam encounters in passing through the tube. When allowances are made for the length of the tube that contains the sample and the sample concentration, it is found that the amount of rotation, as well as its direction, is a characteristic of each individual optically active compound.

Specific rotation is the number of degrees of rotation observed if a 1-dm tube is used and the compound being examined is present to the extent of 1 g per 100 mL. The density for a pure liquid replaces the solution concentration.

$$\text{Specific rotation} = [\alpha] = \frac{\text{observed rotation (degrees)}}{\text{length (dm)} \times (\text{g}/100 \text{ mL})}$$

The temperature of the measurement is indicated by a superscript and the wavelength of the light employed by a subscript written after the bracket; for example, $[\alpha]_{590}^{20}$ implies that the measurement was made at 20°C using 590 nm radiation.

Optically Inactive Chiral Compounds. Although chirality is a necessary prerequisite for optical activity, chiral compounds are not necessarily optically active. With an equal mixture of two enantiomers, no net optical rotation is observed. Such a mixture of enantiomers is said to be *racemic* and is designated as (\pm) and not as *dl*. Racemic mixtures usually have melting points higher than the melting point of either pure enantiomer.

A second type of optically inactive chiral compounds, *meso* compounds, will be discussed next.

Multiple Chiral Centers. The number of stereoisomers increases rapidly with an increase in the number of chiral centers in a molecule. A molecule possessing two chiral atoms should have four optical isomers, that is, four structures consisting of two pairs of enantiomers. However, if a compound has two chiral centers but both centers have the same four substituents attached, the total number of isomers is three rather than four. One isomer of such a compound is not chiral because it is identical with its mirror image; it has an internal mirror plane. This is an example of a diastereomer. The achiral structure is denoted as a *meso* compound. Diastereomers have different physical and chemical properties from the optically active enantiomers. Recognition of a plane of symmetry is usually the easiest way to detect a *meso* compound. The stereoisomers of tartaric acid are examples of compounds with multiple chiral centers (see Figure 1.15), and one of its isomers is a *meso* compound.

Stereochemistry is sometimes harder to discern in ring systems than in open-chained compounds. The smallest ring, cyclopropane, has six equivalent hydrogens, each of which may be substituted. When a substituent such as a methyl group replaces a hydrogen, the molecule remains achiral because a mirror plane is present that bisects the substituted carbon (and its substituent) and the opposite bond. One side of the cyclopropane therefore reflects the other. The presence of a substituent makes the other cyclopropane positions nonequivalent. Thus a second methyl group may be added on the same carbon (opposite side of the ring) or on one of the adjacent carbons on either the same or opposite sides of the ring. Figure 1.16 shows some of these possibilities. *E*-1,2-Dicarboxycyclopropane (a) exists in two distinct forms. They are nonsuperimposable mirror images; *Z*-1,2-Dicarboxycyclopropane (b) has an internal mirror plane and is therefore superimposable on its mirror image. Structure (d) in Figure 1.16 shows a molecular model of this compound. The carboxyl substituents do not appear to reflect each other but recall that they can rotate freely about the single bond.

A cyclic compound that has two differently substituted asymmetric carbons will have $2^2 = 4$ optical isomers. These will consist of pairs of *cis* and *trans* enantiomers. When the asymmetric centers have identical substituents, the *cis* isomer will have an internal reflection plane and is called a *meso* form. The *meso* forms of *cis*-1,2-dicarboxycyclopropane are shown in panels (b) and (d) of Figure 1.16 in a line angle drawing and as a molecular model.

Torsional Asymmetry. Rotation about single bonds of most acyclic compounds is relatively free at ordinary temperatures. There are, however, some examples of compounds in which nonbonded interactions between large substituent groups inhibit free rotation about a sigma bond. In some cases these compounds can be separated into pairs of enantiomers.

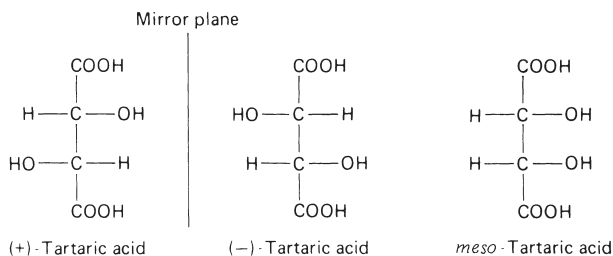


FIGURE 1.15 Isomers of tartaric acid.

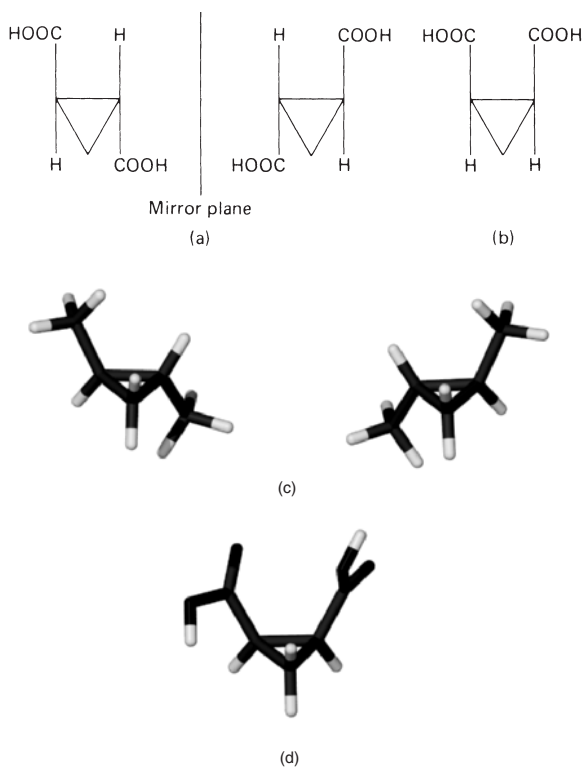


FIGURE 1.16 Isomers of cyclopropane-1,2-dicarboxylic acid. (a) *E*-1,2-Dicarboxycyclopropane (*trans* isomers); (b) *Z*-1,2-Dicarboxycyclopropane isomer. (*meso* isomer); (c) Molecular models of *E*- (*trans*-) 1,2-dimethylcyclopropane shown in the tube representation. Rotation of the right hand structure about a vertical axis through the center of the cyclopropane will superimpose the two methyl groups. The methylene of the rotated structure will be in the back, rather than the front, and not superimposed. (d) A mirror plane through the methylene and the back carbon-carbon bond is a plane of symmetry. The two carboxyl groups appear not to reflect each other in the model shown but they can rotate freely and will reflect each other on an instantaneous basis.

A *chiral axis* is present in chiral biaryl derivatives. When bulky groups are located at the *ortho* positions of each aromatic ring in biphenyl, free rotation about the single bond connecting the two rings is inhibited because of torsional strain associated with twisting rotation about the central single bond. Interconversion of enantiomers is prevented (see Figure 1.17).

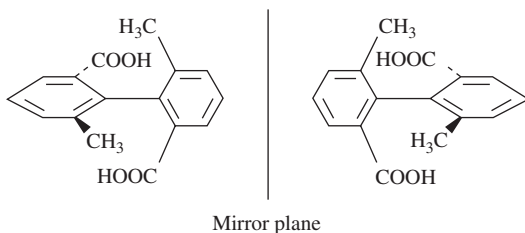


FIGURE 1.17 Isomers of biphenyl compounds with bulky groups attached at the *ortho* positions.

For compounds possessing a chiral axis, the structure can be regarded as an elongated tetrahedron to be viewed along the axis. In deciding upon the absolute configuration it does not matter from which end it is viewed; the nearer pair of ligands receives the first two positions in the order of precedence (see Figure 1.18). For the meaning of (*S*), see the discussion under "Absolute Configuration".

A *chiral plane* is exemplified by the plane containing the benzene ring and the bromine and oxygen atoms in the chiral compound shown in Figure 1.19. Rotation of the benzene ring around the oxygen-to-ring single bonds is inhibited when x is small (although no critical size can be reasonably established).

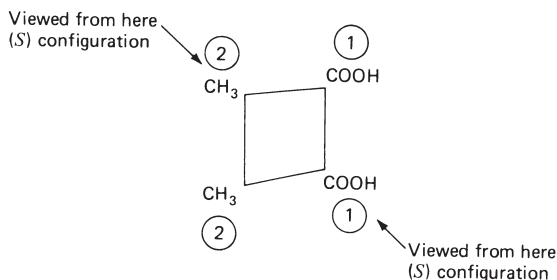


FIGURE 1.18 Example of a chiral axis.

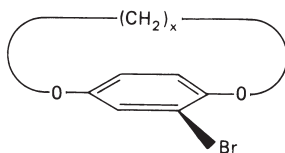


FIGURE 1.19 Example of a chiral plane.

Absolute Configuration. The terms absolute stereochemistry and absolute configuration are used to describe the three-dimensional arrangement of substituents around a chiral element. A general system for designating absolute configuration is based upon the priority system and sequence rules. Each group attached to a chiral center is assigned a number, with number one the highest-priority group. For example, the groups attached to the chiral center of 2-butanol (see Figure 1.20) are assigned these priorities: 1 for OH, 2 for CH_2CH_3 , 3 for CH_3 , and 4 for H. The molecule is then viewed from the side opposite the group of lowest priority (the hydrogen atom), and the arrangement of the remaining groups are noted. If, in proceeding from the group of highest priority to the group of second priority and

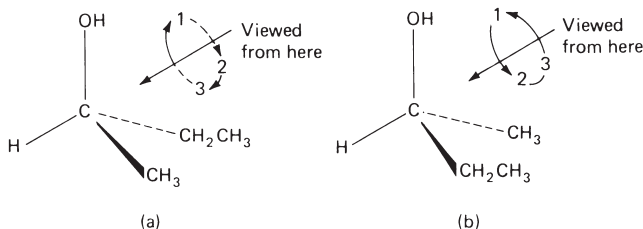


FIGURE 1.20 Viewing angle as a means of designating the absolute configuration of compounds with a chiral axis. (a) (*R*)-2-butanol (sequence clockwise); (b) (*S*)-2-butanol (sequence counterclockwise).

thence to the third, the eye travels in a clockwise direction, the configuration is specified *R* (from the Latin *rectus*, “right”); if the eye travels in a counterclockwise direction, the configuration is specified *S* (from the Latin *sinister*, “left”). The complete name includes both configuration and direction of optical rotation, as for example, (*S*)-(+)-2-butanol.

The relative configurations around the chiral centers of many compounds have been established. One optically active compound is converted to another by a sequence of chemical reactions which are stereospecific; that is, each reaction is known to proceed spatially in a specific way. The configuration of one chiral compound can then be related to the configuration of the next in sequence. In order to establish absolute configuration, one must carry out sufficient stereospecific reactions to relate a new compound to another of known absolute configuration. Historically the configuration of D-(+)-2,3-dihydroxypropanal has served as the standard to which all configuration has been compared. The absolute configuration assigned to this compound has been confirmed by an X-ray crystallographic technique.

Stereochemistry in Biological Systems. Amino acids occur naturally in both D and L (*R* and *S*) enantiomeric configurations. Amino acids that occur in proteins almost always have the L configuration although amino acids that occur in bacterial peptides may have the enantiomeric D configuration. The two configurations are shown in Figure 1.21 for alanine.

The description of α -amino acids as D or L is a holdover from an older nomenclature system. In this system (*S*)-alanine is called L-alanine. The enantiomer would be D- or (*R*)-serine. The L (*laevo*, turned to the left; D = *dextro*, turned to the right) designation refers to the α -carbon in the essential amino acids. In alanine, there is a single α -carbon that is asymmetric. When two asymmetric centers are present as in L-threonine, the stereochemistry of both carbons must be considered. The common form of L-threonine is the 2*S*,3*R* stereoisomer.

Threonine (center) is shown in Figure 1.22 along with the simplest chiral amino acid, alanine. The only cyclic amino acid, proline, is pictured as well in the common L-configuration.

Extended Arrangements of Peptides and Proteins. Amino acids are linked from the carboxyl to the amine with formation of an amide bond, often referred to as the peptide link. The repeating ($-\text{N}-\text{C}-\text{CO}-$) unit is called the peptide or protein backbone. Peptides and proteins differ only in the number of amino acids present in the biopolymer chain. The cutoff is arbitrarily set. Often, but not always, a peptide is designated as having fewer than 100 amino acids and the protein possesses more. Backbone amide groups have been found to play a role in enzyme catalysis.

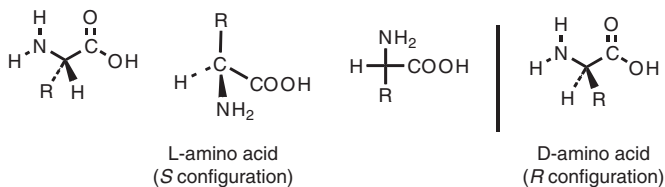


FIGURE 1.21 Stereochemistry of α -amino acids. The most common, L configuration is shown at the left.

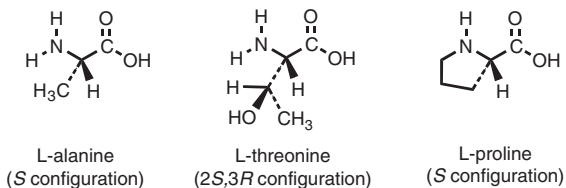


FIGURE 1.22 Structures of alanine, threonine, and proline.

The extended chains, that is, the backbones, may further organize into assemblies that have characteristic properties. The two most important of these are the α -helix and the β -sheet. The latter is illustrated in Figure 1.23. Panel (a) shows the extensive hydrogen bond organization of peptide chains that are oriented in opposite directions. The arrows indicate the nitrogen to carbonyl (arrowhead) direction. The lower panel (b) shows an alternate H-bond organization when the two peptide chains are parallel rather than antiparallel.

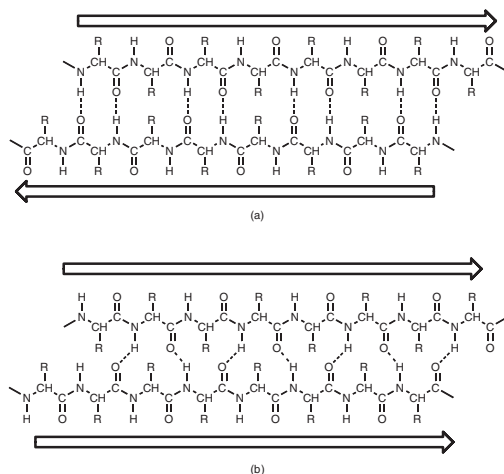


FIGURE 1.23 Hydrogen bonded interactions of peptide chains to form β -sheets. The chains are arranged antiparallel in panel (a) and parallel in panel (b).

An alternate organization for peptide chains is the α -helix. It is essentially a coil in which a carbonyl group H-bonds an amide nitrogen between every fourth residue. The resulting structure exhibits one full turn for each 3.6 amino acids, which spans 5.4 Å per turn. The resulting α -helix is a tight coil that lacks any significant interior space. A schematic representation of the H-bonded coil is shown in Figure 1.24.

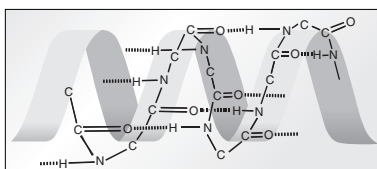


FIGURE 1.24

A number of other arrangements are possible for peptide or protein chains. A discussion of them is beyond the scope of this Handbook.

Chemical Abstracts Indexing System

When compounds of complex structure are considered, the number of name possibilities grows rapidly. To avoid having index entries for all possible names, Chemical Abstracts Service has developed what might be called the principle of inversion. The indexing system employs inverted entries to bring together related compounds in an alphabetically arranged index. The *index heading parent* from the Chemical Substance Index appears in the Formula Index in lightface before the “comma of inversion.” The *substituents* follow the “comma of

inversion" in alphabetical order. Any *name modification* appears on a separate line. If necessary, the chemical description is completed by citation of an associated ion, a functional derivative, a "salt with" or "compound with" terms and/or a stereochemical descriptor.

Quite naturally there is a certain amount of arbitrariness in this system, although the IUPAC nomenclature is followed. The preferred *Chemical Abstracts* index names for chemical substances have been, with very few exceptions, continued unchanged (since 1972) as set forth in the *Ninth Collective Index Guide* and in a journal article.* Any revisions appear in the updated *Index Guide*; new editions appear at 18-month intervals. Appendix VI is of particular interest to chemists. Reprints of the Appendix may be purchased from Chemical Abstracts Service, Marketing Division, P.O. Box 3012, Columbus, Ohio 43210.

PHYSICAL PROPERTIES OF PURE SUBSTANCES

TABLE 1.14 Empirical Formula Index for Organic Compounds

The alphanumeric designations are keyed to Table 1.15

Cl ₂ H ₂ Si: d226	CH ₂ Cl ₂ : d190	CH ₄ S: m33
Cl ₃ HSi: t247	CH ₂ Cl ₄ Si: c165	CH ₃ AsO ₃ : m125
Cl ₆ OSi ₂ : h28	CH ₂ I ₂ : d404	CH ₃ N: m115
	CH ₂ N ₂ : c285, d47	CH ₃ NO ₃ S: a205
	CH ₂ N ₄ : t136	CH ₅ N ₃ : g29
C ₁	CH ₂ O: f27	CH ₅ N ₃ O: s3
	(CH ₂ O) _x : p1	CH ₅ N ₃ S: t162
CBrClF ₂ : b255	CH ₂ O ₂ : f32	CH ₆ N ₂ : m270
CBrCl ₃ : b358	CH ₂ S ₃ : t434	CH ₆ N ₄ : a180, a181
CBrF ₃ : b360	CH ₃ Br: b300	CH ₆ N ₄ O: c11
CBr ₂ F ₂ : d75	CH ₃ Br ₃ Ge: m254	CN ₄ O ₈ : t126a
CClF ₃ : c253	CH ₃ Cl: c137	
CCINO ₃ S: c240	CH ₃ ClHg: m295	C ₂
CCl ₂ F ₂ : d170	CH ₃ ClO ₂ S: m32	
CCl ₃ D: c127	CH ₃ Cl ₃ Ge: m437	
CCl ₃ F: t232	CH ₃ Cl ₃ Si: t238	C ₂ Br ₂ ClF ₃ : d72
CCl ₃ NO ₂ : t239	CH ₃ DO: m35	C ₂ Br ₂ Cl ₄ : d99
CCl ₄ O ₂ S: t236	CH ₃ F: f18	C ₂ Br ₂ F ₄ : d100
CCl ₄ S: t235	CH ₃ I: i40	C ₂ Br ₂ O ₂ : o50
CD ₄ O: m36	CH ₃ NO: f28	C ₂ ClF ₃ : c252
CHBrCl ₂ : b266	CH ₃ NO ₂ : m314, n56	C ₂ Cl ₂ F ₃ I: d188
CHBr ₂ Cl: d71	CH ₃ NO ₃ : m313	C ₂ Cl ₂ F ₄ : d227
CHBr ₃ : t206	CH ₃ N ₅ : a289	C ₂ Cl ₂ O ₂ : o51
CHClF ₂ : c85	CH ₄ : m29	C ₂ Cl ₃ F ₃ : t251
CHCl ₂ F: d183	CH ₄ Cl ₂ Si: d199, m222	C ₂ Cl ₃ N: t217
CHCl ₃ : c126	CH ₄ N ₂ O: f34, u12	C ₂ Cl ₄ : t29
CHF ₃ : t295	CH ₄ N ₂ O ₂ S: f30	C ₂ Cl ₄ F ₂ : d347, d348, t26
CHF ₃ O ₃ S: t296	CH ₄ N ₂ S: t163	C ₂ Cl ₄ O: t218
CHI ₃ : i36	CH ₄ N ₄ O ₂ : n54	C ₂ Cl ₆ : h29
CHN ₃ O ₆ : t385	CH ₄ O: m34	C ₂ D ₃ N: a30
CH ₂ BrCl: b256	CH ₄ O ₂ : m275	C ₂ D ₄ O ₂ : a21
CH ₂ Br ₂ : d88	CH ₄ O ₃ S: m30	C ₂ D ₆ OS: d615

* *J. Chem. Doc.*, **14**(1): 3–15 (1974).

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to table 1.15*

C ₂ F ₄ : t63	C ₂ H ₃ Cl ₅ Si: d182	C ₂ H ₅ ClS: c156
C ₂ F ₆ : h44	C ₂ H ₃ DO ₂ : a20	C ₂ H ₅ Cl ₂ OPS: e117
C ₂ F ₆ O ₅ S ₂ : t297	C ₂ H ₃ FO: a43	C ₂ H ₅ Cl ₂ O ₂ P: e116
C ₂ HBrClF ₃ : b258	C ₂ H ₃ FO ₂ : f6	C ₂ H ₅ Cl ₃ Si: c153, t231
C ₂ HBr ₂ F ₃ : d103	C ₂ H ₃ F ₃ : t291	C ₂ H ₅ DO: e22
C ₂ HBr ₂ N: d63	C ₂ H ₃ F ₃ O: t292	C ₂ H ₅ F: f17
C ₂ HBr ₃ : t205	C ₂ H ₃ IO: a48	C ₂ H ₅ FO ₃ S: e134
C ₂ HBr ₃ O: t201	C ₂ H ₃ IO ₂ : i25	C ₂ H ₅ I: i34
C ₂ HBr ₃ O ₂ : t202	C ₂ H ₃ N: a29	C ₂ H ₅ IO: i35
C ₂ HClF ₂ O ₂ : c83	C ₂ H ₃ NO: m287	C ₂ H ₅ N: e131
C ₂ HClF ₃ : d232	C ₂ H ₃ NS: m289, m426	C ₂ H ₅ NO: a5, a6, m248
C ₂ HCl ₃ : t230	C ₂ H ₃ N ₃ : t199	C ₂ H ₅ NO ₂ : e186, g25, m181, n53
C ₂ HCl ₃ O: d141	C ₂ H ₃ N ₃ S ₂ : a290	C ₂ H ₅ NO ₃ : e185
C ₂ HCl ₃ O ₂ : t216	C ₂ H ₄ BrCl: b254	C ₂ H ₅ NS: t141
C ₂ HCl ₅ : p9	C ₂ H ₄ BrNO: b218	C ₂ H ₅ N ₃ O ₂ : b215, o53
C ₂ HF ₃ O ₂ : t287	C ₂ H ₄ Br ₂ : d77, d78	C ₂ H ₆ : e14
C ₂ H ₂ : a41	C ₂ H ₄ ClNO: c22	C ₂ H ₆ BrN: b281
C ₂ H ₂ BrClO: b224	C ₂ H ₄ Cl ₂ : d176, d177	C ₂ H ₆ Cd: d501
C ₂ H ₂ Br ₂ : d80, d81	C ₂ H ₄ Cl ₂ O: d197	C ₂ H ₆ ClN: c106
C ₂ H ₂ Br ₂ F ₂ : d74	C ₂ H ₄ Cl ₆ Si ₂ : b204	C ₂ H ₆ ClNO ₂ S: d609
C ₂ H ₂ Br ₂ O: b223	C ₂ H ₄ FNO: f5	C ₂ H ₆ ClO ₂ PS: d504
C ₂ H ₂ Br ₂ O ₂ : d62	C ₂ H ₄ F ₂ : d346	C ₂ H ₆ Cl ₃ Si: d174
C ₂ H ₂ Br ₄ : t9	C ₂ H ₄ INO: i24	C ₂ H ₆ Hg: d546
C ₂ H ₂ ClF ₃ : c251	C ₂ H ₄ I ₂ : d403	C ₂ H ₆ N ₂ : a7
C ₂ H ₂ ClN: c27	C ₂ H ₄ N ₂ : a106	C ₂ H ₆ N ₂ O: a25, m444, n79
C ₂ H ₂ Cl ₂ : d178, d179, d180	C ₂ H ₄ N ₂ O ₄ : o54	C ₂ H ₆ N ₂ O ₂ : m271
C ₂ H ₂ Cl ₂ O: c31	C ₂ H ₄ N ₂ O ₆ : e126	C ₂ H ₆ N ₂ O ₄ S: a107
C ₂ H ₂ Cl ₂ O ₂ : d138	C ₂ H ₄ N ₂ S ₂ : d710	C ₂ H ₆ N ₂ S: m431
C ₂ H ₂ Cl ₄ : t27, t28	C ₂ H ₄ N ₄ : a295, d235	C ₂ H ₆ N ₄ O ₂ : o52
C ₂ H ₂ F ₃ NO: t286	C ₂ H ₄ N ₄ O ₂ : a324	C ₂ H ₆ O: d518, e21
C ₂ H ₂ O: k1	C ₂ H ₄ O: a4, e129	C ₂ H ₆ OS: d614, m18
C ₂ H ₂ O ₂ : g27	C ₂ H ₄ OS: t142	C ₂ H ₆ O ₂ : e16, e128
C ₂ H ₂ O ₃ : g28	C ₂ H ₄ O ₂ : a19, h86, m250	C ₂ H ₆ O ₂ S: d613
C ₂ H ₂ O ₄ : o48, o49	C ₂ H ₄ O ₂ S: m14	C ₂ H ₆ O ₃ S: d612, m297
C ₂ H ₃ Br: b284	C ₂ H ₄ O ₃ : h87, p59	C ₂ H ₆ O ₄ S: d610, h114
C ₂ H ₃ BrO: a35	C ₂ H ₄ O ₅ S: s23	C ₂ H ₆ O ₅ S ₂ : m31
C ₂ H ₃ BrO ₂ : b220	C ₂ H ₄ S: e130	C ₂ H ₆ S: d611, e20
C ₂ H ₃ Br ₂ Cl ₃ Si: d82	C ₂ H ₅ AlCl ₂ : e57	C ₂ H ₆ S ₂ : d516, e18
C ₂ H ₃ Br ₃ O: t204	C ₂ H ₅ Br: b277	C ₂ H ₆ Te: d617
C ₂ H ₃ Cl: c109	C ₂ H ₅ BrNaO ₂ S: b278	C ₂ H ₆ Zn: d624
C ₂ H ₃ ClF ₂ : c84	C ₂ H ₅ BrO: b279, b308	C ₂ H ₇ AsO ₂ : d484
C ₂ H ₃ ClO: a37	C ₂ H ₅ Cl: c102	C ₂ H ₇ ClSi: c92
C ₂ H ₃ ClO ₂ : c24, m187	C ₂ H ₅ ClHg: e165	C ₂ H ₇ N: d461, e58
C ₂ H ₃ Cl ₃ : t226, t227	C ₂ H ₅ ClO: c103, c155	C ₂ H ₇ NO: a163, a164
C ₂ H ₃ Cl ₃ O: t228	C ₂ H ₅ ClO ₂ S: e19	C ₂ H ₇ NO ₃ S: a161
C ₂ H ₃ Cl ₃ Si: t252		

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table I.15*

C ₂ H ₇ NO ₄ S: a169	C ₃ H ₄ Cl ₂ O ₂ : m219	C ₃ H ₆ Cl ₄ Si: c229
C ₂ H ₇ NS: a162	C ₃ H ₄ Cl ₃ NO: m436	C ₃ H ₆ I ₂ : d405
C ₂ H ₇ N ₅ : b133	C ₃ H ₄ F ₄ O: t64	C ₃ H ₆ N ₂ : a274, d505
C ₂ H ₇ O ₃ P: d541	C ₃ H ₄ N ₂ : i4, p245	C ₃ H ₄ N ₂ O: i7
C ₂ H ₈ N ₂ : d539, d540, e15	C ₃ H ₄ N ₂ O: c286	C ₃ H ₆ N ₂ O ₂ : m4, m269
C ₂ H ₈ N ₂ O: h120	C ₃ H ₄ N ₂ OS: t152	C ₃ H ₆ N ₂ S: a292, i5
	C ₃ H ₄ N ₂ O ₂ : h84	C ₃ H ₆ N ₂ OS: a58
	C ₃ H ₄ N ₂ S: a291	C ₃ H ₆ N ₆ : t198
	C ₃ H ₄ O: p204, p242	C ₃ H ₆ O: a26, a81, e10, m446, p211, p227, t345
	C ₃ H ₄ O ₂ : a63, o59, p210	C ₃ H ₄ OS: m420, t161
	C ₃ H ₄ O ₃ : e124, o60	C ₃ H ₆ O ₂ : d647, e11, e135, h89, m111, p213
	C ₃ H ₄ O ₄ : m3	C ₃ H ₆ O ₂ S: m21, m293
	C ₃ H ₅ Br: a85, b225, b335, b336	C ₃ H ₆ O ₃ : d397, d398, d503, L1, L2, m38, m259, t388
	C ₃ H ₅ BrO: b276	C ₃ H ₆ O ₃ S: p198
	C ₃ H ₅ BrO ₂ : b337, b338, m143	C ₃ H ₆ S: p206, p228, t345a
	C ₃ H ₅ Br ₃ : t208	C ₃ H ₆ S ₃ : t431
	C ₃ H ₅ Cl: c216	C ₃ H ₇ Br: b332, b333
	C ₃ H ₅ ClO: c101, c215, p216	C ₃ H ₇ BrO: b334
	C ₃ H ₅ ClOS: e101	C ₃ H ₇ Cl: c210, c211
	C ₃ H ₅ ClO ₂ : c218, c219, e98, m182	C ₃ H ₇ ClO: c111, c152, c213, c214
	C ₃ H ₅ Cl ₃ : t244	C ₃ H ₇ ClOS: c136
	C ₃ H ₅ Cl ₃ O: t245	C ₃ H ₇ ClO ₂ : c212
	C ₃ H ₅ Cl ₃ Si: a102	C ₃ H ₇ ClO ₂ S: p197
	C ₃ H ₅ FO: f7	C ₃ H ₇ Cl ₂ OP: p236
	C ₃ H ₅ F ₃ O ₃ S: m438	C ₃ H ₇ Cl ₃ Si: d194, p237
	C ₃ H ₅ I: a92, i50	C ₃ H ₇ I: i48, i49
	C ₃ H ₅ N: p215	C ₃ H ₇ N: a82, p226
	C ₃ H ₅ NO: a62, c290, h168, h169	C ₃ H ₇ NO: a28, d522, m110, p212
	C ₃ H ₅ NO ₂ : o55	C ₃ H ₇ NO ₂ : a73, a74, a75, a76, e91, m258, n73, n74
	C ₃ H ₅ NS: e161, m421	C ₃ H ₇ NO ₂ S: c370
	C ₃ H ₅ N ₃ O: c288	C ₃ H ₇ NO ₃ : i105, n75, p233, s4
	C ₃ H ₅ N ₃ O ₉ : g21	C ₃ H ₇ NO ₅ S: a288
	C ₃ H ₅ N ₃ S: c292	C ₃ H ₇ NS: d620
	C ₃ H ₆ : c364, p205	C ₃ H ₇ NS ₂ : d517
	C ₃ H ₆ BrCl: b257	C ₃ H ₇ O ₅ P: c17
	C ₃ H ₆ BrNO ₄ : b316	C ₃ H ₈ : p191
	C ₃ H ₆ Br ₂ : d92, d93	C ₃ H ₈ ClN: c224
	C ₃ H ₆ Br ₂ O: d94	C ₃ H ₈ Cl ₂ Si: c75, c150
	C ₃ H ₆ ClNO: d502	
	C ₃ H ₆ Cl ₂ : d218, d219	
	C ₃ H ₆ Cl ₂ O: d220	
	C ₃ H ₆ Cl ₂ Si: d200	
C ₃		
C ₃ Br ₂ F ₆ : d85		
C ₃ Cl ₃ NO ₂ : t219		
C ₃ Cl ₃ N ₃ : t250		
C ₃ Cl ₃ N ₃ O ₃ : t234		
C ₃ Cl ₆ : h31		
C ₃ Cl ₆ O: h23		
C ₃ D ₆ O: a27		
C ₃ HCl ₅ O: p7		
C ₃ H ₂ ClN: c32		
C ₃ H ₂ Cl ₂ O ₂ : m6		
C ₃ H ₂ Cl ₄ : t33		
C ₃ H ₂ Cl ₄ O: t21		
C ₃ H ₂ Cl ₄ O ₂ : t229		
C ₃ H ₂ F ₆ O: h45		
C ₃ H ₂ N ₂ : m5		
C ₃ H ₂ N ₂ O ₃ : i6		
C ₃ H ₂ O ₂ : p241		
C ₃ H ₃ Br: b344		
C ₃ H ₃ Cl: c232		
C ₃ H ₃ ClO: a65		
C ₃ H ₃ Cl ₃ O: e13		
C ₃ H ₃ N: a64		
C ₃ H ₃ NOS ₂ : r3		
C ₃ H ₃ NO ₂ : c287		
C ₃ H ₃ NS: t140		
C ₃ H ₃ N ₃ O ₂ S: a249		
C ₃ H ₃ N ₃ O ₃ : c299		
C ₃ H ₄ : a78, p240		
C ₃ H ₄ BrClO: b340, b341		
C ₃ H ₄ BrN: b339		
C ₃ H ₄ Br ₂ : d95		
C ₃ H ₄ Br ₂ O ₂ : d96		
C ₃ H ₄ ClN: c220		
C ₃ H ₄ Cl ₂ : d221, d222		
C ₃ H ₄ Cl ₂ O: c221, c222, d139		

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

C ₃ H ₈ IN: d549 C ₃ H ₈ N ₂ O: d623, e230 C ₃ H ₈ N ₂ O ₂ : e92, f29 C ₃ H ₈ N ₂ S: d621 C ₃ H ₈ O: e171, p202, p203 C ₃ H ₈ OS ₂ : d425, m305 C ₃ H ₈ O ₂ : d441, m65, p194, p195 C ₃ H ₈ O ₂ S: m20 C ₃ H ₈ O ₃ : g16 C ₃ H ₈ S: e182, p199, p200 C ₃ H ₈ S ₂ : p196 C ₃ H ₉ Al: t327 C ₃ H ₈ BO ₃ : t319 C ₃ H ₉ B ₃ O ₆ : t320 C ₃ H ₉ BrGe: b363 C ₃ H ₉ BrSi: b364 C ₃ H ₉ ClGe: c254 C ₃ H ₉ ClSi: c255 C ₃ H ₉ IOS: t378 C ₃ H ₉ IS: t377 C ₃ H ₉ ISi: i55 C ₃ H ₉ N: i88, m246, p220, t328 C ₃ H ₉ NO: a269, a270, a271, a272, m69, m119, t329 C ₃ H ₉ NO ₂ : a268 C ₃ H ₉ N ₃ Si: a319 C ₃ H ₉ O ₃ P: d551, t364 C ₃ H ₉ O ₄ P: t363 C ₃ H ₁₀ N ₂ : m247, p192, p193 C ₃ H ₁₀ N ₂ O: d43 C ₃ H ₁₁ Br ₂ N ₃ S: a171	C ₄ HBrO ₃ : b299 C ₄ HCl ₃ N ₂ : t246 C ₄ HF ₂ O ₂ : h2 C ₄ H ₂ : b376 C ₄ H ₂ Br ₂ S: d101 C ₄ H ₂ Cl ₂ N ₂ : d223 C ₄ H ₂ Cl ₂ O ₂ : f38 C ₄ H ₂ Cl ₂ O ₃ : d208 C ₄ H ₂ Cl ₂ S: d228 C ₄ H ₂ F ₆ O ₂ : t294 C ₄ H ₂ O ₃ : m2 C ₄ H ₂ O ₄ : a42 C ₄ H ₃ BrS: b353 C ₄ H ₃ ClS: c242 C ₄ H ₃ Cl ₂ N ₃ O: d193 C ₄ H ₃ IS: i52 C ₄ H ₄ : b407 C ₄ H ₄ BrNO ₂ : b351 C ₄ H ₄ Br ₂ O ₂ : d69 C ₄ H ₄ Br ₂ O ₄ : d98 C ₄ H ₄ ClNO ₂ : c239 C ₄ H ₄ Cl ₂ : d168 C ₄ H ₄ Cl ₂ O ₂ : s19 C ₄ H ₄ Cl ₂ O ₃ : c25 C ₄ H ₄ N ₂ : b380, p244, p247, p267, s18 C ₄ H ₄ N ₂ O ₂ : d400, p268 C ₄ H ₄ N ₂ O ₂ S: d388 C ₄ H ₄ N ₂ O ₃ : b1 C ₄ H ₄ N ₂ O ₅ : a79 C ₄ H ₄ N ₄ : d40 C ₄ H ₄ O: f40 C ₄ H ₄ O ₂ : d422 C ₄ H ₄ O ₃ : s16 C ₄ H ₄ O ₄ : f37, m1 C ₄ H ₄ S: t154 C ₄ H ₅ BrO ₄ : b350 C ₄ H ₅ Cl: c63, c70 C ₄ H ₅ ClO: c283, c366, m28 C ₄ H ₅ ClO ₂ : a87 C ₄ H ₅ ClO ₃ : e191 C ₄ H ₅ Cl ₂ O ₂ : e226 C ₄ H ₅ F ₃ O ₂ : e227 C ₄ H ₅ N: b400, c365, m27, p269 C ₄ H ₅ NO: m290	C ₄ H ₅ NO ₂ : e106, m193, s17 C ₄ H ₅ NO ₂ S: e32 C ₄ H ₅ NO ₃ : h182 C ₄ H ₅ NS: a93 C ₄ H ₅ N ₃ : a284, i11 C ₄ H ₅ N ₃ O: a198 C ₄ H ₅ N ₃ OS: a191 C ₄ H ₅ N ₃ O ₂ : a154, a155, c289, m322 C ₄ H ₆ : b373, b374, b490, b491 C ₄ H ₆ Br ₂ O ₂ : d70 C ₄ H ₆ ClN: c73 C ₄ H ₆ Cl ₂ : d165, d166, d167 C ₄ H ₆ Cl ₂ O: c74 C ₄ H ₆ Cl ₂ O ₂ : m220 C ₄ H ₆ Cl ₃ NSi: c294 C ₄ H ₆ N ₂ : a151, m280, m281, m282 C ₄ H ₆ N ₂ O ₂ : e114 C ₄ H ₆ N ₂ S: a229 C ₄ H ₆ N ₄ O: d39 C ₄ H ₆ N ₄ O ₃ : a77 C ₄ H ₆ O: b406, c282, d356, d545a, m24, m396 C ₄ H ₆ O ₂ : b386, b401, b402, b403, b492, b497, b498, c367, m26, m114, v2 C ₄ H ₆ O ₂ S: d368 C ₄ H ₆ O ₃ : a22, a24, m334, o56, p225 C ₄ H ₆ O ₄ : d566, s14 C ₄ H ₆ O ₄ S: m23, t148 C ₄ H ₆ O ₅ : h180, h181, o61 C ₄ H ₆ O ₆ : t1, t2 C ₄ H ₇ Br: b240, b241, b242 C ₄ H ₇ BrO ₂ : b244, b280, b307, e75, m146 C ₄ H ₇ Cl: c68, c69, c163, c164 C ₄ H ₇ ClO: b501, c67, c115, i78 C ₄ H ₇ ClO ₂ : c71, c72, e94, m189 C ₄ H ₇ Cl ₂ NSi: c291 C ₄ H ₇ Cl ₃ O: t237
C ₄		
C ₄ Cl ₂ F ₆ : d185 C ₄ Cl ₂ F ₈ : d206 C ₄ Cl ₂ O ₃ : d189 C ₄ Cl ₃ F ₇ : h3 C ₄ Cl ₆ : h25 C ₄ D ₆ O ₃ : a23 C ₄ F ₆ O ₃ : t288		

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table I.15*

<p> $C_4H_7Cl_3O_2Si$: c13 $C_4H_7FO_2$: e133 C_4H_7N: b499, i76 C_4H_7NO: h145, i98, m25, m334, p231, p275 $C_4H_7NO_2$: m331 $C_4H_7NO_3$: a46, e192, p12 $C_4H_7NO_4$: a314, i10 C_4H_7NS: m419 $C_4H_7N_3O$: c278 C_4H_8: b395, b396, b397, c300, m383 C_4H_8BrCl: b251 $C_4H_8Br_2$: d67, d68 $C_4H_8Br_2O$: b149 $C_4H_8Cl_2$: d162, d163, d164 $C_4H_8Cl_2O$: b158, d181 $C_4H_8Cl_2Si$: a89 $C_4H_8N_2O$: a105, a150 $C_4H_8N_2O_2$: d526, s13 $C_4H_8N_2O_3$: a313, g26 $C_4H_8N_2S$: a101, t79 C_4H_8O: b393, b404, b405, b493, e3, e232, i73, m96, m377, m385, t66 C_4H_8OS: e220, t107, t164 $C_4H_8O_2$: b398, b399, b495, d646, e51, h106, i75, m389, m390, p229 $C_4H_8O_2S$: e164, m294, t106 $C_4H_8O_3$: e23, e150, h116, h127, m64, m291, m298 $C_4H_8O_3S$: m384 C_4H_8S: a95, t81 $C_4H_8S_2$: d707 C_4H_9Br: b238, b239, b310, b311 C_4H_9BrO: b285 C_4H_9Cl: c64, c65, c161, c162 C_4H_9ClO: c66, c110 $C_4H_9ClO_2$: c89, c104, m67 C_4H_9ClSi: c93 $C_4H_9Cl_3Si$: b483, c225 $C_4H_9Cl_3Sn$: b481 </p>	<p> C_4H_9F: f20 C_4H_9I: i30, i31, i43, i44 C_4H_9Li: b457, b458 C_4H_9N: p270 C_4H_9NO: a321, b394, b494, d458, e52, i74, m388, m448 $C_4H_9NO_2$: a138, a139, a222, b464, b465, h115, i71, n50 $C_4H_9NO_2S$: a204 $C_4H_9NO_3$: a187, a188, a189, a190, i70, n51 C_4H_9NSi: c298 $C_4H_9N_3O_2$: c277 C_4H_{10}: b378, m375 $C_4H_{10}ClN$: d467 $C_4H_{10}ClO_2PS$: d292 $C_4H_{10}ClO_3P$: d291 $C_4H_{10}Cl_2Si$: b160, m392 $C_4H_{10}N_2$: p179 $C_4H_{10}N_2O$: a231 $C_4H_{10}N_2O_4S$: a8 $C_4H_{10}O$: b391, b392, d300, m381, m382, m393 $C_4H_{10}OS$: e153 $C_4H_{10}OS_2$: b186 $C_4H_{10}O_2$: b381, b382, b383, b384, b385, b453, d438, d439, e34, m95 $C_4H_{10}O_2S$: m430, t149 $C_4H_{10}O_2S_2$: d424, h118 $C_4H_{10}O_3$: b181, b390, t351 $C_4H_{10}O_3S$: d338 $C_4H_{10}O_4S$: d336 $C_4H_{10}S$: b388, b389, d337, i104, m378, m379, m380, m395 $C_4H_{10}S_2$: b387, d294a $C_4H_{10}S_3$: b187 $C_4H_{10}Zn$: d344 $C_4H_{11}ClSi$: c166 $C_4H_{11}N$: b377, b417, b418, d267, d268, d520, i63 $C_4H_{11}NO$: a136, a137, a221, d315, d465, e38, e62 </p>	<p> $C_4H_{11}NO_2$: a165, a220, d245, d440 $C_4H_{11}NO_3$: t423 $C_4H_{11}O_2PS_2$: d296 $C_4H_{11}O_3P$: d314 $C_4H_{12}BrN$: t93 $C_4H_{12}ClN$: t94 $C_4H_{12}Ge$: t109 $C_4H_{12}IN$: t95 $C_4H_{12}N_2$: b379, b452, d521, m376, m377 $C_4H_{12}N_2O$: a166 $C_4H_{12}N_2S_2$: c369 $C_4H_{12}OSi$: m108 $C_4H_{12}O_3Si$: t326a $C_4H_{12}O_4Si$: t92 $C_4H_{12}Pb$: t112 $C_4H_{12}Si$: t120 $C_4H_{12}Sn$: t123 $C_4H_{13}N_3$: d298 $C_4H_{14}OSi_2$: t105 $C_4H_{16}O_4Si_4$: t103 </p> <hr/> <p style="text-align: center;">C_5</p> <hr/> <p> C_5Cl_3N: p12 C_5Cl_6: h27 C_5D_8N: p249 $C_5H_3Br_2N$: d97 $C_5H_3ClO_2$: f48 $C_5H_3Cl_2N$: d224 C_5H_4BrN: b345, b346 C_5H_4ClN: c233 C_5H_4FN: f23 $C_5H_4F_8O$: o18 $C_5H_4N_2O_3$: n76 $C_5H_4N_4O$: h186 $C_5H_4N_4O_3$: u13 $C_5H_4O_2$: t156 $C_5H_4O_2$: f39 $C_5H_4O_2S$: t157 $C_5H_4O_3$: c271, f42 $C_5H_4ClN_2$: a149 $C_5H_5ClN_2O_2$: c167 $C_5H_5F_3O_2$: t293 </p>
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

<p> C_5H_5N: p248 C_5H_5NO: h173, h174, h175, p262 $C_5H_5NO_2$: d401, h177 $C_5H_5NO_3S$: p263 $C_5H_5N_3O_2$: a248 $C_5H_5N_3O_4$: a160 $C_5H_5N_5$: a69 C_5H_6: m166 $C_5H_6Br_2N_2O_2$: d76 $C_5H_6Cl_2N_2O_2$: d173 $C_5H_6Cl_2O_2$: d195, g15 $C_5H_6Cl_4O_2$: t225 $C_5H_6N_2$: a281, a282, a283, g14, m397, v7 $C_5H_6N_2O$: a47, a197 $C_5H_6N_2OS$: h128 $C_5H_6N_2O_2$: d391 $C_5H_6N_2O_2$: e107 C_5H_6O: m59, m252 C_5H_6OS: f44 $C_5H_6O_2$: f46 $C_5H_6O_3$: g12 $C_5H_6O_4$: c270, m245 $C_5H_6O_4S_3$: b155 C_5H_6S: m427 $C_5H_7BrO_2$: m145 $C_5H_7BrO_3$: e79 $C_5H_7ClO_3$: m183, m188 C_5H_7N: m404 C_5H_7NO: f47 $C_5H_7NO_2$: e105 C_5H_7NS: t158 $C_5H_7N_3$: a228, d44 $C_5H_7N_3O$: a192 C_5H_8: c358, m147, m148, m171, p16, p17, p18, p19, p57 $C_5H_8Br_2O_2$: e115 $C_5H_8Br_4$: p21 $C_5H_8F_4O$: m414 $C_5H_8N_2$: d542, d603, e159, p272 $C_5H_8N_2O$: m449 $C_5H_8N_2O_2$: d538 $C_5H_8N_4O_{12}$: p22 </p>	<p> C_5H_8O: c356, c368, d363, e8, m172, p51 $C_5H_8O_2$: a80, e56, g13, i84, m58, m161, m162, m163, m192, m217, m296, p31, p32, p40, p40a, p50, p208 $C_5H_8O_3$: e196, m112, o58 $C_5H_8O_4$: d545, g11, m274, m412 C_5H_9Br: b263 $C_5H_9BrO_2$: e81, e82, m144 C_5H_9Cl: c79 C_5H_9ClO: c192, d600, m179, p44 C_5H_9ClOS: b437, c229 $C_5H_9ClO_2$: b436, e99, e100, i65, m186 $C_5H_9F_3O_2Si$: t376 C_5H_9N: d602, m178, p33, t78 C_5H_9NO: b455, b456, c357, e193, m406 $C_5H_9NO_2$: m118, p273 $C_5H_9NO_4$: g9 $C_5H_9N_3$: i8 C_5H_{10}: c352, m158, m159, m160, p47, p48, p49 $C_5H_{10}Br_2$: d91 $C_5H_{10}ClNO$: d288 $C_5H_{10}Cl_2$: d209 $C_5H_{10}Cl_2O_2Si$: c12 $C_5H_{10}Cl_2Si$: c351 $C_5H_{10}N_2$: d293, d474 $C_5H_{10}N_2O$: d543, p180 $C_5H_{10}N_2O_3$: g10 $C_5H_{10}O$: a91, c355, d596, i108, m157, m164, m165, m173, m174, m415, p27, p41, p42, t76 $C_5H_{10}OS$: m425 $C_5H_{10}O_2$: d454, d598, e208, h139, h156, h157, i66, i87, m102, m175, m176, m177, m286, p36, p219, t68 </p>	<p> $C_5H_{10}O_2S$: e183, m306, m417 $C_5H_{10}O_3$: d289, d451, e162, m68, m278 $C_5H_{10}O_4$: b184 $C_5H_{10}O_5$: a310, r5, x8 $C_5H_{11}Br$: b305, b322, b323 $C_5H_{11}BrO_2$: b269 $C_5H_{11}BrO_2Si$: t370 $C_5H_{11}Cl$: c91, c148, c149, c191 $C_5H_{11}ClSi$: a86 $C_5H_{11}Cl_2N$: b159 $C_5H_{11}I$: i42, i47 $C_5H_{11}N$: a90, m405, p183 $C_5H_{11}NO$: d304, d597, h167, m307, t69 $C_5H_{11}NO_2$: a253, a254, b128, e231, i81, v1 $C_5H_{11}NO_2S$: m37 $C_5H_{11}NO_3$: n58 $C_5H_{11}NS_2$: d295 $C_5H_{11}O_3P$: t365 C_5H_{12}: d592, m149, p28 $C_5H_{12}ClN$: d475 $C_5H_{12}Cl_2O_2Si$: b157 $C_5H_{12}N_2$: a267, m368, m369 $C_5H_{12}N_2O$: b487, t124 $C_5H_{12}N_2O_2$: b430, o46 $C_5H_{12}N_2S$: t122 $C_5H_{12}N_2S_2$: p271 $C_5H_{12}O$: b460, d452, d595, e209, m153, m154, m155, m156, p37, p38, p39 $C_5H_{12}OSi$: t379 $C_5H_{12}O_2$: d594, m57, p30 $C_5H_{12}O_2S$: e221 $C_5H_{12}O_3$: h141, m66, t352, t425 $C_5H_{12}O_3S$: p34 $C_5H_{12}O_4$: p20, t114 $C_5H_{12}O_5$: x7 $C_5H_{12}S$: b463, e210, m150, m151, m152, p35 </p>
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

$C_5H_{12}Si$: t380 $C_5H_{13}N$: a251, a252, d601, m167, m168, m169, p53 $C_5H_{13}NO$: a213, a214, a255, d472, d473, e47, i89, p221 $C_5H_{12}NOSi$: t368 $C_5H_{13}NO_2$: a176, d442, d471, d523, m223 $C_5H_{13}N_3$: t110 $C_5H_{14}N_2$: d593, p29, t113 $C_5H_{14}OSi$: e50, t372 $C_5H_{14}O_2Si$: d255 $C_5H_{15}N_3$: a175	$C_6H_3N_3O_6$: t382, t383 $C_6H_3N_3O_7$: p173 C_6H_4BrCl : b247, b248, b249 $C_6H_4BrClO_2S$: b231 C_6H_4BrF : b288, b289, b290 $C_6H_4BrNO_2$: b314 $C_6H_4BrN_3O_4$: b271 $C_6H_4Br_2$: d65 $C_6H_4Br_2N_2O_2$: d89 $C_6H_4Br_3N$: t203 C_6H_4ClF : c116, c117, c118 C_6H_4ClFO : c122 C_6H_4ClI : c135 $C_6H_4ClNO_2$: c175, c176, c177, c234, c235 $C_6H_4ClNO_3$: c186 $C_6H_4ClNO_3S$: n35 $C_6H_4ClO_2P$: p110 $C_6H_4Cl_2$: d152, d153, d154 $C_6H_4Cl_2N_2O_2$: d202 $C_6H_4Cl_2O$: d210, d211, d212, d213 $C_6H_4Cl_2O_2$: d171 $C_6H_4Cl_2O_2S$: c43 $C_6H_4Cl_3N$: t220, t221 $C_6H_4Cl_4Si$: c208 $C_6H_4FNO_2$: f21 $C_6H_4F_2$: d345 $C_6H_4INO_2$: i45 $C_6H_4I_2$: d402 $C_6H_4N_2$: c295, c296, c297 $C_6H_4N_2O_2$: b43 $C_6H_4N_2O_4$: d626 $C_6H_4N_2O_5$: d635 $C_6H_4N_4$: a273 $C_6H_4N_4O_6$: t381 $C_6H_4O_2$: b59 $C_6H_5BO_2$: c21 C_6H_5Br : b229 C_6H_5BrO : b325, b326 C_6H_5BrS : b354 C_6H_5Cl : c41 C_6H_5ClHg : p126 $C_6H_5ClN_2O_2$: c172, c173a, c173, c174	C_6H_5ClO : c194, c195, c196 $C_6H_5ClO_2$: c87, c88 $C_6H_5ClO_2S$: b23 C_6H_5ClS : c243 C_6H_5ClSe : p151 $C_6H_5Cl_2N$: d142, d143, d144, d145, d146, d147 $C_6H_5Cl_2OP$: p137 $C_6H_5Cl_2O_2P$: p105 $C_6H_5Cl_2P$: d216 $C_6H_5Cl_2PS$: p138 $C_6H_5Cl_3Si$: p155 C_6H_5D : b9 C_6H_5F : f11 C_6H_5FO : f22 $C_6H_5FO_2S$: b24 $C_6H_5F_2O_2$: e137 C_6H_5I : i27 C_6H_5NO : n78, p251, p252, p253 C_6H_5NOS : t153 $C_6H_5NO_2$: n30, n83, p255, p256, p257 $C_6H_5NO_3$: h176, n60, n61 $C_6H_5NO_4$: c272 $C_6H_5N_3$: b62 $C_6H_5N_3O$: h103 $C_6H_5N_3O_4$: d625 C_6H_6 : b8a $C_6H_6AsNO_6$: h153 C_6H_6BrN : b225, b226, b227 C_6H_6ClN : c33, c34, c35 C_6H_6ClNO : a148, c141 $C_6H_6ClNO_2S$: c42 $C_6H_6Cl_2N_2$: d215 $C_6H_6Cl_6$: h26 C_6H_6FN : f9 C_6H_6HgO : p127 C_6H_6IN : i26 $C_6H_6N_2O$: e43, p250, p254 $C_6H_6N_2O_2$: n24, n25, n26 $C_6H_6N_2O_3$: a244, a245, m84
<hr/> C_6 <hr/>		
C_6BrD_5 : b230 C_6BrF_5 : b321 $C_6Cl_4O_2$: t24, t25 $C_6Cl_5NO_2$: p10 C_6Cl_6 : h24 C_6D_6 : b10 C_6D_{12} : c313 C_6F_6 : h43 C_6HBr_5O : p6 $C_6HCl_4NO_2$: t30 C_5HCl_5 : p8 C_6HCl_5O : p11 $C_6H_2BrFN_2O_4$: b272 $C_6H_2Cl_2O_4$: d172 $C_6H_2Cl_3NO_2$: t242a $C_6H_2Cl_4$: t22, t23 $C_6H_3Br_2F$: d84 $C_6H_3Br_2NO_2$: d90 $C_6H_3Br_3O$: t207 $C_6H_3ClFNO_2$: c121 $C_6H_3ClN_2O_4$: c94, c95 $C_6H_3ClN_2O_4S$: d627 $C_6H_3Cl_2NO_2$: d203, d204, d205 $C_6H_3Cl_3$: t222, t223, t224 $C_6H_3Cl_3O$: t240, t241 $C_6H_3Cl_3O_2S$: d155 $C_6H_3FN_2O_4$: d633		

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

$C_6H_6N_4O_4$: d637 C_6H_6O : p64 C_6H_6OS : a57, m428 $C_6H_6O_2$: a44, d377, d378, d379, m251 $C_6H_6O_2S$: b20, t155 $C_6H_6O_3$: h146, m253, t304, t305 $C_6H_6O_3S$: b22 $C_6H_6O_4$: d460 $C_6H_6O_5S$: d382 $C_6H_6O_6$: p207 $C_6H_6O_8S_2$: d381 C_6H_6S : t159 $C_6H_7AsO_3$: b11 $C_6H_7BO_2$: b12 $C_6H_7ClN_2$: c202, c203, c204, c205 C_6H_7N : a298, a299, m398, m399, m400 C_6H_7NO : a257, a258, a259, m101, m403, p264, p265 $C_6H_7NO_2S$: b21 $C_6H_7NO_3S$: a118, a119, a120, s23 $C_6H_7NO_5S_2$: a117 C_6H_7NS : a293 $C_6H_7N_3O$: p258 $C_6H_7N_3O_2$: n67, n68, n69 $C_6H_7O_2P$: p135 $C_6H_7O_3P$: p136 $C_6H_8AsNO_3$: a115, a116 $C_6H_8Cl_2O_2$: h62, m221 $C_6H_8N_2$: a223, a224, a225, a226, a227, d238, m121, m257, p107, p108, p109, p118 $C_6H_8N_2O$: a208, o63 $C_6H_8N_2O_2S$: b25, s22 $C_6H_8N_2O_3S$: d32 $C_6H_8N_4$: p181 C_6H_8O : c331, d525, h40, m216 $C_6H_8O_2$: b375, c322, d364, h42, m214, v4	$C_6H_8O_3$: a36, d365, f43, h183 $C_6H_8O_4$: d524, d544 $C_6H_8O_6$: a312, g8, i59 $C_6H_8O_7$: c273 C_6H_9Br : b262 C_6H_9ClO : c78 $C_6H_9ClO_3$: e95, e96 $C_6H_9F_3O_2$: b484 C_6H_9NO : v11 C_6H_9NOS : m418 $C_6H_9NO_2$: b438 $C_6H_9NO_6$: n21 $C_6H_9N_3$: a158 $C_6H_9N_3O_2$: a159, c284, h83 C_6H_{10} : c330, d488, h41, h82, m351 $C_6H_{10}N_2$: e172, p184 $C_6H_{10}N_2O_2$: c323 $C_6H_{10}N_2O_4$: d279 $C_6H_{10}N_3O_5$: a14 $C_6H_{10}N_4$: p26 $C_6H_{10}O$: c328, d26, d361, e5, e6, h78, m215, m350, m352 $C_6H_{10}O_2$: a96, c353, d359, e40, e104, e112, e166, h61, h71, h76, m349 $C_6H_{10}O_3$: d436, e53, e54, h121, p214 $C_6H_{10}O_4$: d325, d608, e17, h57, m272 $C_6H_{10}O_4S$: t151 $C_6H_{10}O_4S_2$: d709 $C_6H_{10}O_5$: d326 $C_6H_{10}O_6$: d616 $C_6H_{10}O_8$: t84 $C_6H_{10}S$: d27 $C_6H_{11}Br$: b261 $C_6H_{11}BrO_2$: b295, e76, e77, e78 $C_6H_{11}Cl$: c77 $C_6H_{11}ClO$: h73 $C_6H_{11}ClO_2$: b433, c151, e97	$C_6H_{11}Cl_3Si$: c344 $C_6H_{11}I$: i32 $C_6H_{11}N$: d25, h63, m339, m416 $C_6H_{11}NO$: c329, e217, f35, m376, o57, t352 $C_6H_{11}NO_2$: e61 C_6H_{12} : c312, d498, d499, e84, h75, m213, m347, m348 $C_6H_{12}Br_2$: d86 $C_6H_{12}ClN$: c160 $C_6H_{12}ClNO$: c112 $C_6H_{12}Cl_2$: d187 $C_6H_{12}Cl_2O$: b161 $C_6H_{12}Cl_2O_2$: b156, d169 $C_6H_{12}Cl_3O_3P$: t417 $C_6H_{12}Cl_3O_4P$: t416 $C_6H_{12}F_3NOSi$: m440 $C_6H_{12}NO_3P$: d293a $C_6H_{12}N_2$: d45, t269 $C_6H_{12}N_3O_3$: s15 $C_6H_{12}N_3O_4S_2$: c371 $C_6H_{12}N_3S_4$: b174 $C_6H_{12}N_2Si$: t373 $C_6H_{12}N_4$: h52 $C_6H_{12}O$: a100, b488, c327, d497, d618, e87, h54, h72, h77, i72, m346, o47 $C_6H_{12}O_2$: b412, b413, b414, d500, e49, e88, e89, h66, h142, i62, m227, m302, m340, m341, m342, t77 $C_6H_{12}O_3$: d435, d457, d515, e37, e152, e154, i99, p2, p232, t67 $C_6H_{12}O_6Si$: d23 $C_6H_{12}O_6$: f36, g1, g6, i23, m11, s6 $C_6H_{12}O_7$: g4 $C_6H_{12}S$: c326 $C_6H_{13}Br$: b294 $C_6H_{13}BrO_2$: b267 $C_6H_{13}Cl$: c129 $C_6H_{13}ClO$: c130
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The alphanumeric designations are keyed to Table 1.15

<p> $C_6H_{13}ClO_2$: c81 $C_6H_{13}ClO_3$: c105 $C_6H_{13}Cl_3O_3Si$: t415 $C_6H_{13}I$: i39 $C_6H_{13}N$: c334, h51, m371, m372, m373, m374 $C_6H_{13}NO$: d260, d553, e184, h144, p187 $C_6H_{13}NO_2$: a183, a184, h122, i79, L4, L5 $C_6H_{13}NO_4$: b182 $C_6H_{13}NO_4S$: m451 $C_6H_{13}NO_5$: g5, t428 C_6H_{14}: d489, d490, h55, m336, m337 $C_6H_{14}ClN$: d272 $C_6H_{14}Cl_4OSi_2$: b168 $C_6H_{14}N_2$: a182, a219, c318, c319 $C_6H_{14}N_2O$: a172, h123 $C_6H_{14}N_2O_2$: L12 $C_6H_{14}N_4O_2$: a311 $C_6H_{14}O$: b449, d417, d492, d492, d494, d495, d496, d701, e83, h68, h69, h70, m343, m344, m345 $C_6H_{14}OSi$: a97, e33, t374 $C_6H_{14}O_2$: b410, d251, d252, d491, e179, h58, h59, h60, i86, m338 $C_6H_{14}O_2S$: d704 $C_6H_{14}O_3$: b191, d253, e35, e156, h65, h172, t322 $C_6H_{14}O_4$: e127, t270 $C_6H_{14}O_4S$: d703 $C_6H_{14}O_6$: d738, m10, s5 $C_6H_{14}O_6S_2$: b188 $C_6H_{14}S$: b451, h64 $C_6H_{14}Si$: a104 $C_6H_{15}Al$: t263 $C_6H_{15}As$: t266 $C_6H_{15}B$: t268 $C_6H_{15}Bi$: t267 $C_6H_{15}ClO_2Si$: c154 $C_6H_{15}ClO_3Si$: c231 $C_6H_{15}ClSi$: b446 </p>	<p> $C_6H_{15}Ga$: t274 $C_6H_{15}In$: t276 $C_6H_{15}N$: d411, d696, e85, e86, h80, m353a, t264 $C_6H_{15}NO$: a185, a216, a217, b419, b448, d270 $C_6H_{15}NOSi$: m439 $C_6H_{15}NO_2$: d254, e118 $C_6H_{15}NO_3$: t264 $C_6H_{15}NO_6S$: t424 $C_6H_{15}N_3$: a174 $C_6H_{15}O_3B$: t260 $C_6H_{15}O_3P$: d420, t282 $C_6H_{15}O_3PS$: t285 $C_6H_{15}O_4P$: t280 $C_6H_{15}P$: t281 $C_6H_{15}Sb$: t265 $C_6H_{16}Cl_2Si_2$: t104 $C_6H_{16}N_2$: d302, h56, t108 $C_6H_{16}OSi$: p218 $C_6H_{16}Br_2OSi_2$: b150 $C_6H_{16}O_2Si$: d249 $C_6H_{16}O_3SSi$: m22 $C_6H_{16}O_3Si$: t266b $C_6H_{16}Si$: t284 $C_6H_{17}NO_3Si$: a280 $C_6H_{17}NO_5S$: b180 $C_6H_{17}N_3$: i9 $C_6H_{18}LiNSi_2$: L11 $C_6H_{18}N_2Si$: b172 $C_6H_{18}N_3ClSi$: c257a $C_6H_{18}N_3OP$: h53 $C_6H_{18}N_4$: t272 $C_6H_{18}OSi_2$: h50 $C_6H_{18}O_3Si_3$: h48 $C_6H_{19}NOSi_2$: b210 $C_6H_{19}NSi_2$: h49 C_6N_4: t37 </p>	<p> $C_7H_3ClF_3NO_2$: c182, c183, c184 $Cl_7H_3ClN_2O_5$: d630 $C_7H_3ClN_2O_6$: c96 $C_7H_3Cl_3O$: d160, d161 $C_7H_4BrF_3$: b233, b234 C_7H_4ClFO: f14 $C_7H_4ClF_3$: c51, c52, c53 C_7H_4ClN: c47, c48 C_7H_4ClNO: c206 $C_7H_4ClNO_3$: n41, n42 $C_7H_4ClNO_4$: c178, c179, c180, n66 $C_7H_4Cl_2O$: c55, c56, d150 $C_7H_4Cl_2O_2$: d156, d157, d158 $C_7H_4Cl_3F$: t233 $C_7H_4Cl_4S$: t34 $C_7H_4F_3NO_2$: n88, n89 $C_7H_4F_2O$: d718 $C_7H_4I_2O_3$: h111 $C_7H_4N_2O_2$: n40 $C_7H_4N_2O_6$: d628, d629 $C_7H_4N_2O_7$: d638 $C_7H_4O_3S$: h104 $C_7H_4O_4S$: s24 C_7H_5BrO: b66, b228 $C_7H_5BrO_2$: b232 $C_7H_5BrO_3$: b348 $C_7H_5ClF_3N$: a144, a145, a146 $C_7H_5ClN_2$: a141 C_7H_5ClO: b67, c38, c39 C_7H_5ClOS: p103 $C_7H_5ClO_2$: c45, c46, c46a, c237, c238, p102 $C_7H_5ClO_3$: c193 $C_7H_5Cl_2F$: c119 $C_7H_5Cl_2N$: d196 $C_7H_5Cl_2NO$: d151 $C_7H_5Cl_3$: t248, t249 C_7H_5FO: b69, f10 $C_7H_5FO_2$: f12, f13 $C_7H_5F_3$: t300 $C_7H_5F_3N_2O_2$: a241, a242 $C_7H_5F_3O$: t290 </p>
	C_7	
<p> C_7F_5N: p23 $C_7H_3BrClF_3$: b250 $C_7H_3BrF_3NO_2$: b315 </p>		

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

<p> $C_7H_5F_4N$: a179 $C_7H_5IO_2$: i29 $C_7H_5IO_3$: i51 $C_7H_5I_2NO_2$: a156 C_7H_5N: b51 C_7H_5NO: b63, p121 $C_7H_5NO_3$: n27, n28 $C_7H_5NO_3S$: s1 $C_7H_5NO_4$: n37, n38, n39, p259, p260, p261 $C_7H_5NO_5$: h154 C_7H_5NS: b60, p122 $C_7H_5NS_2$: m17 $C_7H_5N_3O_2$: a238, n36, n55 $C_7H_5N_3O_2S$: a240 $C_7H_5N_3O_6$: t386 C_7H_6BrClO: b252 $C_7H_6BrNO_2$: n46 $C_7H_6BrNO_3$: h155 $C_7H_6Br_2$: b236, d102 C_7H_6ClF: c123, c124, c125, f16 C_7H_6ClNO: c40 $C_7H_6ClNO_2$: a140, c187, c188, c189, n47 $C_7H_6ClNO_3$: c140 $C_7H_6Cl_2$: c59, c60, d229, d230, d231 $C_7H_6Cl_2O$: d191, d192 $C_7H_6F_3N$: a129, a130, a131 $C_7H_6INO_2$: a203 $C_7H_6N_2$: a124, a125, a126, b38 $C_7H_6N_2O_3$: n29 $C_7H_6N_2O_4$: a237, d639, d640, d641 $C_7H_6N_2O_5$: d631, d33a $C_7H_6N_2S$: a128, m15 C_7H_6O: b3 C_7H_6OS: t143 $C_7H_6O_2$: b44, h94, h95, h96, m240 $C_7H_6O_2S$: m16 $C_7H_6O_3$: d375, d376, f41, h99, h100, h101 </p>	<p> $C_7H_6O_4$: d383, d384, d385 $C_7H_6O_5$: t306 $C_7H_6O_6S$: s28 C_7H_7Br: b85, b355, b356, b357 C_7H_7BrO: b235, b301, b302, b303 C_7H_7Cl: b89, c244, c245, c246 $C_7H_7ClN_4O_2$: c241 C_7H_7ClO: c57, c139, c158, c159 $C_7H_7ClO_2S$: t177 $C_7H_7ClO_3S$: m49 C_7H_7ClS: c248 $C_7H_7Cl_3Si$: b123, t192 C_7H_7F: f24, f25, f26 C_7H_7FO: f15, f19 $C_7H_7FO_2S$: t178 C_7H_7I: i53, i54 C_7H_7IO: i41 C_7H_7N: v9, v10 C_7H_7NO: a53, a54, a55, b4, f31 $C_7H_7NO_2$: a121, a122, a123, h97, h98, m401, m402, n85, n86, n87 $C_7H_7NO_3$: a286, a287, m81, m82, m323, m324, n44, n45 $C_7H_7NO_4S$: c16 $C_7H_7N_3$: a201, a202, m136 C_7H_8: b129, c310, t167 C_7H_8BrN: b304 C_7H_8ClN: c58, c142, c143, c144, c145, c146 C_7H_8ClNO: c138a, c138 $C_7H_8ClNO_2S$: c247 $C_7H_8Cl_2Si$: d198, m358 $C_7H_8N_2O$: a114, b72, p165 $C_7H_8N_2O_2$: d33, h165, m315, m316, m317 $C_7H_8N_2O_3$: m78, m79, m80 $C_7H_8N_2S$: p154 $C_7H_8N_4O_2$: t138 </p>	<p> C_7H_8O: b78, c279, c280, c281, m48 C_7H_8OS: m429 $C_7H_8O_2$: d389, d390, h105, m87, m88, m89, m276 $C_7H_8O_2S$: t173 $C_7H_8O_3$: e136, f45, m304 $C_7H_8O_3S$: m127, t176 C_7H_8S: m367, p128, t147 C_7H_9ClSi: m357 C_7H_9N: b79, d604, d605, d606, d607, e211, e212, e213, m122, t180, t181, t182 C_7H_9NO: a218, b98, h126, m42, m43, m44 $C_7H_9NO_2$: d456 $C_7H_9NO_2S$: t174 $C_7H_9NO_3S$: a294 C_7H_9NS: m422, m423 $C_7H_9N_3O$: a133 C_7H_{10}: b130 $C_7H_{10}N_2$: a157, a177, a178, d476, m360, t168, t169, t170, t171 $C_7H_{10}N_2O$: m94 $C_7H_{10}N_2OS$: h129 $C_7H_{10}N_2O_2$: e173, m232 $C_7H_{10}N_2O_2S$: a210, t175 $C_7H_{10}O$: m61, m62, n108, t65 $C_7H_{10}O_2$: a40, c359 $C_7H_{10}O_3$: e12, h158, m333, t341 $C_7H_{10}O_4$: d550 $C_7H_{10}O_5$: d459 $C_7H_{11}Si$: m366 $C_7H_{11}Br$: b318 $C_7H_{11}BrO_4$: d286 $C_7H_{11}ClO$: c316 $C_7H_{11}ClO_4$: d290 $C_7H_{11}NO$: c340, h110 $C_3H_{11}NO_2$: a52 $C_7H_{11}NO_3$: m335 $C_7H_{11}NO_5$: a45 $C_7H_{11}NS$: c341 </p>
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table I.15*

<p> C_7H_{12}: c311, h22, m207, m208, n107 $C_7H_{12}O$: c309, c315, m204, m205, m206, m268 $C_7H_{12}O_2$: b417, c317, d355, e121 $C_7H_{12}O_3$: e168, e195 $C_7H_{12}O_4$: d317, d318, d552, d574, d575, d576, h8, m273, t126 $C_7H_{12}O_5$: g17, g18 $C_7H_{12}O_6Si$: m435 $C_7H_{12}O_7$: g3 $C_7H_{13}Br$: b260, b306 $C_7H_{13}BrO_2$: e80 $C_7H_{13}ClO$: h18 $C_7H_{13}N$: a250, d333, q5 $C_7H_{13}NO$: a317, c339 $C_7H_{13}NO_2$: a152 C_7H_{14}: c306, h19, m194 $C_7H_{14}ClN$: c113 $C_7H_{14}N_2$: d416 $C_7H_{14}N_2O$: a278 $C_7H_{14}N_2O_2$: e201 $C_7H_{14}O$: c308, c342, d569, d578, h5, h15, h16, h17, m197, m198, m199, m200, m201, m202, m203, m267 $C_7H_{14}O_2$: b479, c307, d258, e123, e170, e198, h10, i80, m75, m265, p52 $C_7H_{14}O_3$: i68 $C_7H_{14}O_6$: m256 $C_7H_{15}Br$: b291, b292 $C_7H_{15}Cl$: c128 $C_7H_{15}ClO_2$: c82 $C_7H_{15}Cl_3Si$: h21 $C_7H_{15}I$: i37 $C_7H_{15}N$: c324, d591, e202, e203, m209, m211, m211 $C_7H_{15}NO$: d469, e157, h125, m375, p185, p186 $C_7H_{15}NO_2$: p276 $C_7H_{15}NO_3$: c18, m452 $C_7H_{15}O_5P$: e119 </p>	<p> C_7H_{16}: d570, d571, d572, d573, e197, h6, m264, t337 $C_7H_{16}BrNO_2$: a38 $C_7H_{16}ClNO_2$: a39 $C_7H_{16}N_2$: a215, m301, t366 $C_7H_{16}N_2O$: a277 $C_7H_{16}N_2O_2$: p182 $C_7H_{16}O$: d577, h12, h13, h14, m266, t338 $C_7H_{16}O_2$: d257, d331, m394 $C_7H_{16}O_2Si$: d256, e228 $C_7H_{16}O_3$: d700, t278, t321 $C_7H_{16}O_4$: t91 $C_7H_{16}S$: h9 $C_7H_{17}N$: h20, m269a $C_7H_{17}NO$: d275 $C_7H_{17}NO_2$: b420, d274 $C_7H_{17}NO_3$: m255 $C_7H_{17}NO_6S$: t427 $C_7H_{17}NO_7S$: t426 $C_7H_{18}N_2$: d330, h7, i103, t118 $C_7H_{18}N_2O$: b173 $C_7H_{18}N_2O_2$: a276 $C_7H_{18}O_2Si$: b486 $C_7H_{18}O_3Si$: b485, t266a $C_7H_{19}NOSi_2$: b209 $C_7H_{19}NSi$: d343, t371 $C_7H_{19}N_3$: d42, t419 $C_7H_{21}N_3Si$: t420 </p> <hr/> <p style="text-align: center;">C_8</p> <hr/> <p> $C_8Br_4O_3$: t10 $C_8Cl_4O_3$: t31 C_8D_{10}: e67 $C_8HCl_4NO_2$: t32 $C_8H_3NO_5$: n72 $C_8H_4BrNO_2$: b296 $C_8H_4Cl_2O_2$: b14, b15, p171 $C_8H_4Cl_2O_4$: d217 $C_8H_4Cl_6$: b202 $C_8H_4F_3N$: t298 $C_8H_4F_6$: b206 $C_8H_4N_2$: d236, d237 $C_8H_4O_3$: p168 </p>	<p> $C_8H_5Br_5$: p5 $C_8H_5ClO_4$: c209 $C_8H_5Cl_3O_3$: t242 $C_8H_5F_3O$: t289 $C_8H_5F_3O_2S$: t137 $C_8H_5F_6N$: b205 C_8H_5NO: b68 $C_8H_5NO_2$: i21, p170 $C_8H_5NO_3$: h166, i58 $C_8H_5NO_6$: n31, n32, n33, n34 C_8H_6: p82 C_8H_6BrClO: b246 C_8H_6BrN: b329 $C_8H_6Br_2O$: d64 $C_8H_6Br_4$: t11, t12 $C_8H_6ClF_3$: t299 C_8H_6ClN: c201 $C_8H_6ClNO_3$: c171 $C_8H_6Cl_2O$: d140 $C_8H_6Cl_2O_3$: d214 $C_8H_6Cl_4$: t35 $C_8H_6N_2$: q4 $C_8H_6N_2O_2$: a266, n65 $C_8H_6N_2O_6$: d636, m228 C_8H_6O: b42 $C_8H_6O_2$: b13, p169 $C_8H_6O_3$: b70, c14, f33, m239 $C_8H_6O_4$: b16, b17, m241, p167 C_8H_6S: b61 C_8H_7Br: b349 C_8H_7BrO: b221, b222 $C_8H_7BrO_2$: b327, b328 C_8H_7ClO: c28, c29, c30, p81, t187, t188, t189 C_8H_7ClOS: b91 $C_8H_7ClO_2$: b90, c200, m53, p69 $C_8H_7ClO_3$: c86, c197, m184, m185 $C_8H_7ClO_4$: c133 C_8H_7FO: f8 C_8H_7N: i18, p80, t184, t185, t186 </p>
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

C_8H_7NO : m9, m137, t190 $C_8H_7NO_2$: h133, n84 $C_8H_7NO_3$: n22, n23 $C_8H_7NO_3S$: t179 $C_8H_7NO_4$: a116a, m318, m319, m320, m321, n62, n63, n64 $C_8H_7NO_5$: m83 C_8H_7NS : b121, m135 $C_8H_7N_2O_2$: a153 C_8H_8 : s11 C_8H_8BrNO : b219 $C_8H_8Br_2$: d79, d104, d105 C_8H_8ClNO : c23 $C_8H_8ClNO_3S$: a10 $C_8H_8Cl_2$: d233, d234 $C_8H_8Cl_2Si$: p166 $C_8H_8HgO_2$: p125 $C_8H_8N_2$: a260, m128 $C_8H_8N_2OS$: a207 C_8H_8O : a31, e9, m126, p76a C_8H_8OS : m424, p153 $C_8H_8O_2$: b41, b97, h90, h91, h92, m45, m46, m129, m130, m131, m132, p78, p79 $C_8H_8O_2S$: t160 $C_8H_8O_3$: d370, d380, h130, h131, h137, h138, h160, m8, m50, m51, m52, m242, m277, m410, p68, t74 $C_8H_8O_4$: d21, h132 $C_8H_8O_4S$: a33 C_8H_9Br : b282, b283, b368, b369, b370, b371 C_8H_9BrO : b270, b286 $C_8H_9BrO_2$: b268 C_8H_9Cl : c107, c108, c258, c259, c260, c261 C_8H_9ClO : c90 C_8H_9N : b100, c360, i22, m447	C_8H_9NO : a18, a108, a109, a110, b96, m249 $C_8H_9NO_2$: a15, a16, a17, a211, a212, b88, d556, d557, d558, d559, e187, e214, e215, e216, m47, m116, m117, p115, t75 $C_8H_9NO_3$: a206, h163, h164, m85, n59 $C_8H_9NO_4$: d444 C_8H_{10} : e68, m244, x4, x5, x6 $C_8H_{10}N_2O$: d560 $C_8H_{10}N_4O_2$: c1, d240 $C_8H_{10}O$: b131, d579, d580, d581, d582, d583, d584, e28, e199, m105, m106, m107, m138, m139, m140, p112, p113 $C_8H_{10}O_2$: b18, d431, d432, d433, m54, p72, p111 $C_8H_{10}O_3$: c320, d446, h135, h159 $C_8H_{10}O_3S$: m434 $C_8H_{10}O_4$: d263 $C_8H_{10}S$: b105 $C_8H_{11}ClSi$: d585 $C_8H_{11}N$: b103, d477, d478, d479, d480, d481, d482, d483, e63, e64, e65, e180, e181, m141, m142, p114, t367 $C_8H_{11}NO$: a173, a256, a261, a262, a300, d470, e24, h117, m55, m71, m72, m73, p266 $C_8H_{11}NO_2$: d427, d428, d429 $C_8H_{11}NO_3S$: m433 $C_8H_{11}NO_3$: e132 $C_8H_{11}NO_3S$: d463 $C_8H_{11}N_5$: p93 C_8H_{12} : c345, v6 $C_8H_{12}N_2$: d239, d586, t119, x9 $C_8H_{12}N_2O_2$: d410 $C_8H_{12}N_2O_3$: d280 $C_8H_{12}N_4$: a323	$C_8H_{12}O$: e234 $C_8H_{12}O_2$: d508, e219, h185, n111 $C_8H_{12}O_3$: e194 $C_8H_{12}O_4$: d305, d316 $C_8H_{12}O_6Si$: t195 $C_8H_{12}Si$: d587 $C_8H_{13}N$: e235 C_8H_{14} : c349, d532, o17, o44, v5 $C_8H_{14}N_2$: p188 $C_8H_{14}O$: c348, d510, e7a, m262, o45 $C_8H_{14}O_2$: b459, c333, c363, d537, i69, m195 $C_8H_{14}O_3$: b415, b496, d712, e90 $C_8H_{14}O_4$: b447, d320, d335, d536a, e149, o24 $C_8H_{14}O_4S$: d619 $C_8H_{14}O_5S_2$: d708 $C_8H_{14}O_6$: d339, d340 $C_8H_{14}O_6Si$: t194 $C_8H_{15}ClO$: e145, o37 $C_8H_{15}N$: o27 $C_8H_{15}NO$: d367 $C_8H_{15}NO_2$: d468, e204, e205, e206 C_8H_{16} : c346, d506, d507, e108, o39, t357 $C_8H_{16}ClN$: c227 $C_8H_{16}O$: c347, d509, e109, e110, o34, o35, o36, o40 $C_8H_{16}O_2$: b431, c321, e142, e143, h79, i67, m261, o29, p234 $C_8H_{16}O_4$: e36, t125 $C_8H_{17}Br$: b320 $C_8H_{17}Cl$: c190 $C_8H_{17}Cl_3Si$: o43 $C_8H_{17}I$: i46 $C_8H_{17}N$: c350, d511 $C_8H_{17}NO_2$: p189 $C_8H_{17}NO_3S$: c335 $C_8H_{17}O_3P$: t283
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table I.15*

C_8H_{18} : d533, e140, e174, e175, m260, o22, t100, t353, t354, t355 $C_8H_{18}ClNO_2$: a49 $C_8H_{18}Cl_2O_2Si_3$: d186 $C_8H_{18}Cl_2Si$: d184 $C_8H_{18}Cl_2Sn$: d136a $C_8H_{18}F_3NOSi_2$: b212 $C_8H_{18}N_2$: c314 $C_8H_{18}N_2O$: m224, m367 $C_8H_{18}N_2O_4S$: h124 $C_8H_{18}O$: d115, d407, e144, o30, o31, o32, o33 $C_8H_{18}OSi_2$: d713 $C_8H_{18}OSn$: d137 $C_8H_{18}O_2$: d122, d535, e141, o25, o26, t356 $C_8H_{18}O_2S$: d135 $C_8H_{18}O_3$: b176, b411, d698, t277 $C_8H_{18}O_3S$: d134 $C_8H_{18}O_3Si$: t262 $C_8H_{18}O_4$: b189 $C_8H_{18}O_4S$: d131 $C_8H_{18}O_5$: t51 $C_8H_{18}S$: d132, d133, o28 $C_8H_{18}S_2$: b153, b154, d113, d114 $C_8H_{18}Si_2$: b208 $C_8H_{19}N$: d107, d406, d418, d536, e147, o41, t102 $C_8H_{19}NO$: d412 $C_8H_{19}NO_2$: b444, d247, d248 $C_8H_{19}NO_5$: b183 $C_8H_{19}O_3P$: d127 $C_8H_{20}BrN$: t48 $C_8H_{20}ClN$: t49 $C_8H_{20}Ge$: t56 $C_8H_{20}N_2$: d534, o23, t101, t273 $C_8H_{20}O_3SSi$: m19 $C_8H_{20}O_3Si$: t261 $C_8H_{20}O_4Si$: t47 $C_8H_{20}O_5P_2$: t59 $C_8H_{20}O_7P_2$: t58	$C_8H_{20}Pb$: t57 $C_8H_{20}Si$: t60 $C_8H_{20}Sn$: t62 $C_8H_{21}NO$: t50 $C_8H_{21}NOSi_2$: b207 $C_8H_{21}NO_2Si$: a275 $C_8H_{22}N_2O_3Si$: a167a, t324 $C_8H_{22}N_4$: b145 $C_8H_{22}O_2Si_2$: b211 $C_8H_{23}N_5$: t54 $C_8H_{24}Cl_2O_3Si_4$: d207 $C_8H_{24}O_2Si_3$: o21 $C_8H_{24}O_4Si_4$: o20 $C_8H_{28}N_4Si_4$: o19 <div style="text-align: center;">C_9</div> $C_9F_{15}N_3$: t432 $C_9H_2Cl_6O_3$: h30 $C_9H_3Cl_3O_3$: b32 $C_9H_4O_5$: b31, c15 $C_9H_5BrClNO$: b255 $C_9H_5Br_2NO$: d87 C_9H_5ClNO : c132 $C_9H_5Cl_2N$: d225 C_9H_6BrN : b347 C_9H_6ClN : c236 C_9H_6ClNO : c134 $C_9H_6N_2O_2$: n77, t172 $C_9H_6O_2$: b56, c276 $C_9H_6O_3$: h108, h109 $C_9H_6O_4$: i16 $C_9H_6O_6$: b28, b29, b30 C_9H_7BrO : b259 C_9H_7ClO : c268 $C_9H_7ClO_2$: c76 $C_9H_7Cl_3O_3$: t243 C_9H_7N : i110, q3 C_9H_7NO : h178, i20 $C_9H_7NO_3$: h143, m285 $C_9H_7NO_4S$: h179 $C_9H_7N_3O_4S_2$: a247 C_9H_8 : i17 $C_9H_8Cl_2O_2$: n109 $C_9H_8N_2$: m409	$C_9H_8N_2O_5$: n43 C_9H_8O : c266, i15 $C_9H_8O_2$: c266, d353 $C_9H_8O_3$: h107 $C_9H_8O_4$: a56, p124 C_9H_9BrO : b342 C_9H_9Cl : c217 C_9H_9ClO : c223 $C_9H_9ClO_3$: c199, c249 C_9H_9N : d486, m283, m284 C_9H_9NO : m93 $C_9H_9NO_2$: a9 $C_9H_9NO_2S$: t191 $C_9H_9NO_3$: a11, a12, b71 $C_9H_9N_3O$: a265 C_9H_{10} : a84, i13, m411, v3 $C_9H_{10}F_3NO_2$: m123 $C_9H_{10}N_2$: a301, p119a $C_9H_{10}N_2O$: p147 $C_9H_{10}N_2O_2$: p83 $C_9H_{10}N_2O_3$: a132 $C_9H_{10}O$: a98, a99, c269, d360, i14, m113, p144, p145, p209, p217 $C_9H_{10}O_2$: b77, d485, e9a, e25, e26, e69, h170, h171, m39, m40, m41, m356, p74, p146 $C_9H_{10}O_2S$: b120 $C_9H_{10}O_3$: d430, e29, e30, e39, e48, e151, e218, m91, m279, m292, p75 $C_9H_{10}O_4$: d434, m288, m445 $C_9H_{10}O_8$: c354 $C_9H_{11}Br$: b297, b331, b361, b362 $C_9H_{11}BrO$: b343 $C_9H_{11}ClO_3S$: c114 $C_9H_{11}Cl_3Si$: c226, m354 $C_9H_{11}N$: a83, a199, a200, c332, t71, t80 $C_9H_{11}NO$: d462, m355, m432 $C_9H_{11}NO_2$: d464, e27, e59, e60, p84
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

<p> $C_9H_{11}NO_3$: t437 C_9H_{12}: e158, i91, n91, p222, t333, t334, t335, v8 $C_9H_{12}Cl_2Si$: m353 $C_9H_{12}N_2O_4$: a246 $C_9H_{12}N_2O_6$: u14 $C_9H_{12}O$: b95, d547, d548, i106, i107, p142, p143, p235, t358, t359, t362 $C_9H_{12}O_2$: b110, e31, i85, n110, p73, p140, t348 $C_9H_{12}O_3$: m196, t315 $C_9H_{12}O_3S$: e222 $C_9H_{12}S$: p141 $C_9H_{13}N$: b480, d487, d622, e72, e169, e223, e224, i90, t330 $C_9H_{13}NO$: a264, b80, m86, n112 $C_9H_{13}NO_2$: a263 $C_9H_{13}N_3O_2$: t438 $C_9H_{14}BrN$: p159 $C_9H_{14}Br_3N$: p162 $C_9H_{14}ClN$: p160 $C_9H_{14}IN$: p161 $C_9H_{14}N_2$: n94 $C_9H_{14}O$: d527, d529, i82, t340 $C_9H_{14}OSi$: t375 $C_9H_{14}O_2Si$: d443 $C_9H_{14}O_3$: b192 $C_9H_{14}O_3Si$: p158 $C_9H_{14}O_5$: d262, d321 $C_9H_{14}O_6$: p201 $C_9H_{14}Si$: p163 $C_9H_{15}NO$: c361 $C_9H_{15}NO_2$: d568 $C_9H_{15}NO_5$: d261 $C_9H_{15}NSi$: t369 C_9H_{16}: h46 $C_9H_{16}Cl_2Si$: c333a $C_9H_{16}N_2$: d46 $C_9H_{16}O$: d528 $C_9H_{16}O_2$: c325 $C_9H_{16}O_3$: b467 </p>	<p> $C_9H_{16}O_4$: d303, d307, d322, d530, n95 $C_9H_{17}ClO$: n101 $C_9H_{17}N$: a88, n97 $C_9H_{17}NO$: m180 $C_9H_{17}NO_2$: e177, e178 C_9H_{18}: i94, n102, p224, t339 $C_9H_{18}NO$: t117 $C_9H_{18}N_2O_3Si$: t325 $C_9H_{18}O$: d531, n100, n103 $C_9H_{18}O_2$: e138, m329, n98 $C_9H_{18}O_3$: d111 $C_9H_{19}Br$: b317 $C_9H_{19}N$: i95, t332 $C_9H_{19}NO$: d116 $C_9H_{19}NO_2$: e120 $C_9H_{19}NO_3S$: c337 C_9H_{20}: n92, t346 $C_9H_{20}Cl_2Si$: m330 $C_9H_{20}N_2$: a296 $C_9H_{20}N_2S$: d136 $C_9H_{20}O$: n99, t347 $C_9H_{20}O_2$: b450, n96 $C_9H_{20}O_3$: d699, t279 $C_9H_{20}O_3Si$: a103 $C_9H_{20}O_4$: t408 $C_9H_{20}O_5$: t53 $C_9H_{21}BO_3$: t406 $C_9H_{21}ClO_3Si$: c230 $C_9H_{21}ClSi$: c257 $C_9H_{21}N$: n104, t407 $C_9H_{21}NO_3$: t309 $C_9H_{21}N_3$: t275 $C_9H_{21}O_3B$: t310 $C_9H_{21}O_3P$: t313 $C_9H_{22}N_2$: d327, n93 $C_9H_{22}O_3Si$: p238 $C_9H_{23}NO_3Si$: a279 $C_9H_{24}N_4$: b147 </p> <hr/> <p style="text-align: center;">C_{10}</p> <hr/> <p> $C_{10}H_2O_6$: b27 $C_{10}H_4Cl_2O_2$: d201 </p>	<p> $C_{10}H_6N_2$: b99 $C_{10}H_6N_2O_4$: d634 $C_{10}H_6N_2O_4S$: d48 $C_{10}H_6O_2$: n11 $C_{10}H_6O_3$: h152 $C_{10}H_6O_8$: b26 $C_{10}H_7Br$: b312 $C_{10}H_7BrO$: b313 $C_{10}H_7Cl$: c168, c169 $C_{10}H_7NO_2$: n57, n81, p123 $C_{10}H_7NO_8S_2$: n82 $C_{10}H_8$: a326, n2 $C_{10}H_8BrNO_2$: b287 $C_{10}H_8N_2$: d705 $C_{10}H_8O$: n9, n10 $C_{10}H_8O_2$: d392, d393, d394, d395, m191 $C_{10}H_8O_3$: h140 $C_{10}H_8O_3S$: n18 $C_{10}H_8O_7S_2$: h150, h151 $C_{10}H_8O_8S_2$: d396 $C_{10}H_9ClCrN_2O_3$: b143 $C_{10}H_9N$: m407, m408, n17 $C_{10}H_9NO$: a51, a236 $C_{10}H_9NO_2$: i19 $C_{10}H_9NO_3S$: a234 $C_{10}H_9NO_4S$: a193, a194, a195, a196 $C_{10}H_9NO_6$: d561 $C_{10}H_9NO_6S_2$: a232, a233 $C_{10}H_9N_3$: d706 $C_{10}H_{10}ClFO$: c120 $C_{10}H_{10}ClNO_2$: c26 $C_{10}H_{10}N_2$: a285, n4, n5 $C_{10}H_{10}N_2O$: m365 $C_{10}H_{10}O$: d362, m190, p96, p98 $C_{10}H_{10}O_2$: b64, s2 $C_{10}H_{10}O_3$: b73, m60 $C_{10}H_{10}O_4$: d588, d589, d590, h136, p152 $C_{10}H_{11}BrO$: b312a $C_{10}H_{11}ClO_3$: c198 $C_{10}H_{11}ClO_4$: t317 $C_{10}H_{11}IO_4$: i28 $C_{10}H_{11}N$: p101 </p>
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

$C_{10}H_{11}NO_2$: a32, d448 $C_{10}H_{11}NO_4$: c10 $C_{10}H_{11}NO_6$: m226 $C_{10}H_{12}$: d244, t73 $C_{10}H_{12}NO$: b408 $C_{10}H_{12}N_2$: a170, b81, b102 $C_{10}H_{12}N_2O_2$: p77 $C_{10}H_{12}O$: a94, b500, e55, i77, m97, m386, m387, m391, p94, p95 $C_{10}H_{12}O_2$: e200, h112, h162, m70, m92, m98, m99, m100, p99, p100, p223 $C_{10}H_{12}O_3$: d426, e41, e163, m300, p71, p230 $C_{10}H_{12}O_4$: d447, m225, t314 $C_{10}H_{12}O_5$: d306, p239, t316 $C_{10}H_{12}O_6$: d514 $C_{10}H_{13}Br$: b298 $C_{10}H_{13}BrO$: b243 $C_{10}H_{13}Cl$: b434 $C_{10}H_{13}NO$: p129 $C_{10}H_{13}NO_2$: e45 $C_{10}H_{13}NO_2S$: b92 $C_{10}H_{13}N_5O_4$: a70 $C_{10}H_{14}$: b423, b424, b425, d282, d283, d284, i64, i100, i101, i102, t97, t98, t99 $C_{10}H_{14}NO_5PS$: p3 $C_{10}H_{14}N_2$: n20, p139 $C_{10}H_{14}N_2O$: d323, d334 $C_{10}H_{14}N_4O_4$: d399 $C_{10}H_{14}N_5O_7P$: a72 $C_{10}H_{14}O$: b469, b470, b471, b472, b473, b477, c20, c362, i92, i102a, p58, t116, t254 $C_{10}H_{14}O_2$: b432, b454, d450 $C_{10}H_{14}O_3$: c6, c9 $C_{10}H_{14}O_4$: m90, t318 $C_{10}H_{15}BrO$: b245	$C_{10}H_{15}N$: b421, d277, d278, d564, e233, i93, p97, t96 $C_{10}H_{15}NO$: d273, e1, e2 $C_{10}H_{15}NO_2$: d451, p106 $C_{10}H_{15}N_5O_{10}P_2$: a71 $C_{10}H_{16}$: a67, c2, d649, L6, L7, m453, p25, p175, p176, t5, t6, t253 $C_{10}H_{16}ClN$: b126 $C_{10}H_{16}Cl_2O_2$: d11 $C_{10}H_{16}N_2O_8$: e125 $C_{10}H_{16}O$: c3, c4, d352, d562, d563, L8, p177, p178, p243, t351 $C_{10}H_{16}OSi$: d519 $C_{10}H_{16}O_4$: c5, d266 $C_{10}H_{16}O_4S$: c7 $C_{10}H_{16}O_5$: d265, d301 $C_{10}H_{16}Si$: b127 $C_{10}H_{17}N$: a66, p274 $C_{10}H_{17}NO$: c343, m450 $C_{10}H_{18}$: d1, d2, p174 $C_{10}H_{18}N_2O_7$: h119 $C_{10}H_{18}O$: b216, b441, b442, c265, d3, g2, i60, i83, i109, L9, m13, p190, t7, t350 $C_{10}H_{18}O_2$: e112 $C_{10}H_{18}O_3$: d599, t70 $C_{10}H_{18}O_4$: b175, d9, d121, d332, d565 $C_{10}H_{18}O_4S$: d341 $C_{10}H_{18}O_6$: d421 $C_{10}H_{19}ClO$: d17 $C_{10}H_{19}N$: d12, t331 $C_{10}H_{19}NO_2$: e207 $C_{10}H_{20}$: c301, d18 $C_{10}H_{20}Br_2$: d73 $C_{10}H_{20}N_2S_4$: t61 $C_{10}H_{20}O$: b439, b440, c274, d6, d16, d357, d366, e148, m12, m303 $C_{10}H_{20}O_2$: d14, e146, e190, m63, m170 $C_{10}H_{20}O_5$: p45	$C_{10}H_{20}O_5Si$: t326 $C_{10}H_{21}Br$: b265 $C_{10}H_{21}Cl$: c80 $C_{10}H_{21}I$: i33 $C_{10}H_{21}N$: d294 $C_{10}H_{21}NO$: a230 $C_{10}H_{22}$: d7 $C_{10}H_{22}N_2$: d41 $C_{10}H_{22}O$: d15, d651, t72 $C_{10}H_{22}O_2$: d10, d106 $C_{10}H_{22}O_3$: d697, t413 $C_{10}H_{22}O_3S$: d13 $C_{10}H_{22}O_4$: t412 $C_{10}H_{22}O_5$: b190 $C_{10}H_{22}O_7$: d648 $C_{10}H_{23}N$: d19, d650 $C_{10}H_{23}NO$: d108 $C_{10}H_{23}NO_2$: d259 $C_{10}H_{24}N_2$: d8, t55, t111 $C_{10}H_{24}N_2O_2$: d645 $C_{10}H_{24}N_4$: b146 $C_{10}H_{24}OSi$: m109 $C_{10}H_{24}O_3Si$: m441 $C_{10}H_{24}O_6Si$: t429 $C_{10}H_{27}O_3N_3Si$: t323 $C_{10}H_{30}O_3Si_4$: d5 $C_{10}H_{30}O_5Si_5$: d4
<div style="text-align: center;">C_{11}</div>		
$C_{11}H_4F_{20}O$: i1 $C_{11}H_7N$: c293 $C_{11}H_8O$: n1 $C_{11}H_8O_2$: h147, m310, n3 $C_{11}H_8O_3$: h148, h149 $C_{11}H_9Br$: b309 $C_{11}H_9Cl$: c157 $C_{11}H_9N$: p148 $C_{11}H_{10}$: m308, m309 $C_{11}H_{10}N_2S$: n19 $C_{11}H_{10}O$: m76, m77 $C_{11}H_{11}N$: n6 $C_{11}H_{12}N_2O$: a309 $C_{11}H_{12}N_2O_2$: t436 $C_{11}H_{12}O_2$: d358, e103, m104		

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

$C_{11}H_{12}O_3$: e70 $C_{11}H_{13}ClO$: b428 $C_{11}H_{13}ClO_3$: c250 $C_{11}H_{13}NO$: b119 $C_{11}H_{13}NO_2$: t183 $C_{11}H_{13}NO_3$: a302, a303 $C_{11}H_{13}N_3O$: a113 $C_{11}H_{13}N_3O_3S$: d567 $C_{11}H_{14}O$: m103, p43 $C_{11}H_{14}O_2$: b426, b427, d455, e46 $C_{11}H_{14}O_3$: b409, b468, b476, e167 $C_{11}H_{14}O_4$: e155 $C_{11}H_{14}O_4Si$: d24 $C_{11}H_{15}NO$: d269 $C_{11}H_{15}NO_2$: d276, d466, e122 $C_{11}H_{16}$: b482, p24, p54 $C_{11}H_{16}N_2$: b114 $C_{11}H_{16}O$: b86, b461, b462, p56 $C_{11}H_{16}O_2$: a68 $C_{11}H_{16}O_3$: m299 $C_{11}H_{16}O_4$: d714 $C_{11}H_{17}N$: b429, e160 $C_{11}H_{17}NO$: e225 $C_{11}H_{17}NO_2$: b104 $C_{11}H_{17}O_3P$: b93 $C_{11}H_{18}O$: d308, n105, p4 $C_{11}H_{18}O_5$: d264 $C_{11}H_{19}ClO$: u11 $C_{11}H_{19}N$: a209 $C_{11}H_{20}O$: p55, u7 $C_{11}H_{20}O_2$: u9 $C_{11}H_{20}O_4$: d119, d287, d309 $C_{11}H_{21}BrO_2$: b367 $C_{11}H_{22}$: u8 $C_{11}H_{22}N_2$: d695 $C_{11}H_{22}O$: u1, u5, u6, u10 $C_{11}H_{22}O_2$: m218, u3 $C_{11}H_{22}O_4Si$: e7 $C_{11}H_{23}NO_2$: a297 $C_{11}H_{24}$: u2 $C_{11}H_{24}O$: d310, u4 $C_{11}H_{24}O_3Si$: t311	$C_{11}H_{24}O_4$: t410 $C_{11}H_{24}O_6$: p46 $C_{11}H_{24}O_6Si$: t430 $C_{11}H_{26}N_2$: d129 $C_{11}H_{26}N_2O_6$: b214 <hr/> C_{12} <hr/> $C_{12}Br_{10}O$: b197 $C_{12}H_4Cl_6S_2$: b203 $C_{12}H_5ClO_3$: c170 $C_{12}H_6Br_4O_4S$: s25 $C_{12}H_6O_3$: n7 $C_{12}H_6O_{12}$: b19 $C_{12}H_7NO_2$: n8 $C_{12}H_8$: a3 $C_{12}H_8Br_2$: d66 $C_{12}H_8Cl_2OS$: b166 $C_{12}H_8Cl_2O_2S$: b165 $C_{12}H_8N_2$: p63 $C_{12}H_8N_2O_2$: a235 $C_{12}H_8N_2O_4S_2$: b194, b195 $C_{12}H_8O$: d50 $C_{12}H_8O_6$: b132 $C_{12}H_8S$: d52 $C_{12}H_9Br$: b237 $C_{12}H_9BrO$: b330 $C_{12}H_9ClO_2S$: c207 $C_{12}H_9N$: c8, d665, n16 $C_{12}H_9NO$: b74, b75, b76 $C_{12}H_9NO_2$: n48, n49 $C_{12}H_9NO_3$: n70, n71 $C_{12}H_9NS$: p66 $C_{12}H_{10}$: a2, b134 $C_{12}H_{10}ClN$: c61, c62 $C_{12}H_{10}ClO_3P$: d662 $C_{12}H_{10}ClP$: c99 $C_{12}H_{10}Cl_2Si$: d175 $C_{12}H_{10}Hg$: d675 $C_{12}H_{10}N_2$: a322 $C_{12}H_{10}N_2O$: n80, p89 $C_{12}H_{10}N_2O_2$: n52 $C_{12}H_{10}N_2O_2S$: a243 $C_{12}H_{10}N_3O_3P$: d682	$C_{12}H_{10}O$: d667, m311, m312, p131, p132 $C_{12}H_{10}OS$: d690 $C_{12}H_{10}O_2$: d387, h88, n14, n15 $C_{12}H_{10}O_2S$: d689, t150 $C_{12}H_{10}O_3$: n12 $C_{12}H_{10}O_3S$: b139 $C_{12}H_{10}O_4$: q1 $C_{12}H_{10}O_4S$: s27, t145 $C_{12}H_{10}S$: d688 $C_{12}H_{10}S_2$: d664 $C_{12}H_{10}Se_2$: d663 $C_{12}H_{11}ClNO_2P$: p134 $C_{12}H_{11}N$: a134, a135, b117, b118, d655 $C_{12}H_{11}NO$: n13, p70 $C_{12}H_{11}N_3$: p87 $C_{12}H_{11}O_3P$: d681 $C_{12}H_{12}$: d554, d555 $C_{12}H_{12}N_2$: b136, d673, p131 $C_{12}H_{12}N_2O$: o62 $C_{12}H_{12}N_2O_2$: b40 $C_{12}H_{12}N_2O_2S$: d36, d37 $C_{12}H_{12}N_4$: d31 $C_{12}H_{12}O$: e44 $C_{12}H_{12}O_2Si$: d687 $C_{12}H_{12}O_3$: t196 $C_{12}H_{12}O_6$: t193, t336 $C_{12}H_{13}N_3$: d34 $C_{12}H_{14}N_2O_3S$: a167 $C_{12}H_{14}N_4O_2S$: s21 $C_{12}H_{14}O_3$: e176 $C_{12}H_{14}O_4$: d329 $C_{12}H_{15}N$: d369 $C_{12}H_{15}NO$: b116 $C_{12}H_{15}N_3O_3$: t197 $C_{12}H_{16}$: c338, m212, p104 $C_{12}H_{16}O_2$: m364 $C_{12}H_{16}O_3$: d246 $C_{12}H_{17}N$: b115, c337 $C_{12}H_{17}NO$: d319, d342 $C_{12}H_{18}$: b489, c304, d414, d415, h47, p117, t435 $C_{12}H_{18}Cl_2N_4OS$: t139
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table I.15*

$C_{12}H_{18}O$: d419, d513 $C_{12}H_{18}O_2$: b474, b475 $C_{12}H_{18}O_4$: b445 $C_{12}H_{19}N$: d413, h81 $C_{12}H_{20}O_2$: b185, b217, e102, L10 $C_{12}H_{20}O_3Si$: p157 $C_{12}H_{20}O_4$: d118 $C_{12}H_{20}O_4Si$: t8 $C_{12}H_{21}N$: t431 $C_{12}H_{21}N_3$: t422 $C_{12}H_{22}$: c305, d241 $C_{12}H_{22}O$: c303, e4 $C_{12}H_{22}O_3$: h67 $C_{12}H_{22}O_4$: d130, d324, d512, d702, d721 $C_{12}H_{22}O_{11}$: L3, m7, s20 $C_{12}H_{23}ClO$: d728 $C_{12}H_{23}N$: d242, d724 $C_{12}H_{23}NO$: a318 $C_{12}H_{24}$: d729 $C_{12}H_{24}N_2$: d694 $C_{12}H_{24}O$: c302, d731, m443, t349 $C_{12}H_{24}O_2$: d726, e113 $C_{12}H_{24}O_6$: h74 $C_{12}H_{25}Br$: b275 $C_{12}H_{25}Cl$: c100 $C_{12}H_{25}Cl_3Si$: d736 $C_{12}H_{26}$: d719 $C_{12}H_{26}O$: d350, d727, t354a $C_{12}H_{26}O_2$: d722, d723 $C_{12}H_{26}O_3$: b151 $C_{12}H_{26}O_4$: t411 $C_{12}H_{26}O_4S$: d735 $C_{12}H_{26}S$: d725 $C_{12}H_{27}Al$: t307 $C_{12}H_{27}BO_3$: t209 $C_{12}H_{27}ClSn$: t215 $C_{12}H_{27}N$: d349, d732, t210 $C_{12}H_{27}O_3P$: t214 $C_{12}H_{27}O_4P$: t212 $C_{12}H_{27}P$: t213 $C_{12}H_{28}BrN$: t135 $C_{12}H_{28}N_2$: d720	$C_{12}H_{28}O_4Si$: t88, t134 $C_{12}H_{28}O_4Ti$: t166 $C_{12}H_{28}O_8Si$: t89 $C_{12}H_{36}O_4Si_4Ti$: t90
C_{13}	
$C_{13}H_5N_3O_7$: t384 $C_{13}H_8ClNO_3$: c181 $C_{13}H_8ClNOS$: p67 $C_{13}H_8Cl_2O$: d159 $C_{13}H_8N_2O_7$: b193 $C_{13}H_8O$: f3 $C_{13}H_8OS$: t165 $C_{13}H_8O_2$: x3 $C_{13}H_9BrO$: b232 $C_{13}H_9ClO$: c49, c50 $C_{13}H_9ClO_2$: c131 $C_{13}H_9N$: a61 $C_{13}H_{10}$: f2 $C_{13}H_{10}ClNO$: a142, a143, d659 $C_{13}H_{10}Cl_2O_2$: m233 $C_{13}H_{10}N_2$: p90 $C_{13}H_{10}N_2O_3$: a239 $C_{13}H_{10}O$: b53, x1 $C_{13}H_{10}O_2$: b135, h102, p91 $C_{13}H_{10}O_3$: d386, d661, p150 $C_{13}H_{10}O_5$: t83 $C_{13}H_{11}Br$: b274 $C_{13}H_{11}Cl$: c97 $C_{13}H_{11}ClO$: c44 $C_{13}H_{11}NO$: a127, b5 $C_{13}H_{11}NO_2$: h161, p85 $C_{13}H_{11}NO_3$: p86 $C_{13}H_{12}$: d676 $C_{13}H_{12}N_2$: b54, d38, d670 $C_{13}H_{12}N_2O$: d693 $C_{13}H_{12}N_2S$: d692, t146 $C_{13}H_{12}N_4O$: p88 $C_{13}H_{12}N_4S$: d691 $C_{13}H_{12}O$: b138, d677, h113, m56, p76 $C_{13}H_{12}S$: b113	$C_{13}H_{13}ClSi$: c98 $C_{13}H_{13}N$: d678, m230, m93 $C_{13}H_{13}NO$: b106 $C_{13}H_{13}N_3$: d671 $C_{13}H_{14}N_2$: d35, m238, t344 $C_{13}H_{14}N_2O_3$: a59 $C_{13}H_{14}N_4O$: d660 $C_{13}H_{14}Si$: m231 $C_{13}H_{16}O_2$: m74 $C_{13}H_{16}O_3$: e71 $C_{13}H_{16}O_4$: d328 $C_{13}H_{17}NO_2$: e74 $C_{13}H_{20}$: p116 $C_{13}H_{20}N_2O_2$: d271 $C_{13}H_{20}O$: i56, i57 $C_{13}H_{22}ClN$: b125 $C_{13}H_{22}N_2$: d243 $C_{13}H_{22}O_2$: n106 $C_{13}H_{22}O_3Si$: b124 $C_{13}H_{26}$: t258 $C_{13}H_{26}N_2$: m236, t343 $C_{13}H_{26}O_2$: e229, t257 $C_{13}H_{27}Br$: b359 $C_{13}H_{28}$: t256 $C_{13}H_{28}O_4$: t409 $C_{13}H_{29}NO_4$: b169
C_{14}	
$C_{14}H_6Cl_2O_2$: d148, d149 $C_{14}H_7ClO_2$: c36, c37 $C_{14}H_8ClNO_3$: c185 $C_{14}H_8O_2$: a305, p62 $C_{14}H_8O_3$: h93 $C_{14}H_8O_4$: d371, d372, d373, d374 $C_{14}H_8O_5S$: a308 $C_{14}H_8O_8$: a306, d312 $C_{14}H_9Br$: b324 $C_{14}H_9ClO_3$: c54 $C_{14}H_9Cl_5$: b167 $C_{14}H_9NO_2$: a111, a112 $C_{14}H_9NO_3$: a186	

TABLE 1.14 Empirical Formula Index for Organic Compounds (continued)

The alphanumeric designations are keyed to Table 1.15

C ₁₄ H ₁₀ : a304, d654, p61 C ₁₄ H ₁₀ Br ₂ O: b273 C ₁₄ H ₁₀ ClNO ₃ : a147 C ₁₄ H ₁₀ Cl ₂ O ₄ : b162 C ₁₄ H ₁₀ Cl ₄ : b163 C ₁₄ H ₁₀ N ₂ O ₂ : d28, d29, d30 C ₁₄ H ₁₀ O ₂ : b34 C ₁₄ H ₁₀ O ₃ : b45, b65, x2 C ₁₄ H ₁₀ O ₄ : b137, d54, t82 C ₁₄ H ₁₁ N: d653, p120 C ₁₄ H ₁₁ NOS: a50 C ₁₄ H ₁₂ : d351, s9 C ₁₄ H ₁₂ Cl ₂ O: b164 C ₁₄ H ₁₂ N ₂ O: b37 C ₁₄ H ₁₂ N ₂ O ₂ : b35 C ₁₄ H ₁₂ O: a34, d22, m133, m134 C ₁₄ H ₁₂ O ₂ : b46, b83, b84, b107, b108, d652 C ₁₄ H ₁₂ O ₃ : b36, h35 C ₁₄ H ₁₃ ClO: c147 C ₁₄ H ₁₃ N: e93, i12 C ₁₄ H ₁₃ NO: b82 C ₁₄ H ₁₃ NO ₂ : b50 C ₁₄ H ₁₄ : d666 C ₁₄ H ₁₄ N ₂ : a168 C ₁₄ H ₁₄ N ₂ O ₃ : a325 C ₁₄ H ₁₄ O: d58 C ₁₄ H ₁₄ OS: b200 C ₁₄ H ₁₄ O ₂ : b109 C ₁₄ H ₁₄ S ₂ : b199, d57 C ₁₄ H ₁₅ N: d56, d668 C ₁₄ H ₁₅ O ₃ P: d61 C ₁₄ H ₁₆ N ₂ : d669 C ₁₄ H ₁₆ O ₂ Si: d437 C ₁₄ H ₁₆ O ₄ : d281 C ₁₄ H ₁₈ O ₄ : d285 C ₁₄ H ₂₀ N ₂ O ₆ S: m120 C ₁₄ H ₂₀ O ₅ : b39 C ₁₄ H ₂₂ : p130a C ₁₄ H ₂₂ O: d123, d124, d125, d126 C ₁₄ H ₂₂ O ₂ : d112 C ₁₄ H ₂₃ N: d109, o42 C ₁₄ H ₂₃ N ₃ O ₁₀ : d299 C ₁₄ H ₂₆ O ₃ : h11 C ₁₄ H ₂₆ O ₄ : d408	C ₁₄ H ₂₇ ClO: t41 C ₁₄ H ₂₈ : t42, t43 C ₁₄ H ₂₈ O ₂ : t39 C ₁₄ H ₂₉ Br: b352 C ₁₄ H ₂₉ Cl ₃ Si: t46 C ₁₄ H ₃₀ : t38 C ₁₄ H ₃₀ O: t40 C ₁₄ H ₃₁ N: t44 C ₁₄ H ₃₂ N ₂ O ₄ : t87 <div>C₁₅</div> C ₁₅ H ₁₀ O ₂ : b101, m124 C ₁₅ H ₁₁ NO: d679 C ₁₅ H ₁₂ N ₂ O ₂ : d672 C ₁₅ H ₁₂ O: d354, d685 C ₁₅ H ₁₂ O ₂ : d53 C ₁₅ H ₁₃ NO: a13 C ₁₅ H ₁₄ O: d684 C ₁₅ H ₁₄ O ₂ : b49, b141, d686 C ₁₅ H ₁₄ O ₃ : b111 C ₁₅ H ₁₆ O: m359 C ₁₅ H ₁₆ O ₂ : i97 C ₁₅ H ₁₇ N ₃ : d711 C ₁₅ H ₁₈ OSi: e42 C ₁₅ H ₂₂ O ₃ : d117 C ₁₅ H ₂₄ : t312 C ₁₅ H ₂₄ O: d120 C ₁₅ H ₂₆ O: h184 C ₁₅ H ₂₆ O ₆ : g19 C ₁₅ H ₃₀ N ₂ : t342 C ₁₅ H ₃₀ N ₃ OP: t405 C ₁₅ H ₃₀ O: p14 C ₁₅ H ₃₀ O ₂ : m413 C ₁₅ H ₃₂ : p13 C ₁₅ H ₃₂ O ₃ Si ₄ : p164 C ₁₅ H ₃₂ O ₁₀ : t389 <div>C₁₆</div> C ₁₆ H ₁₀ : b52, fl, p246 C ₁₆ H ₁₁ NO ₂ : p149 C ₁₆ H ₁₂ N ₂ O ₅ S: a60 C ₁₆ H ₁₂ N ₄ O ₉ S ₂ : t3	C ₁₆ H ₁₃ N: p130 C ₁₆ H ₁₄ : d656, d657, e66 C ₁₆ H ₁₄ O: d658 C ₁₆ H ₁₄ O ₆ S: s26 C ₁₆ H ₁₅ NO ₄ : d445 C ₁₆ H ₁₆ O ₂ : b47, b112 C ₁₆ H ₁₆ O ₃ : d449 C ₁₆ H ₁₈ ClN ₃ S: m237 C ₁₆ H ₁₉ ClSi: b435 C ₁₆ H ₂₀ N ₂ : d59 C ₁₆ H ₂₀ O ₂ Si: d250 C ₁₆ H ₂₂ O ₄ : d128, d409 C ₁₆ H ₂₂ O ₁₁ : g7 C ₁₆ H ₂₆ O ₃ : d730 C ₁₆ H ₂₆ O ₇ : t52 C ₁₆ H ₃₂ : h37 C ₁₆ H ₃₂ O ₂ : h35 C ₁₆ H ₃₄ Br: b293 C ₁₆ H ₃₃ I: i38 C ₁₆ H ₃₃ NO: d297 C ₁₆ H ₃₄ : h4, h32 C ₁₆ H ₃₄ O: h36 C ₁₆ H ₃₄ O ₂ : h33 C ₁₆ H ₃₄ S: d644, h34 C ₁₆ H ₃₅ N: d643, h38 C ₁₆ H ₃₅ O ₄ P: b178 C ₁₆ H ₃₆ BF ₄ N: t19 C ₁₆ H ₃₆ BrN: t14 C ₁₆ H ₃₆ ClN: t15 C ₁₆ H ₃₆ FN: t16 C ₁₆ H ₃₆ IN: t18 C ₁₆ H ₃₆ O ₄ Si: t13 C ₁₆ H ₃₆ Sn: t20 C ₁₆ H ₃₇ NO ₄ S: t17 <div>C₁₇</div> C ₁₇ H ₆ O ₇ : b55 C ₁₇ H ₁₀ O: b8 C ₁₇ H ₁₂ O ₃ : p119 C ₁₇ H ₁₃ N ₃ O ₅ S ₂ : p172 C ₁₇ H ₁₆ O ₄ : d60 C ₁₇ H ₁₈ O ₃ : b478 C ₁₇ H ₂₀ N ₂ O: b171 C ₁₇ H ₂₀ N ₄ O ₆ : r4
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TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table I.15*

$C_{17}H_{21}NO_4$: c275 $C_{17}H_{22}N_2$: m234 $C_{17}H_{23}NO_3$: a315 $C_{17}H_{34}O_2$: m263 $C_{17}H_{36}$: h1 $C_{17}H_{37}N$: m229	$C_{18}H_{38}S$: o4 $C_{18}H_{39}ClSi$: t302 $C_{18}H_{39}N$: o13, t301 $C_{18}H_{39}O_7P$: t414 $C_{18}H_{40}Si$: t303	$C_{20}H_{40}O$: o16 $C_{20}H_{42}$: i2
C_{18}	C_{19}	C_{21}
$C_{18}H_9Cl_6O_4P$: t418 $C_{18}H_{10}O_6$: h85 $C_{18}H_{12}$: b6, b7, t396 $C_{18}H_{12}N_5O_6$: d683 $C_{18}H_{14}$: t4 $C_{18}H_{14}O$: d680 $C_{18}H_{14}O_8$: d55 $C_{18}H_{15}As$: t394 $C_{18}H_{15}N$: t392 $C_{18}H_{15}N_3Si$: a320 $C_{18}H_{15}O_3P$: t403 $C_{18}H_{15}O_4P$: t399 $C_{18}H_{15}P$: t400 $C_{18}H_{15}PS$: t402 $C_{18}H_{15}PSe$: t401 $C_{18}H_{15}Sb$: t393 $C_{18}H_{16}O_2$: b422 $C_{18}H_{16}Si$: t404 $C_{18}H_{18}O_3$: e73 $C_{18}H_{20}O_2$: b48 $C_{18}H_{25}NO_3$: i61 $C_{18}H_{30}O$: t211 $C_{18}H_{30}O_2$: o7 $C_{18}H_{31}N$: d733 $C_{18}H_{32}O_2$: o1 $C_{18}H_{32}O_{16}$: r1 $C_{18}H_{34}O_2$: o10, o11 $C_{18}H_{34}O_4$: d110 $C_{18}H_{36}$: d734, o8 $C_{18}H_{36}O$: o12 $C_{18}H_{36}O_2$: e139, o5 $C_{18}H_{37}Br$: b319 $C_{18}H_{37}Cl_3Si$: o15 $C_{18}H_{37}N$: o9 $C_{18}H_{37}NO$: o2 $C_{18}H_{38}$: o3 $C_{18}H_{38}O$: o6	$C_{19}H_{15}Br$: b366 $C_{19}H_{15}Cl$: c256 $C_{19}H_{16}$: t397 $C_{19}H_{16}O$: t398 $C_{19}H_{18}BrP$: m442 $C_{19}H_{20}Br_4O_4$: i96 $C_{19}H_{20}O_4$: b87 $C_{19}H_{22}N_2O$: c264 $C_{19}H_{30}O_5$: m243 $C_{19}H_{32}$: p156 $C_{19}H_{34}ClN$: b122 $C_{19}H_{34}O_2$: m325 $C_{19}H_{36}O_2$: m327 $C_{19}H_{37}NO$: o14 $C_{19}H_{38}O_2$: m326 $C_{19}H_{40}$: n90, t115 $C_{19}H_{40}Cl_2Si$: m328	$C_{21}H_{15}NO$: b142 $C_{21}H_{15}N_3O_3$: t390 $C_{21}H_{21}N$: t200 $C_{21}H_{22}N_2O_2$: s10 $C_{21}H_{24}O_2$: b144 $C_{21}H_{28}N_2O$: b170 $C_{21}H_{36}O$: p15 $C_{21}H_{39}N_3$: t255
	C_{20}	C_{22}
	$C_{20}H_{10}Br_2O_5$: d83 $C_{20}H_{12}$: b57, b58, d49 $C_{20}H_{12}O_5$: f4 $C_{20}H_{14}O_4$: p65 $C_{20}H_{15}Br$: b365 $C_{20}H_{18}O_3Si$: t391 $C_{20}H_{19}N_3$: b2 $C_{20}H_{22}O_6$: t271 $C_{20}H_{24}N_2O_2$: q2 $C_{20}H_{24}O_6$: d51 $C_{20}H_{28}O_2P$: d674 $C_{20}H_{30}O_2$: a1 $C_{20}H_{31}N$: d20 $C_{20}H_{35}N$: t45 $C_{20}H_{36}O_2$: e188 $C_{20}H_{38}O_2$: e189 $C_{20}H_{40}$: i3	$C_{22}H_{23}N_3O_9$: a316 $C_{22}H_{30}O_2S$: t144 $C_{22}H_{34}O_4$: b443 $C_{22}H_{39}N$: h39 $C_{22}H_{42}O_4$: d312 $C_{22}H_{44}O_2$: b466, d716 $C_{22}H_{46}$: d715 $C_{22}H_{46}O$: d717
		C_{23}
		$C_{23}H_{16}O_6$: m235 $C_{23}H_{26}N_2O_4$: b372
		C_{24}
		$C_{24}H_{16}N_2O_2$: b198 $C_{24}H_{18}$: t395 $C_{24}H_{20}BNa$: t128 $C_{24}H_{20}O_4Si$: t127 $C_{24}H_{20}Si$: t132 $C_{24}H_{20}Sn$: t133 $C_{24}H_{22}N_2O$: b140 $C_{24}H_{38}O_4$: b179, d313 $C_{24}H_{40}O_5$: c263 $C_{24}H_{46}O_4$: d643a $C_{24}H_{50}$: t36 $C_{24}H_{51}N$: t387

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)*The alphanumeric designations are keyed to Table 1.15*

$C_{24}H_{51}O_3P$: d423, t421 $C_{24}H_{52}O_4Si$: t85 $C_{24}H_{54}OSn_2$: b201	$C_{27}H_{46}O$: c262 $C_{27}H_{50}ClN$: b94	$C_{32}H_{68}O_4Si$: t86 $C_{36}H_{75}O_3P$: d642 $C_{38}H_{30}NiO_2P_2$: b213 $C_{39}H_{74}O_6$: g20 $C_{40}H_{56}$: c19 $C_{40}H_{82}O_6P_2$: b196
C_{26}	C_{28}	
$C_{26}H_{20}$: t131 $C_{26}H_{26}N_2O_2S$: b152 $C_{26}H_{26}OSi_3$: t130 $C_{26}H_{50}O_4$: b177, d311	$C_{28}H_{22}$: t129 $C_{28}H_{31}ClN_2O_3$: r2 $C_{28}H_{32}O_2Si_3$: t121	C_{45} to C_{57}
C_{27}	C_{30} to C_{40}	$C_{45}H_{86}O_6$: g24 $C_{48}H_{40}O_4Si_4$: o38 $C_{51}H_{98}O_6$: g23 $C_{57}H_{104}O_6$: g22
$C_{27}H_{19}NO$: b148 $C_{27}H_{42}ClNO_2$: b33	$C_{30}H_{50}$: s8 $C_{30}H_{62}$: s7 $C_{30}H_{63}O_3P$: t308 $C_{32}H_{66}$: d737	

TABLE 1.15 Physical Constants of Organic Compounds*See also the special tables of fats, oils, and waxes.*

Names of the compounds in the table starting on p. 1.82 are arranged alphabetically. Usually substitutive nomenclature is employed; exceptions generally involve ethers, sulfides, sulfones, and sulfoxides. Each compound is given a number within its letter classification; thus compound c195 is 3-chlorophenol. The section "Nomenclature of Organic Compounds" should be consulted to familiarize oneself with present nomenclature systems.

Synonyms or *Alternate Names* are found at the bottom of each spread in their alphabetical listing; the number following the name refers to the numerical place of this compound in the table. For example, epichlorohydrin, c101, indicates that this compound is found listed under the name 1-chloro-2,3-epoxypropane.

Formulas are presented in a semistructural form when no ambiguity is possible. Complicated systems are drawn in complete structural form and located at the bottom of each page and keyed to the number of the entry.

Beilstein Reference. In the column so headed is found the reference to the volume and page numbers of the fourth edition of Beilstein: (Handbuch der Organischen Chemie) (Springer-Verlag, New York). Thus the entry 9, 202 refers to an entry in volume 9 appearing on page 202. When the volume number has a superscript attached, reference is made to the appropriate supplementary volume. For example, 12², 404 indicates that the compound will be found listed in the second supplement to volume 12 on page 404. The earliest Beilstein entry is listed. Supplementary information may be found in the supplements to the basic series; such coordinating references (series number, volume number, and page number of the main edition) along with the system number are found at the top of each *odd-numbered* page. Similarly, a back reference such as H 93; E II 64; E III 190 in a volume of Supplementary Series IV means that previous items on

TABLE 1.14 Empirical Formula Index for Organic Compounds (*continued*)

The alphanumeric designations are keyed to Table 1.15

$C_{24}H_{51}O_3P$: d423, t421 $C_{24}H_{52}O_4Si$: t85 $C_{24}H_{54}OSn_2$: b201	$C_{27}H_{46}O$: c262 $C_{27}H_{50}ClN$: b94	$C_{32}H_{68}O_4Si$: t86 $C_{36}H_{75}O_3P$: d642 $C_{38}H_{30}NiO_2P_2$: b213 $C_{39}H_{74}O_6$: g20 $C_{40}H_{56}$: c19 $C_{40}H_{82}O_6P_2$: b196
C_{26}	C_{28}	C_{45} to C_{57}
$C_{26}H_{20}$: t131 $C_{26}H_{26}N_2O_2S$: b152 $C_{26}H_{26}OSi_3$: t130 $C_{26}H_{50}O_4$: b177, d311	$C_{28}H_{22}$: t129 $C_{28}H_{31}ClN_2O_3$: r2 $C_{28}H_{32}O_2Si_3$: t121	$C_{45}H_{86}O_6$: g24 $C_{48}H_{40}O_4Si_4$: o38 $C_{51}H_{98}O_6$: g23 $C_{57}H_{104}O_6$: g22
C_{27}	C_{30} to C_{40}	
$C_{27}H_{19}NO$: b148 $C_{27}H_{42}ClNO_2$: b33	$C_{30}H_{50}$: s8 $C_{30}H_{62}$: s7 $C_{30}H_{63}O_3P$: t308 $C_{32}H_{66}$: d737	

TABLE 1.15 Physical Constants of Organic Compounds

See also the special tables of fats, oils, and waxes.

Names of the compounds in the table starting on p. 1.82 are arranged alphabetically. Usually substitutive nomenclature is employed; exceptions generally involve ethers, sulfides, sulfones, and sulfoxides. Each compound is given a number within its letter classification; thus compound c195 is 3-chlorophenol. The section "Nomenclature of Organic Compounds" should be consulted to familiarize oneself with present nomenclature systems.

Synonyms or *Alternate Names* are found at the bottom of each spread in their alphabetical listing; the number following the name refers to the numerical place of this compound in the table. For example, epichlorohydrin, c101, indicates that this compound is found listed under the name 1-chloro-2,3-epoxypropane.

Formulas are presented in a semistructural form when no ambiguity is possible. Complicated systems are drawn in complete structural form and located at the bottom of each page and keyed to the number of the entry.

Beilstein Reference. In the column so headed is found the reference to the volume and page numbers of the fourth edition of Beilstein: (Handbuch der Organischen Chemie) (Springer-Verlag, New York). Thus the entry 9, 202 refers to an entry in volume 9 appearing on page 202. When the volume number has a superscript attached, reference is made to the appropriate supplementary volume. For example, 12², 404 indicates that the compound will be found listed in the second supplement to volume 12 on page 404. The earliest Beilstein entry is listed. Supplementary information may be found in the supplements to the basic series; such coordinating references (series number, volume number, and page number of the main edition) along with the system number are found at the top of each *odd-numbered* page. Similarly, a back reference such as H 93; E II 64; E III 190 in a volume of Supplementary Series IV means that previous items on

this compound are found in the same volume of the Basic Series on page 93, of Supplementary Series II on page 64, and of Supplementary Series III on page 190. The absence of a back reference implies that the compound involved is described *for the first time* in the series concerned.

Formula Weights are based on the International Atomic Weights of 1973 and are computed to the nearest hundredth.

Density values are given at room temperature unless otherwise indicated by the superscript figure; thus 0.9711¹¹² indicates a density of 0.9711 for the substance at 112°C. A density of 0.899₄¹⁶ indicates a density of 0.899 for the substance at 16°C relative to water at 4°C.

Refractive Index, unless otherwise specified, is given for the sodium line at 589.6 nm. The temperature at which the measurement was made is indicated by the superscript figure; otherwise it is assumed to be room temperature.

Melting Point is recorded in certain cases as 250 d and in some other cases as d 250, the distinction being made in this manner to indicate that the former is a melting point with decomposition at 250°C, while the latter decomposition occurs only at 250°C and higher temperatures. Where a value such as -2H₂O, 120 is given, it indicates a loss of 2 mol of water per formula weight of the compound at a temperature of 120°C.

Boiling Point is given at atmospheric pressure (760 mmHg) unless otherwise indicated; thus 82¹⁵mm indicates that the boiling point is 82°C when the pressure is 15 mmHg. Also, subl 550 indicates that the compound sublimes at 550°C.

Flash Point is given in degrees Celsius, usually closed up. Because values will vary with the specific procedure employed, and sometimes the method was not stated, the values listed for the flash point should be considered only as indicative. See also Table 4.13, Properties of Combustible Mixtures in Air.

Solubility is given in parts by weight (of the formula weight) per 100 parts by weight of the solvent and at room temperature. Other temperatures are indicated by the superscript. In the case of gases, the solubility is often expressed as 5¹⁰ mL, which indicates that at 10°C, 5 mL of the gas is soluble in 100 g of the solvent.

Abbreviations Used in the Table

abs, absolute	EtOH, ethanol, 95%	s, soluble
acet, acetone	expl, explodes	sec, secondary
alc, ethanol	glyc, glycerol	sl, slight or slightly
alk, alkali (i.e., aqueous NaOH or KOH)	h, hot	soln, solution
anhyd, anhydrous	HOAc, acetic acid	solv, solvent
aq, aqueous; water	hyd, hydrolysis	subl, sublimes
as, asymmetrical	hygr, hygroscopic	s, symmetrical
atm, atmosphere	i, insoluble	sym, symmetrical
BuOH, butanol	ign, ignites	tert, tertiary
bz, benzene	i-PrOH, isopropanol	v, very
c, cold	l (-), levorotatory	v s, very soluble
chl, chloroform, CHCl ₃	L, designates configuration	v sl s, very slightly soluble
conc, concentrated	m, meta position	vac, vacuo or vacuum
d, decomposes or decomposed	Me, methyl	vols, volumes
d (+), dextrorotatory	MeEtKe, methyl ethyl ketone	>, greater than
-d ₂ , deuterium substitution	MeOH, methanol	<, less than
D, designates configuration	misc, miscible; soluble in all proportions	~, approximately
deliq, deliquescent	NaOH, aqueous sodium hydroxide	α, alpha position
dil, dilute	o, ortho position	β, beta position
diox, dioxane	org, organic	γ, gamma position
DL (or dl), inactive (i.e., 50% D and 50% L)	p, para position	δ, delta position
DMF, dimethylformamide	PE, petroleum ether	ε, epsilon position
EtAc, ethyl acetate	pyr, pyridine	ω, omega position (farthest from parent functional group)
eth, diethyl ether		

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a1	(-)-Abietic acid		302.44	9 ² , 424	—		172–175			i aq; s alc, bz, chl, eth, acet, dil alk
a2	Acenaphthene		154.21	5, 586	1.069 ⁹⁵ ₉₅		93.45	279		i aq; 3.2 alc; 20 bz
a3	Acenaphthylene		152.20	5, 625	0.899 ¹⁶ ₄		80–83	280		i aq; v s alc, eth
a4	Acetaldehyde	CH ₃ CHO	44.05	1, 594	0.8053 ⁰ ₄	1.3311 ²⁰	–123.5	20.2	–27	misc aq, alc
a5	Acetaldoxime	CH ₃ CH=NOH	59.07	1, 608	0.966	1.415 ²⁰	46.5	114.5	38	v s aq, alc; eth
a6	Acetamide	CH ₃ CONH ₂	59.07	2 ² , 177	0.9711 ¹¹²	1.4158 ¹¹⁰	80.1	221.15		70 aq; 50 alc; s chl, hot bz
a7	Acetamidine HCl	CH ₃ (=NH)NH ₂ ·HCl	94.54	2, 185			170–172			v s aq, alc; i acet, eth
a8	<i>N</i> -(2-Acetamido)-2-aminoethane-sulfonic acid	H ₂ N(CO)CH ₂ NHCH ₂ -CH ₂ SO ₃ H	182.20				> 220 d			
a9	4-Acetamidobenzaldehyde	CH ₃ CONHC ₆ H ₄ CHO	163.18	14, 38			154–156			s aq, bz; sl s alc
a10	4-Acetamidobenzene-sulfonyl chloride	CH ₃ CONHC ₆ H ₄ SO ₂ Cl	233.67	14, 439			149			d aq; v s alc, eth
a11	2-Acetamidobenzoic acid	CH ₃ CONHC ₆ H ₄ COOH	179.18	14, 337			185–187			sl s aq; v s alc, bz, eth, acet
a12	4-Acetamidobenzoic acid	CH ₃ CONHC ₆ H ₄ COOH	179.18	14, 432			260–262			i aq; s alc; sl s eth
a13	2-Acetamidofluorene		223.28	12, 1331			194			i aq; s alc, glycols
a14	<i>N</i> -(2-Acetamido)-iminodiacetic acid	H ₂ NCOCH ₂ N(CH ₂ COOH) ₂	190.16				219 d			
a15	2-Acetamidophenol	CH ₃ CONHC ₆ H ₄ OH	151.17	13, 370			207–209			
a16	3-Acetamidophenol	CH ₃ CONHC ₆ H ₄ OH	151.17	13, 415			146–149			
a17	4-Acetamidophenol	CH ₃ CONHC ₆ H ₄ OH	151.17	13, 460	1.293 ²¹ ₄		170			s alc, acet

a18	Acetanilide	$\text{CH}_3\text{CONHC}_6\text{H}_5$	135.17	12, 237	1.219 ₄ ¹⁵		114.2	304	173	0.56 aq ²⁵ ; 29 alc; 2bz; 27 chl; 25 acet; 5 eth
a19	Acetic acid	CH_3COOH	60.65	2, 96	1.0492 ₄ ²⁰	1.3716 ²⁰	16.63	117.90	40	misc aq, alc, eth, CCl_4
a20	Acetic acid- <i>d</i>	CH_3COOD	61.05		1.07	1.3715 ²⁰		115.5	40	misc aq, alc, eth, CCl_4
a21	Acetic- <i>d</i> ₃ , acid- <i>d</i>	CD_3COOD	64.08		1.11	1.3709 ²⁰		115.5	40	misc aq, alc, eth
a22	Acetic anhydride	$(\text{CH}_3\text{CO})_2\text{O}$	102.09	2, 166	1.082 ₄ ¹⁵	1.3904 ²⁰	-73.1	140.0	130	13 aq; s chl, eth
a23	Acetic anhydride- <i>d</i> ₆	$(\text{CD}_3\text{CO})_2\text{O}$	108.14			1.3875 ²⁰		65 ^{65mm}	54	d aq, alc
a24	Acetoacetic acid	$\text{CH}_3\text{COCH}_2\text{COOH}$	102.09	3, 630			36-37	d violently 100		misc aq, alc, eth
a25	Acetohydrazide	$\text{CH}_3\text{CONHNH}_2$	74.08	2, 191				129 ^{18mm}		
a26	Acetone	CH_3COCH_3	58.08	1, 635	0.7908 ₄ ²⁰	1.3588 ²⁰	-95.35	56.24	-20	misc aq, alc, chl,
a27	Acetone- <i>d</i> ⁶	CD_3COCD_3	64.13		0.88	1.3554 ²⁰		55.5	-17	
a28	Acetone oxime	$(\text{CH}_3)_2\text{C}=\text{NOH}$	73.10	1, 649	0.901		60-63	135		v s aq, alc, eth

ACES, a8

Acetal, d251

Acetaldehyde ammonia, a163

Acetaldehyde diethyl acetal, d251

Acetaldehyde dimethyl acetal, d438

Acetamidoacetic acid, a46

2-Acetamidopentanedioic acid, a45

Acethydrazide, a25

Acetic acid hydrazide, a25

Acetoacetanilide, a32

2-Acetoacetanilide, a302

4-Acetoacetanilide, a303

Acetoacetic esters, e53, e54

Acetoin, h106

Acetonaphthones, m311, m312

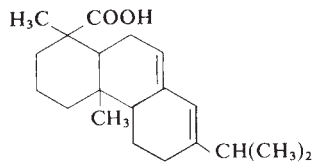
Acetonecarboxylic acid, a24

Acetone cyanohydrin, h145

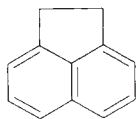
Acetone dimethyl acetal, d452

Acetone dimethyl acetal, d452

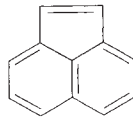
Acetone ketal of glycerine, d515



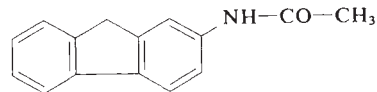
a1



a2



a3



a13

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a29	Acetonitrile	CH_3CN	41.05	2, 183	0.7857 ²⁰	1.3441 ²⁰	−43.8	81.60	5	misc aq, alc, chl
a30	Acetonitrile- <i>d</i> ₃	CD_3CN	44.08		0.84	1.3420 ²⁰		80.7	5	misc aq, alc, chl
a31	Acetophenone	$\text{C}_6\text{H}_5\text{COCH}_3$	120.15	7, 271	1.0238 ²⁵	1.5322 ²⁵	19.62	202.08	82	0.55 aq; s alc, eth
a32	2-Acetylacetanilide	$\text{C}_6\text{H}_5\text{NHCOCH}_2\text{COCH}_3$	177.20	12, 518			85			sl s aq; s alc, hot bz, chl, eth, acids, alk
a33	4-Acetylbenzene-sulfonic acid, Na salt	$\text{CH}_3\text{COC}_6\text{H}_4\text{SO}_3^-\text{Na}^+$	222.02	11 ² , 186			>300			
a34	4-Acetylbiphenyl	$\text{C}_6\text{H}_5\text{C}_6\text{H}_4\text{COCH}_3$	196.25	7 ² , 337			116–118	325–327		i aq; v s alc, acet
a35	Acetyl bromide	CH_3COBr	122.95	2, 174	1.663 ₄ ¹⁶		−96	75–77	1	d aq, alc; misc bz, chl, eth
a36	2-Acetylbutyrolactone		128.13		1.1846 ₄ ²⁰	1.4585 ²⁰		107 ^{5mm}		21 aq
a37	Acetyl chloride	CH_3COCl	78.50	2, 173	1.104 ₄ ²⁰	1.3886 ²⁰	−112.9	50.8	4	d aq, alc; misc bz, chl, eth
a38	Acetylcholine bromide	$(\text{CH}_3)_3\text{NBrCH}_2\text{CH}_2\text{—OCOCH}_3$	226.14	4 ¹ , 428			114–116			v s aq (d hot aq); s alc; i eth
a39	Acetylcholine chloride	$(\text{CH}_3)_3\text{NClCH}_2\text{CH}_2\text{—OCOCH}_3$	181.66	4, 281			150–152			v s aq; alc; d hot aq; i eth
a40	2-Acetylcyclopentanone		126.16	7, 558	1.043	1.4905 ²⁰		72–75 ^{80mm}	72	
a41	Acetylene	$\text{HC}\equiv\text{CH}$	26.02	1, 228	0.90(g)		−81 ^{891mm}	−83.95 subl		90 aq; 14 alc; v s bz, eth; acet dissolves 25 acet ^{15°}
a42	Acetylenedicarboxylic acid	$\text{HOCC}\equiv\text{CCOOH}$	114.06	2, 801			180 d			v s aq, alc, eth
a43	Acetyl fluoride	CH_3COF	62.04	2, 172	1.032		>−60	20		5 aq(d); misc alc, bz, eth

a44	2-Acetylfuran		110.11	17, 286	1.098	1.5065 ²⁰	29–30	67 ^{10mm}	71	
a45	<i>N</i> -Acetyl-L-glutamic acid	HOOCCH ₂ CH ₂ CH— (NHC(=O)CH ₃)COOH	189.17	4 ² , 908			200–201			
a46	<i>N</i> -Acetylglycine	CH ₃ CONHCH ₂ COOH	117.10	4, 354			207–209			2.7 aq ¹⁵ ; s alc; i eth
a47	<i>N</i> -Acetylimidazole		110.12				93–96			
a48	Acetyl iodide	CH ₃ COI	169.96	2, 174	2.0674 ²⁰ ₄	1.5491 ²⁰		108		d aq, alc; s bz, eth
a49	Acetyl-2-methylcholine chloride	CH ₃ COOCH(CH ₃)CH ₂ — NC1(CH ₃) ₃	195.69				171–173			v s aq, alc, chl; i eth
a50	2-Acetylphenothiazine		241.31				180–185			
a51	2-Acetylphenylacetone nitrile	C ₆ H ₅ CH(CN)COCH ₃	159.19	10, 699			89–92			
a52	<i>N</i> -Acetyl-4-piperidone		141.17		1.146	1.5026 ²⁰		218	> 112	

Acetonylacetone, h61

Acetophenetidin, e45

Acetophenetidide, e45

p-Acetotoluide, m355

Acetoxime, a28

2-Acetoxybenzoic acid, a56

1-Acetoxy-1,3-butadiene, b375

Aceturic acid, a46

Acetylacetaldehyde dimethyl acetal, d435

Acetylacetone, p31

N-Acetylanthranilic acid, a11

Acetylbenzene, a31

Acetylcyclopropane, c368

Acetylene dichlorides, d179, d180

Acetylene tetrabromide, t9

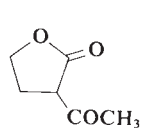
Acetylene tetrachloride, t28

N-Acetylethanolamine, h115

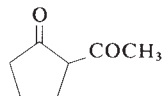
3-Acetyl-6-methyl-2*H*-pyran-2,4-(3*H*)-dione, d21

2-(Acetyloxy)benzoic acid, a56

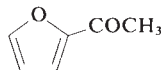
3-Acetyl-1-propanol, h157



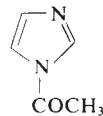
a36



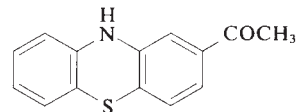
a40



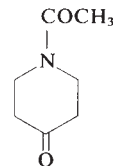
a44



a47



a50



a52

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a53	2-Acetylpyridine	(C ₅ H ₄ N)COCH ₃	121.14	21, 279	1.080	1.5203 ²⁰		188–189	>112	v s alc, eth
a54	3-Acetylpyridine	(C ₅ H ₄ N)COCH ₃	131.14	21, 279	1.102	1.5336 ²⁰		220	150	v s acids, alc, eth; s aq
a55	4-Acetylpyridine	(C ₅ H ₄ N)COCH ₃	121.14	21, 279	1.095	1.5290 ²⁰		212	>112	0.33 aq ²⁵ ; 20 alc; 5.9 chl; 5 eth; sl s bz
a56	Acetylsalicylic acid	HOOC ₆ H ₄ OOCCH ₃	180.16	10, 67	1.35		135			0.33 aq ²⁵ ; 20 alc; 5.9 chl; 5 eth; sl s bz
a57	2-Acetylthiophene	(C ₄ H ₃ S)COCH ₃	126.18	17, 287	1.168 ²² ₄	1.5564 ²⁰	10–11	214		sl s aq; misc alc, eth
a58	<i>N</i> -Acetylthiourea	CH ₃ CONHC(S)NH ₂	118.16	3, 191			165–169			s hot aq, alc; sl s eth
a59	<i>N</i> -Acetyl-DL-tryptophan		246.27	22 ² , 469			204–206			s aq, alc; v s eth
a60	Acid alizarin violet N		366.33	16 ² , 127						
a61	Acridine		179.22	20, 459			107–110 subl 110	346		s alc, eth, CS ₂ , PE
a62	Acrylamide	H ₂ C=CHCONH ₂	71.08	2, 400	1.122 ³⁰ ₄		84.5	125 ^{25mm}		215 aq ³⁰ ; 86 alc ³⁰ ; 63 acet; 2.7 chl; v s eth
a63	Acrylic acid	H ₂ C=CHCOOH	72.06	2, 397	1.0511 ²⁰	1.4224 ²⁰	13	140–141	54	misc aq, alc, bz, eth, chl, acet
a64	Acrylonitrile	H ₂ C=CHCN	53.06	2, 400	0.8060 ²⁰ ₄	1.3911 ²⁰	–83.7	77.4	0	7.3 aq; misc org solv
a65	Acryloyl chloride	H ₂ C=CHCOCl	90.51	2, 400	1.114	1.4350 ²⁰		72–76	16	d aq; v s chl
a66	1-Adamantanamine		151.25				206–208			sl s aq
a67	Adamantane		136.24		1.09	1.568	268 sealed tube	subl 205		

a68	1-Adamantane-carboxylic acid	180.25			174–175		
a69	Adenine	135.13	26, 420		>360 d	subl 220	0.05 aq; sl s alc; i chl, eth
a70	Adenosine	267.25	31, 27		234–236		s aq; i alc

N-Acetylsulfanilyl chloride, a10

Aconitic acid, p207

Acrolein, p204

Acrolein diethyl acetal, d258

Acrolein dimethyl acetal, d454

Acrylaldehyde, p207

1-Adamantanemethylamine, a209

Adenosine monophosphate, a72

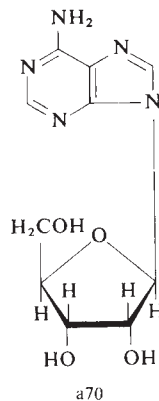
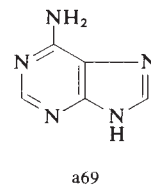
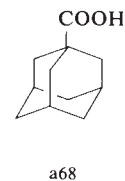
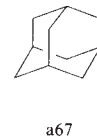
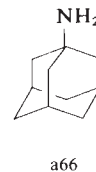
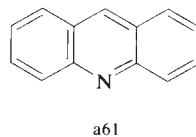
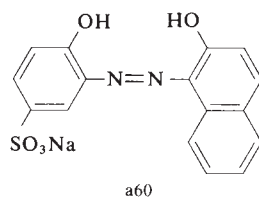
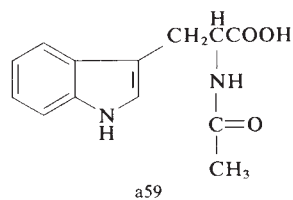


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a71	Adenosine-5'-diphosphoric acid		427.22							
a72	Adenosine-5'-phosphoric acid		347.22				200 d			v s hot aq, HCl
a73	D- α -Alanine	$\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$	89.09	4, 385			291–293 d			
a74	DL- α -Alanine	$\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$	89.09	4, 387	1.402		289 d	subl		16.7 aq ²⁵ ; 8.7 alc ²⁵ ; i eth
a75	L- α -Alanine	$\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$	89.09	4, 381			315–316			16.7 aq ²⁵ ; 8.7 alc ²⁵ ; i eth
a76	β -Alanine	$\text{H}_2\text{NCH}_2\text{CH}_2\text{COOH}$	89.09	4, 401	1.437 ⁻⁵		197–198 d			v s aq; sl s alc; i eth
a77	Allantoin		158.12	25, 474			238			0.45 aq; 0.2 alc
a78	Allene	$\text{H}_2\text{C}=\text{C}=\text{CH}_2$	40.06	1, 248	1.787	1.4168	–136.2	–34.5		
a79	Alloxan monohydrate		160.09	24, 500			253 d			s alc, acet, HOAc; sl s chl, PE, EtAc
a80	Allyl acetate	$\text{H}_2\text{C}=\text{CHCH}_2\text{OCOCH}_3$	100.12	2, 136	0.928 ₄ ^{0.928}	1.404 ²⁰		104	6	i aq; misc alc, eth
a81	Allyl alcohol	$\text{H}_2\text{C}=\text{CHCH}_2\text{OH}$	58.08	2, 436	0.854 ₄ ²⁰	1.4127 ²⁰	–50 glass	97.1	22	misc aq, alc, chl, eth
a82	Allylamine	$\text{H}_2\text{C}=\text{CHCH}_2\text{NH}_2$	57.10	4, 205	0.760 ₂₀ ²⁰	1.4205 ²⁰	–88.2	53.3	–28	misc aq, alc, chl, eth
a83	N-Allylaniline	$\text{C}_6\text{H}_5\text{NHCH}_2\text{CH}=\text{CH}_2$	133.19	12, 170	0.982 ²⁵	1.5630 ²⁰		218–220	89	i aq; s alc, eth
a84	Allylbenzene	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}=\text{CH}_2$	118.18	5, 484	0.892 ₀ ²⁰	1.5122 ²⁰		156–157	33	i aq; s alc, eth
a85	Allyl bromide	$\text{H}_2\text{C}=\text{CHCH}_2\text{Br}$	120.98	1, 201	1.451 ₂₅ ²⁵	1.465 ²⁵	–50	70	7	i aq; misc org solv
a86	Allylchlorodimethylsilane	$\text{H}_2\text{C}=\text{CHCH}_2\text{Si}(\text{CH}_3)_2\text{Cl}$	134.7		0.8964 ²	1.4195 ²⁰		110–112		
a87	Allyl chloroformate	$\text{H}_2\text{C}=\text{CHCH}_2\text{OCCl}$	120.54		1.13	1.423		27	31	

a88	Allylcyclohexylamine	$C_6H_{11}NHCH_2CH=CH_2$	139.24		0.962	1.4664 ²⁰		66 ^{12mm}	53	
a89	Allyldichloromethylsilane	$H_2C=CHCH_2Si(CH_3)Cl_2$	155.1		1.0758 ²⁰	1.4419 ²⁰		119–120		
a90	<i>N</i> -Allyl- <i>N,N</i> -dimethylamine	$H_2C=CHCH_2N(CH_3)_2$	85.0			1.4010 ²⁰		63–64		
a91	Allyl ethyl ether	$H_2C=CHCH_2OCH_2CH_3$	86.13	1,438	0.7651 ²⁰	1.3881 ²⁰		64–66		i aq; misc alc, eth
a92	Allyl iodide	$H_2C=CHCH_2I$	167.98	1,202	1.846 ²⁰		–99.3	103.1		i aq; misc alc, eth

Adenosine 5'-(trihydrogen diphosphate), a71

5'-Adenylic acid, a72

Adipic acid, h57

Adipic acid monoethyl ester, e149

Adiponitrile, d238

Adipolyl chloride, h62

ADP, a71

Alaninols, a271, a272

Alizarin, d371

Allylacetic acid, p50

Allylacetone, h78

4-Allylanisole, a94

Allyl carbamide, a105

Allyl chloride, c216

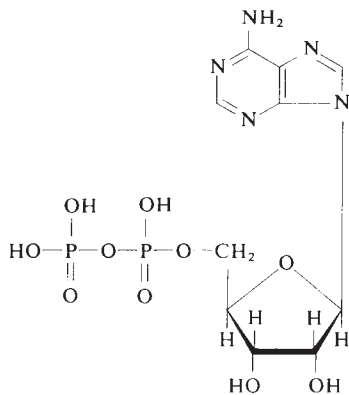
Allyl cyanide, b400

Allyldimethylchlorosilane, a86

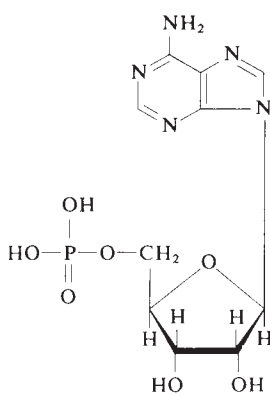
Allyl glycidyl ether, a96

1-Allyl-2-hydroxybenzene, a98

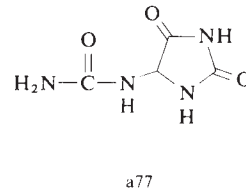
Allyl iodide, i50



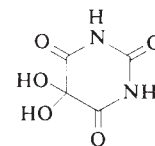
a71



a72




a77



a79

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

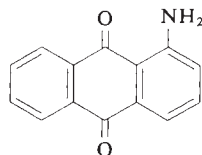
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a93	Allyl isothiocyanate	$\text{H}_2\text{C}=\text{CHCH}_2\text{NCS}$	99.16	4, 214	1.013 ₄ ²⁰	1.5300 ²⁰	−80	150	46	0.2 aq; misc org solv
a94	1-Allyl-4-methoxybenzene	$\text{H}_2\text{C}=\text{CHCH}_2\text{C}_6\text{H}_4\text{OCH}_3$	148.21	6, 571	0.9645 ₄ ²¹	1.5195 ²⁰		215–216		a slc, chl
a95	Allyl methyl sulfide	$\text{H}_2\text{C}=\text{CHCH}_2\text{SCH}_3$	88.17	1, 440	0.803	1.4714 ²⁰		91–93	18	
a96	1-Allyloxy-2,3-epoxypropane	$\text{H}_2\text{C}-\text{CHCH}_2\text{OCH}_2$ 	114.14		0.962	1.4332 ²⁰		154	57	
a97	Allyloxytrimethylsilane	$\text{H}_2\text{C}=\text{CHCH}_2\text{OSi}(\text{CH}_3)_3$	130.3		0.7830	1.4075 ²⁵		100–101		
a98	2-Allylphenol	$\text{H}_2\text{C}=\text{CHCH}_2\text{C}_6\text{H}_4\text{OH}$	134.18	6, 572	1.0255 ₁₅ ¹⁵	1.5455 ²⁰	−6	220	88	s alc, eth
a99	Allyl phenyl ether	$\text{H}_2\text{C}=\text{CHCH}_2\text{OC}_6\text{H}_5$	134.18	6, 144	0.983 ₄ ¹⁵	1.5200 ²⁰		192	62	i aq; s alc; misc eth
a100	Allyl propyl ether	$\text{H}_2\text{C}=\text{CHCH}_2\text{OC}_3\text{H}_7$	100.16	1 ³ , 1882	0.7670 ₄ ²⁰	1.3919 ²⁰		90–92	38	s alc; misc eth
a101	1-Allyl-2-thiourea	$\text{H}_2\text{C}=\text{CHCH}_2\text{NHC}(\text{S})\text{NH}_2$	116.18	4, 211	1.219 ₂₀ ²⁰		78			3.3 aq; s alc; i bz; v sl s eth
a102	Allyltrichlorosilane	$\text{H}_2\text{C}=\text{CHCH}_2\text{SiCl}_3$	175.5		1.2011 ₄ ²⁰	1.4460 ²⁰		117.5		
a103	Allyltriethoxysilane	$\text{H}_2\text{C}=\text{CHCH}_2\text{Si}(\text{OC}_2\text{H}_5)_3$	204.3		0.9030 ²⁰	1.4072 ²⁰		176 ^{740mm}		
a104	Allyltrimethylsilane	$\text{H}_2\text{C}=\text{CHCH}_2\text{Si}(\text{CH}_3)_3$	114.27		0.7193 ₄ ²⁰	1.4074 ²⁰		85–86	7	
a105	Allylurea	$\text{H}_2\text{C}=\text{CHCH}_2\text{NHCONH}_2$	100.12	4, 209			78			v s aq, alc; v sl s eth
a106	Aminoacetonitrile	$\text{H}_2\text{NCH}_2\text{CN}$	56.07	4, 344				58 ^{15mm} d		s acids, alc
a107	Aminoacetonitrile hydrogen sulphate	$\text{H}_2\text{NCH}_2\text{CN} \cdot \text{H}_2\text{SO}_4$	154.14	4, 344			101	d 165		v s aq; sl s alc; i eth
a108	2'-Aminoacetophenone	$\text{H}_2\text{NC}_6\text{H}_4\text{COCH}_3$	135.17	14, 41				70 ^{3mm}		v sl s aq; s alc, eth
a109	3'-Aminoacetophenone	$\text{H}_2\text{NC}_6\text{H}_4\text{COCH}_3$	135.17	14, 45			98–99	289–290		
a110	4'-Aminoacetophenone	$\text{H}_2\text{NC}_6\text{H}_4\text{COCH}_3$	135.17	14, 46			106	293–295		s hot aq, alc, eth, HOAc; sl s bz

a111	1-Aminoanthraquinone		223.23	14, 177		253–255	subl	i aq; v s alc, bz, chl, eth, HOAc, HCl
a112	2-Aminoanthraquinone		223.23	14, 191		295 d	subl	i aq, eth; s alc, bz
a113	4-Aminoantipyrine		203.25	24, 273		109		s aq, alc, bz; sl s eth
a114	2-Aminobenzamide	$\text{H}_2\text{NC}_6\text{H}_4\text{CONH}_2$	136.15	14, 320		110	300 sl d	v s hot aq, alc; i bz; sl s eth
a115	2-Aminobenzene-arsonic acid	$\text{H}_2\text{NC}_6\text{H}_4\text{AsO}(\text{OH})_2$	217.06	16 ¹ , 463		153		
a116	4-Aminobenzene-arsonic acid	$\text{H}_2\text{NC}_6\text{H}_4\text{AsO}(\text{OH})_2$	217.06	16, 878		> 300		s hot aq, alk CO_3 , mineral acids
a116a	5-Aminobenzene-1,3-dicarboxylic acid	$\text{H}_2\text{NC}_6\text{H}_3(\text{COOH})_2$	181.15	14 ¹ , 636		> 300		
a117	2-Aminobenzene-1,4-disulfonic acid	$\text{H}_2\text{NC}_6\text{H}_3(\text{SO}_3\text{H})_2$	253.24					
a118	2-Aminobenzene-sulfonic acid	$\text{H}_2\text{NC}_6\text{H}_4\text{SO}_3\text{H}$	173.19	14, 681		d 325		1.5 aq ¹⁵ ; v sl s alc, eth

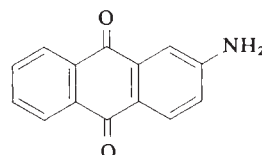
Allyl mercaptan, p206
 4-Allyl-2-methoxyphenol, m99
 2-Allyl-4-methylphenol, m387
 2-Allyl-6-methylphenol, m386

Allyl sulfide, d27
 Aluminon, a316
N-Amidinosarcosine, c277
 Aminoacetaldehyde diethyl acetal, d254

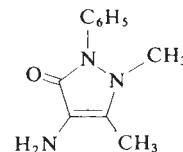
Aminoacetaldehyde dimethyl acetal, d440
 1-Aminoadamantane, a66
 Aminoanisoles, m42, m43, m44
p-Aminoazobenzene, p87



a111



a112



a113

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

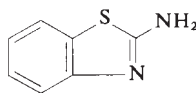
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a119	3-Aminobenzene-sulfonic acid	$\text{H}_2\text{NC}_6\text{H}_4\text{SO}_3\text{H}$	173.19		1.69					2 aq ¹⁵ ; sl s alc
a120	4-Aminobenzene-sulfonic acid	$\text{H}_2\text{NC}_6\text{H}_4\text{SO}_3\text{H}$	173.19	14, 695			d 288			1 aq ²⁰ ; sl s hot MeOH
a121	2-Aminobenzoic acid	$\text{H}_2\text{NC}_6\text{H}_4\text{COOH}$	137.14	14, 310			144–146	subl		v s hot aq, alc, eth
a122	3-Aminobenzoic acid	$\text{H}_2\text{NC}_6\text{H}_4\text{COOH}$	137.14	14, 383	1.511 ⁴		172–174			sl s aq; v s alc; s eth
a123	4-Aminobenzoic acid	$\text{H}_2\text{NC}_6\text{H}_4\text{COOH}$	137.14	14, 418	1.374		187			0.59 aq; 5.6 alc
a124	2-Aminobenzonitrile	$\text{H}_2\text{NC}_6\text{H}_4\text{CN}$	118.14	14, 322			49	268		s alc, eth
a125	3-Aminobenzonitrile	$\text{H}_2\text{NC}_6\text{H}_4\text{CN}$	118.14	14, 391			53	288–290		s hot aq; v s alc, eth
a126	4-Aminobenzonitrile	$\text{H}_2\text{NC}_6\text{H}_4\text{CN}$	118.14	14, 425			85	d		v s hot aq, alc, eth
a127	2-Aminobenzo-phenone	$\text{H}_2\text{NC}_6\text{H}_4\text{COC}_6\text{H}_5$	197.24	14, 76			108	223–226		sl s aq; s alc, eth
a128	2-Aminobenzothiazole		150.20	27, 182			132	d		v s alc, chl, eth
a129	2-Aminobenzotri-fluoride	$\text{H}_2\text{NC}_6\text{H}_4\text{CF}_3$	161.13	12 ² , 453	1.290 ²⁵	1.4785 ²⁵	34	175	55	
a130	3-Aminobenzotri-fluoride	$\text{H}_2\text{NC}_6\text{H}_4\text{CF}_3$	161.13	12, 870	1.290	1.4800 ²⁰	6	187	85	
a131	4-Aminobenzotri-fluoride	$\text{H}_2\text{NC}_6\text{H}_4\text{CF}_3$	161.13	12 ³ , 2151	1.283 ²⁷	1.4815 ²⁵	38	107 ^{39mm}	85	
a132	<i>N</i> -(<i>p</i> -Aminobenzoyl)-glycine	$\text{H}_2\text{NC}_6\text{H}_4\text{CONHCH}_2\text{COOH}$	194.19	14 ² , 258			198–199			i aq; s alc, bz, chl
a133	4-Aminobenzoyl hydrazide	$\text{H}_2\text{NC}_6\text{H}_4\text{CONHNH}_2$	151.17	14 ¹ , 570			227			
a134	2-Aminobiphenyl	$\text{H}_2\text{NC}_6\text{H}_4\text{C}_6\text{H}_5$	169.23	12, 1317			53	299		sl s aq; s alc
a135	4-Aminobiphenyl	$\text{H}_2\text{NC}_6\text{H}_4\text{C}_6\text{H}_5$	169.23	12, 1318			54	191 ^{15mm}		s hot aq, alc, eth
a136	D-(+)-2-Amino-1-butanol	$\text{CH}_3\text{CH}_2\text{CH}(\text{NH}_2)\text{CH}_2\text{OH}$	89.14	4, 291	0.947 ²⁰	1.4521 ²⁰	–2	174	79	misc aq; s alc

a137	L-(–)-2-Amino-1-butanol	$\text{CH}_3\text{CH}_2\text{CH}(\text{NH}_2)\text{CH}_2\text{OH}$	89.14	4, 291	0.947 ²⁰	1.4525 ²⁰	–2	174	82	misc aq; s alc
a138	DL-2-Aminobutyric acid	$\text{CH}_3\text{CH}_2\text{CH}(\text{NH}_2)\text{COOH}$	103.12	4, 408			304	subl 300		21 aq; 0.2 hot alc
a139	4-Aminobutyric acid	$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{COOH}$	103.12	4, 413			195.d			v s aq; i alc, eth
a140	2-Amino-4-chlorobenzoic acid	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{COOH}$	171.58	14, 365			233			
a141	2-Amino-5-chlorobenzonitrile	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{CN}$	152.58				99	132 ^{0.5mm}	> 112	
a142	2-Amino-4'-chlorobenzophenone	$\text{H}_2\text{NC}_6\text{H}_4\text{COC}_6\text{H}_4\text{Cl}$	231.68	14 ¹ , 389			104			
a143	2-Amino-5-chlorobenzophenone	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{COC}_6\text{H}_5$	231.68	14, 79			100			
a144	2-Amino-5-chlorobenzotrifluoride	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{CF}_3$	195.57	12 ³ , 1921	1.386	1.5069 ²⁰		66–67 ^{3mm}		
a145	3-Amino-4-chlorobenzotrifluoride	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{CF}_3$	195.57		1.428	1.4975 ²⁵		82–83 ^{9mm}	none	
a146	5-Amino-2-chlorobenzotrifluoride	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{CF}_3$	195.57				36			

Aminobenzenethiol, a293
Aminobenzoic acid hydrazide, a133
Aminobenzyl cyanide, a260
1-Aminobutane, b417

2-Aminobutane, b377
Aminobutanoic acids, a138, a139
3-Amino-2-butenamide, a150
4-Aminobutyraldehyde diethyl acetal, d247

α -Aminocaproic acid, a183
 ε -Aminocaproic acid, a184



a128

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

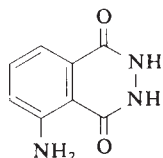
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a147	2-(3-Amino-4-chloro-benzoyl)benzoic acid	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{CO}-\text{C}_6\text{H}_4\text{COOH}$	275.69	14, 661			171–173			
a148	2-Amino-4-chloro-phenol	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{OH}$	143.57	13, 383			138			
a149	2-Amino-5-chloro-pyridine	$\text{H}_2\text{N}(\text{Cl})\text{C}_5\text{H}_3\text{N}$	128.56	22 ² , 332			138	128 ^{11mm}		
a150	3-Aminocrotamide	$\text{CH}_3\text{C}(\text{NH}_2)=\text{CHCONH}_2$	100.12				102			
a151	3-Aminocrotononitrile	$\text{CH}_3\text{C}(\text{NH}_2)=\text{CHCN}$	82.11	3, 660						
a152	1-Amino-1-cyclo-hexanecarboxylic acid	$\text{C}_6\text{H}_{10}(\text{NH}_2)\text{COOH}$	143.19	14, 299			>300			
a153	5-Amino-2,3-dihydro-1,4-phthalazine-dione		177.16	25 ¹ , 698			319–320			
a154	2-Amino-4,6-dihydroxypyrimidine		127.10	24, 468			>300			
a155	4-Amino-2,6-dihydroxypyrimidine		127.10	24, 469			>300			
a156	4-Amino-3,5-diiodobenzoic acid	$\text{I}_2(\text{NH}_2)\text{C}_6\text{H}_2\text{COOH}$	388.93	14, 439			>300			i aq, alc
a157	2-Amino-4,6-dimethylpyridine	$(\text{CH}_3)_2(\text{NH}_2)(\text{C}_5\text{H}_2\text{N})$	122.17	22, 435			64	235		
a158	4-Amino-2,6-dimethylpyridimide		123.16	24 ² , 45			181			156 aq; 18.9 alc
a159	6-Amino-1,3-dimethyluracil		155.16	24, 471			295 d			
a160	5-Amino-2,6-dioxo-1,2,3,6-tetrahydro-4-pyrimidinecarboxylic acid		171.11	25, 264			>300			

a161	2-Aminoethane-sulfonic acid	$\text{H}_2\text{NCH}_2\text{CH}_2\text{SO}_3\text{H}$	125.15	4, 528			d > 300		6.45 aq ¹² ; i abs alc
a162	2-Aminoethanethiol	$\text{HSCH}_2\text{CH}_2\text{NH}_2$	77.14	4, 286			99–100		v s aq; s alc
a163	1-Aminoethanol	$\text{CH}_3\text{CH}(\text{OH})\text{NH}_2$	61.08				97	110 d	s aq; sl s eth
a164	2-Aminoethanol	$\text{H}_2\text{NCH}_2\text{CH}_2\text{OH}$	61.08	4, 274	1.0158 ²⁰	1.4539 ²⁰	10.52	171	misc aq, org solv
a165	2-(2-Aminoethoxy)-ethanol	$\text{H}_2\text{NCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{OH}$	105.14	4 ³ , 642	1.460			218–224	
a166	2-(2-Aminoethyl-amino)ethanol	$\text{H}_2\text{NCH}_2\text{CH}_2\text{NHCH}_2\text{-CH}_2\text{OH}$	104.15	4, 286	1.030	1.4861 ²⁰		241	v s aq, alc; sl s eth
a167	5-(2-Aminoethyl-amino)-1-naphthalenesulfonic acid	$\text{H}_2\text{NCH}_2\text{CH}_2\text{NH-C}_{10}\text{H}_6\text{SO}_3\text{H}$	266.32				>300		
a167a	3-(2-Aminoethyl-amino)propyl-trimethoxy-silane	$\text{H}_2\text{NCH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{-CH}_2\text{Si}(\text{OCH}_3)_3$	222.1		1.01 ₄ ²⁵	1.4418 ²⁵		140 ^{15mm}	150

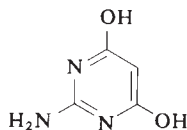
4-Amino-*m*-cresol, a218
Aminocyclohexane, c334
Aminodecane, d19
2-Amino-2-deoxyglucose, g5
2-Amino-5-diethylaminopentane, d327

2-Amino-1,5-dihydro-1-methyl-4 *H*-imidazol-4-one, c278
2-Aminodiphenylamine, p131
1-Amino-1,2-diphenylethane, d668
Aminodiphenylmethane, d678

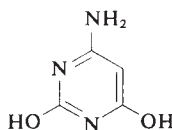
Aminoethane, e58
1-(2-Aminoethyl)amino-2-[(2-aminoethyl)-aminoethyl]aminoethane, t54



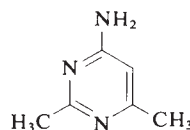
a153



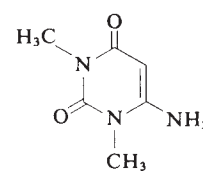
a154



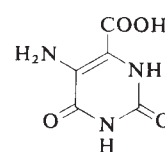
a155



a158



a159



a160

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a168	3-Amino-9-ethyl-carbazole	$\text{H}_2\text{NCH}_2\text{CH}_2\text{OSO}_3\text{H}$	210.28	22 ¹ , 642	0.992	1.4755 ²⁰	98–100	137 ^{0.15mm}	175	i aq, bz, chl, eth; s alc, acet
a169	2-Aminoethyl hydrogen sulfate		141.15	4, 276			280 d			
a170	3-(2-Aminoethyl)-indole		160.22	22 ¹ , 636			118			
a171	<i>S</i> -2-Aminoethyl-isothiuronium bromide HBr	$\text{HOC}_6\text{H}_4\text{CH}_2\text{CH}_2\text{NH}_2$	281.02	13, 625	0.985	1.4983 ²⁰	194–195	175 ^{8mm}	93	misc aq; s alc
a172	<i>N</i> -(2-Aminoethyl)-morpholine		130.19				25.6			
a173	<i>p</i> -(2-Aminoethyl)-phenol		137.18				161–163			
a174	<i>N</i> -(2-Aminoethyl)-piperazine	$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{NH}_2$	129.21	22, 434	0.928	1.4815 ²⁰	–26	152 ^{10mm}	74	misc aq; s alc
a175	<i>N</i> -(2-Aminoethyl)-1,3-propanediamine		117.20				38			
a176	2-Amino-2-ethyl-1,3-propanediol		119.16				1099 ²⁰ ₂₀			
a177	2-(2-Aminoethyl)-pyridine	$\text{H}_2\text{NCH}_2\text{CH}_2(\text{C}_5\text{H}_4\text{N})$	122.17	22, 434	1.021	1.5357 ²⁰		93 ^{12mm}	81 ^{20mm}	i aq; d hot aq
a178	4-(2-Aminoethyl)-pyridine	$\text{H}_2\text{NCH}_2\text{CH}_2(\text{C}_5\text{H}_4\text{N})$	122.17					104 ^{9mm}		
a179	3-Amino-4-fluorobenzo-trifluoride	$\text{H}_2\text{N}(\text{F})\text{C}_6\text{H}_3\text{CF}_3$	179.0							
a180	Aminoguanidine H_2CO_3	$\text{H}_2\text{NNHC}(=\text{NH}) - \text{NH}_2 \cdot \text{H}_2\text{CO}_3$	136.11	3, 117			172 d			

a181	Aminoguanidine nitrate	$\text{H}_2\text{NNHC}(=\text{NH})\cdot\text{HNO}_3$	137.11	3, 117			137			
a182	<i>N</i> -Aminohexamethyl- eneimine	$\text{C}_6\text{H}_{12}\text{N}-\text{NH}_2$	114.19		0.984	1.4850 ²⁰		165	56	
a183	2-Aminohexanoic acid	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{NH}_2)\cdot\text{COOH}$	131.18	4, 433	1.172		d 327			1.15 aq ²⁵ ; 0.42 alc
a184	6-Aminohexanoic acid	$\text{H}_2\text{N}(\text{CH}_2)_4\text{CH}_2\text{COOH}$	131.18	4, 434			204–206			v s aq; i alc
a185	6-Amino-1-hexanol	$\text{H}_2\text{N}(\text{CH}_2)_5\text{CH}_2\text{OH}$	117.19	4 ² , 748			56–58	135 ^{30mm}		
a186	1-Amino-4-hydroxy- anthraquinone		239.23	14, 268			207–209			s eth
a187	L-2-Amino-3-hydroxy- butyric acid	$\text{CH}_3\text{CH}(\text{OH})\text{CH}(\text{NH}_2)\text{COOH}$	119.12	4, 514			d 255– 257			v s aq; i alc, eth, chl

Aminoethylbenzenes, e64, e65

2-(2-Aminoethyl)-2-thiopseudourea, a171

1-Aminoheptane, h20

2-Aminoheptane, m269a

1-Aminohexane, h80

2-Aminohexane, m353a

p-Aminohippuric acid, a132

Aminohydroxybenzoic acids, a286, a287

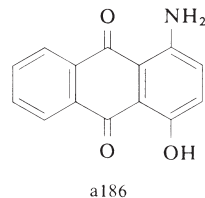
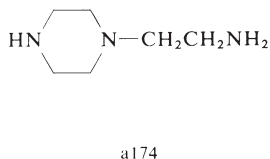
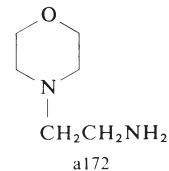
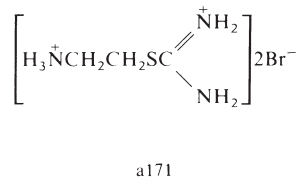
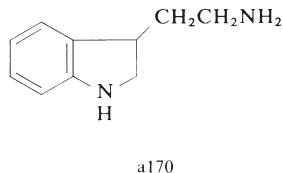
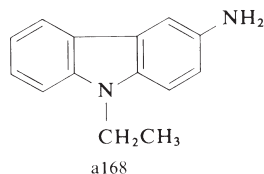


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a188	DL-2-Amino-4-hydroxy-butyric acid	$\text{HOCH}_2\text{CH}_2\text{CH}(\text{NH}_2)\text{COOH}$	119.12	4, 514			188–189			s alc
a189	L-2-Amino-4-hydroxy-butyric acid	$\text{HOCH}_2\text{CH}_2\text{CH}(\text{NH}_2)\text{COOH}$	119.12	4 ³ , 1636			203 d			
a190	DL-4-Amino-3-hydroxy-butyric acid	$\text{H}_2\text{NCH}_2\text{CH}(\text{OH})\text{CH}_2\text{COOH}$	119.12	4 ² , 938			202 d			s aq; sl s alc, eth
a191	4-Amino-6-hydroxy-2-mercapto-pyrimidine hydrate		161.18	24, 476			>300			
a192	2-Amino-4-hydroxy-6-methylpyrimidine		125.13	24, 343			>300			
a193	4-Amino-3-hydroxy-1-naphthalenesulfonic acid		239.25	14, 846			295 d			i aq, alc, bz, eth
a194	4-Amino-5-hydroxyl-1-naphthalenesulfonic acid		239.25	14, 835						sl s aq; i alc, eth
a195	5-Amino-6-hydroxy-2-naphthalenesulfonic acid		239.25							sl s hot aq; i eth
a196	6-Amino-7-hydroxy-2-naphthalenesulfonic acid		239.25	14, 849			>300			
a197	2-Amino-3-hydroxy-pyridine	$\text{H}_2\text{N}(\text{HO})(\text{C}_5\text{H}_3\text{N})$	110.12	22 ² , 408			172–174			
a198	4-Amino-2-hydroxy-pyrimidine		111.10	24, 314			> 300			0.77 aq; sl s alc

a199	1-Aminoindan		133.19	12, 1191	1.038 ¹⁵	1.5613 ²⁰	1.5	97 ^{8mm}	94	sl s aq
a200	5-Aminoindan		133.19	12 ¹ , 511			36	249 ^{745mm}		sl s aq
a201	5-Aminoindazole		133.15	25 ² , 308			178			
a202	6-Aminoindazole		133.15	25, 317			206 d			
a203	2-Amino-5-iodoben- zoic acid	H ₂ N(I)C ₆ H ₃ COOH	263.03	14, 373			221 d			sl s aq, PE; s alc
a204	DL-2-Amino-4-mer- captobutyric acid	HSCH ₂ CH ₂ CH- (NH ₂)COOH	135.19	4 ³ , 1647			232–233			
a205	Aminomethane- sulfonic acid	H ₂ NCH ₂ SO ₃ H	111.12	1, 583			185 d			v s aq

2-Amino-2-(hydroxymethyl)-1,3-propanediol,
t423

α-Amino-4-imidazolepropanoic acid, h83

Aminoiminomethanesulfinic acid, f30

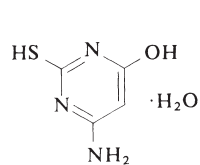
N-(Aminoiminomethyl)-N-methylglycine, c277

2-Aminoisobutyric acid, a222

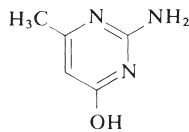
5-Aminoisophthalic acid, a116a

6-Amino-2,4-lutidine, a157

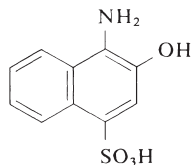
2-Amino-3-mercaptopropanoic acid, c370



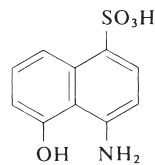
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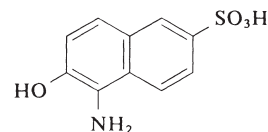
a192



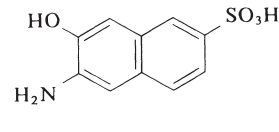
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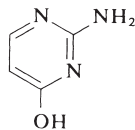
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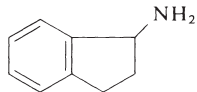
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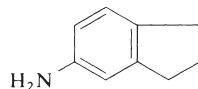
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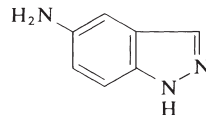
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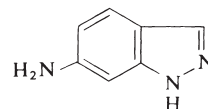
a199



a200



a201



a202

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

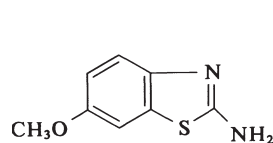
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a206	3-Amino-4-methoxybenzoic acid	$\text{CH}_3\text{O}(\text{NH}_2)\text{C}_6\text{H}_3\text{COOH}$	167.16	14 ¹ , 657			241			
a207	2-Amino-6-methoxybenzothiazole		180.23	27 ² , 334			165–167			
a208	5-Amino-2-methoxypyridine	$\text{CH}_3\text{O}(\text{NH}_2)\text{C}_5\text{H}_3\text{N}$	124.14	22 ² , 408		1.5745 ²⁰	31	90 ¹ mm		
a209	1-(Aminomethyl)adamantane		165.28		0.933	1.5137 ²⁰		83–85 ^{0.3} mm	92	
a210	4-(Aminomethyl)benzenesulfonamide	$\text{H}_2\text{NCH}_2\text{C}_6\text{H}_4\text{SO}_2\text{NH}_2$	186.25				151–152			s dil alk, dil acid
a211	2-Amino-5-methylbenzoic acid	$\text{H}_2\text{N}(\text{CH}_3)\text{C}_6\text{H}_3\text{COOH}$	151.17	14, 481			177 d			sl s aq; s alc, eth
a212	3-Amino-4-methylbenzoic acid	$\text{H}_2\text{N}(\text{CH}_3)\text{C}_6\text{H}_3\text{COOH}$	151.17	14, 487			166			a aq
a213	DL-2-Amino-3-methyl-1-butanol	$(\text{CH}_3)_2\text{CHCH}(\text{NH}_2)\text{CH}_2\text{OH}$	103.17			1.4543 ²⁰		77 ⁸ mm	83	
a214	L-2-Amino-3-methyl-1-butanol	$(\text{CH}_3)_2\text{CHCH}(\text{NH}_2)\text{CH}_2\text{OH}$	103.17		0.926	1.4548 ²⁰		81 ⁸ mm	78	
a215	2-(Aminomethyl)-1-ethylpyrrolidine		128.22		0.887	1.4665 ²⁰		60 ¹⁶ mm		
a216	2-Amino-3-methyl-1-pentanol	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{NH}_2)\text{CH}_2\text{OH}$	117.19			1.4589 ²⁰	30	97 ¹⁴ mm		
a217	2-Amino-4-methyl-1-pentanol	$\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\text{NH}_2)\text{CH}_2\text{OH}$	117.19	4, 298	0.917	1.4511 ²⁰		200	90	
a218	4-Amino-3-methylphenol	$\text{H}_2\text{N}(\text{CH}_3)\text{C}_6\text{H}_3\text{OH}$	123.16	13, 593			179			
a219	4-(Aminomethyl)piperidine		114.19			1.4900 ²⁰	25	200	78	
a220	2-Amino-2-methyl-1,3-propanediol	$\text{HOCH}_2\text{C}(\text{CH}_3)(\text{NH}_2)\text{CH}_2\text{OH}$	105.14	4, 303			110	151 ¹⁰ mm		250 aq ²⁰ ; s alc

a221	2-Amino-2-methyl-1-propanol	$(\text{CH}_3)_2\text{C}(\text{NH}_2)\text{CH}_2\text{OH}$	89.14		0.934 ²⁰ ₂₀	1.4480 ²⁰	30–31	165	67	misc aq; s alc, org solv
a222	2-Amino-2-methylpropionic acid	$(\text{CH}_3)_2\text{C}(\text{NH}_2)\text{COOH}$	103.12	4, 414			335 sealed tube	280 subl		v s aq
a223	2-(Aminomethyl)-pyridine	$\text{H}_2\text{NCH}_2(\text{C}_5\text{H}_4\text{N})$	108.14		1.049	1.5445 ²⁰		85 ^{12mm}		
a224	3-(Aminomethyl)-pyridine	$\text{H}_2\text{NCH}_2(\text{C}_5\text{H}_4\text{N})$	108.14		1.062	1.5510 ²⁰	–21	74 ^{1mm}	100	
a225	2-Amino-3-methylpyridine	$\text{H}_2\text{N}(\text{CH}_3)(\text{C}_5\text{H}_3\text{N})$	108.14	22 ² , 342		1.5782 ²⁰	34	222		v s aq; s alc
a226	2-Amino-4-methylpyridine	$\text{H}_2\text{N}(\text{CH}_3)(\text{C}_5\text{H}_3\text{N})$	108.14	22 ² , 342			100	230		v s aq, alc, DMF
a227	2-Amino-6-methylpyridine	$\text{H}_2\text{N}(\text{CH}_3)(\text{C}_5\text{H}_3\text{N})$	108.14	22 ¹ , 633			45	209		v s aq
a228	2-Amino-4-methylpyrimidine		109.13	24, 84			160	subl		s hot aq; s alc
a229	2-Amino-4-methylthiazole		114.17	27, 159			45	232		v s aq, alc, eth
a230	2-Aminomethyl-3,5,5-trimethylcyclohexanol		171.29		0.969	1.4904 ²⁰	43–48	265	> 112	

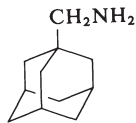
1-Amino-2-methoxyethane, m69
 α -(Aminomethyl)benzyl alcohol, a262

3-Amino- α -methylbenzyl alcohol, a261
 2-Amino-3-methylpentanoic acid, i79

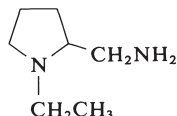
2-Aminomethylthiophene, t158



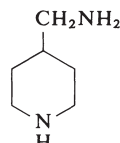
a207



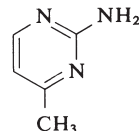
a209



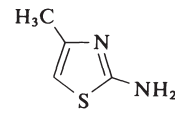
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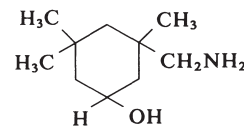
a219



a228



a229



a230

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

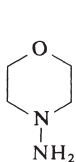
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a231	<i>N</i> -Aminomorpholine		102.14	27, 8	1.059	1.4772 ²⁰		168	58	
a232	2-Amino-1, 5-naphthalenedisulfonic acid		303.31	14, 786			>300			
a233	7-Amino-1,3-naphthalenedisulfonic acid		303.31	14, 784			>300			
a234	4-Amino-1-naphthalenesulfonic acid	H ₂ NC ₁₀ H ₆ SO ₃ H	223.26		1.670 ₄ ²⁵		d			0.031 aq; s dil alk
a235	4-Amino-1,8-naphthalimide		212.21	22 ² , 452			360			
a236	3-Amino-2-naphthol	H ₂ NC ₁₀ H ₆ OH	159.19	13, 685			207			
a237	2-Amino-4-nitrobenzoic acid	H ₂ N(NO ₂)C ₆ H ₃ COOH	182.14	14, 374			270 d			i aq; v s alc, eth
a238	2-Amino-5-nitrobenzonitrile	H ₂ N(NO ₂)C ₆ H ₃ CN	163.14	14 ² , 234			200–207			
a239	2-Amino-5-nitrobenzophenone	C ₆ H ₅ COC ₆ H ₃ (NH ₂)NO ₂	242.23	14, 79			166–168			
a240	2-Amino-6-nitrobenzothiazole		195.20	27 ² , 232			247–249			
a241	2-Amino-5-nitrobenzotrifluoride	H ₂ N(NO ₂)C ₆ H ₃ CF ₃	206.12				90–92			
a242	4-Amino-3-nitrobenzotrifluoride	H ₂ N(NO ₂)C ₆ H ₃ CF ₃	206.12				105–106			
a243	4-Amino-4'-nitrodiphenylsulfide	O ₂ NC ₆ H ₄ SC ₆ H ₄ NH ₂	246.29	13, 534			142			
a244	2-Amino-4-nitrophenol	O ₂ N(NH ₂)C ₆ H ₃ OH	154.13	13 ³ , 192			145			

a245	4-Amino-2-nitro-phenol	$O_2N(NH_2)C_6H_3OH$	154.13	13, 520			127		
a246	D-(-)- <i>threo</i> -2-Amino-1-(<i>p</i> -nitrophenyl)-1,3-propanediol	$HOCH_2CH(NH_2)CH(OH)-C_6H_4NO_2$	212.21				163–165 163–165		
a247	2-Amino-5-(<i>p</i> -nitrophenylsulfonyl)-thiazole		285.30				222–226		
a248	2-Amino-5-nitro-pyridine	$H_2N(C_5H_3N)NO_2$	139.11	22 ¹ , 631			188		sl s aq, bz, eth
a249	2-Amino-5-nitro-thiazole		145.14				202 d		v sl s aq; 0.7 alc; 0.4 eth
a250	<i>exo</i> -2-Aminonorbornane		111.19		0.938	1.4807 ²⁰	49 ^{10mm}	35	

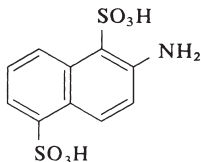
1-Aminonaphthalene, n17

1-Amino-2-naphthol-4-sulfonic acid, a193

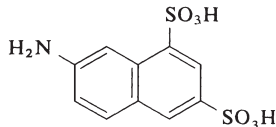
1-Amino-2-naphthol-6-sulfonic acid, a195



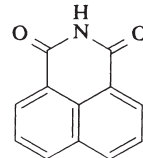
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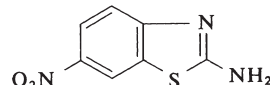
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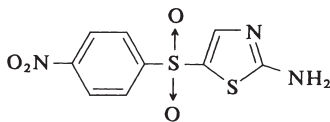
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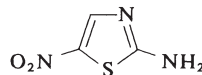
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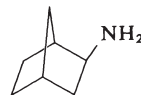
a240



a247



a249



a250

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a251	2-Aminopentane	$\text{H}(\text{CH}_2)_3\text{CH}(\text{NH}_2)\text{CH}_3$	87.17	4, 177	0.739 ²⁰	1.4047 ²⁰		91–92		s aq, alc, eth, PE
a252	3-Aminopentane	$\text{C}_2\text{H}_5\text{CH}(\text{NH}_2)\text{C}_2\text{H}_5$	87.17	4, 178	0.749 ²⁰	1.4055 ²⁰		91	1	misc aq, alc, eth
a253	DL-2-Aminopentanoic acid	$\text{H}(\text{CH}_2)_3\text{CH}(\text{NH}_2)\text{COOH}$	117.15	4, 416			303	320 subl		5.5 aq ¹⁸ ; v sl s alc, chl, eth, PE
a254	5-Aminopentanoic acid	$\text{H}_2\text{N}(\text{CH}_2)_4\text{COOH}$	117.15	4, 418			158–161			v s aq; sl s alc; i eth
a255	5-Amino-1-pentanol	$\text{H}_2\text{N}(\text{CH}_2)_5\text{OH}$	103.17	4 ¹ , 441		1.4615 ²⁰	37	122 ^{16mm}	65	
a256	2-Aminophenethyl alcohol	$\text{H}_2\text{NC}_6\text{H}_4\text{CH}_2\text{CH}_2\text{OH}$	137.18	13 ³ , 1679	1.045	1.5849 ²⁰		148 ^{4mm}	>112	
a257	2-Aminophenol	$\text{H}_2\text{NC}_6\text{H}_4\text{OH}$	109.13	13, 354			170–174			2 aq; 4.3 alc; v s eth; sl s bz
a258	3-Aminophenol	$\text{H}_2\text{NC}_6\text{H}_4\text{OH}$	109.13	13, 401			122–123	164 ^{11mm}		2.5 aq; v s alc, eth
a259	4-Aminophenol	$\text{H}_2\text{NC}_6\text{H}_4\text{OH}$	109.13	13, 427			190	284 d		0.65 aq; s alc, eth
a260	4'-Aminophenylacetonitrile	$\text{H}_2\text{NC}_6\text{H}_4\text{CH}_2\text{CN}$	132.17	14, 457			44	312		sl s hot aq; s alc
a261	1-(3-Aminophenyl)-ethanol	$\text{H}_2\text{NC}_6\text{H}_4\text{CH}(\text{CH}_3)\text{OH}$	137.18	13 ³ , 1654			68–71			
a262	2-Amino-1-phenylethanol	$\text{C}_6\text{H}_5\text{CH}(\text{CH}_2\text{NH}_2)\text{OH}$	137.18	13 ² , 361			56–57	160 ^{17mm}		v s aq; s alc
a263	1S,2S-(+)-2-Amino-1-phenyl-1,3-propanediol	$\text{C}_6\text{H}_5\text{CH}(\text{OH})\text{CH}(\text{NH}_2)\text{CH}_2\text{OH}$	167.21				109–113			
a264	L-2-Amino-3-phenyl-1-propanol	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}(\text{NH}_2)\text{CH}_2\text{OH}$	151.21	13 ³ , 1757			92–94			
a265	3-Amino-1-phenyl-2-pyrazolin-5-one		175.19				210–215			
a266	N-Aminophthalimide		162.15				200–202			
a267	N-Aminopiperidine		100.17	20, 89	0.928	1.4750 ²⁰		146 ^{730mm}	36	
a268	3-Amino-1,2-propanediol	$\text{H}_2\text{NCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$	91.11	4, 301	1.175	1.4920 ²⁰		265 ^{739mm}	>112	

a269	DL-1-Amino-2-propanol	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{NH}_2$	75.11	4, 289	0.973	1.4483 ²⁰	−2	160	73	s aq, alc; i eth
a270	DL-2-Amino-1-propanol	$\text{CH}_3\text{CH}(\text{NH}_2)\text{CH}_2\text{OH}$	75.11	4 ¹ , 432	0.943	1.4495 ²⁰		173–176		v s aq, alc, eth
a271	L-2-Amino-1-propanol	$\text{CH}_3\text{CH}(\text{NH}_2)\text{CH}_2\text{OH}$	75.11	4 ¹ , 432	0.965	1.4495 ²⁰		176	62	v s aq, alc, eth
a272	3-Amino-1-propanol	$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$	75.11	4, 288	0.982	1.4598 ²⁰	12	188	79	s aq, alc
a273	2-Amino-1-propene-1,1,3-tricarbonitrile	$\text{NCC}(\text{CN})=\text{C}(\text{NH}_2)-\text{CH}_2\text{CN}$	132.13				171–173			s aq
a274	3-Aminopropionitrile	$\text{H}_2\text{NCH}_2\text{CH}_2\text{CN}$	70.09					185		
a275	3-Aminopropyl-(diethoxy)methylsilane	$\text{H}_2\text{N}(\text{CH}_2)_3\text{Si}(\text{CH}_3)_2(\text{OCH}_2\text{CH}_3)_2$	191.4		0.916 ²⁰ ₄	1.427 ²⁰		85–88 ^{8mm}		
a276	N-(3-Aminopropyl)-iminodiethanol	$\text{H}_2\text{N}(\text{CH}_2)_3\text{N}-(\text{CH}_2\text{CH}_2\text{OH})_2$	162.23		0.1071	1.4980 ²⁰		170 ^{2mm}	137	
a277	N-(3-Aminopropyl)-morpholine		144.22		0.9872 ²⁰ ₂₀	1.4761 ²⁰	−15	224	98	misc aq, alc, bz
a278	N-(3-Aminopropyl)-2-pyrrolidinone		142.20		1.014	1.5000 ²⁰		120–123 ^{1mm}	>112	

5-Aminoorotic acid, a160

1-Aminopentane, p53

4-Aminophenyl phenyl ether, p70

Aminophenyl sulfones, d36, d37

3-Aminophthalhydrazide, a153

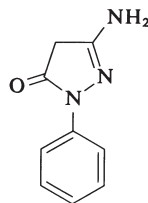
Aminopicolines, a225, a226, a227

1-Aminopropane, p220

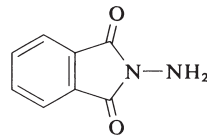
2-Aminopropane, i88

3-Amino-1-propene, a82

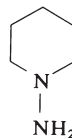
N-(3-Aminopropyl)diethanolamine, a276



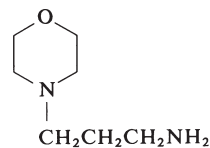
a265



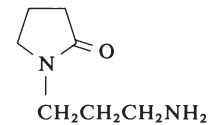
a266



a267



a277



a278

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

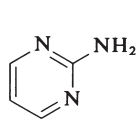
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a279	3-Aminopropyl-triethoxysilane	$\text{H}_2\text{N}(\text{CH}_2)_3\text{Si}(\text{OC}_2\text{H}_5)_3$	221.37		0.9506 ₄ ²⁰	1.4225 ²⁰		217	96	
a280	3-Aminopropyl-trimethoxysilane	$\text{H}_2\text{N}(\text{CH}_2)_3\text{Si}(\text{OCH}_3)_3$	179.2		1.01 ₄ ²⁵	1.420 ²⁵		80 ^{8mm}	104	
a281	2-Aminopyridine	$(\text{C}_5\text{H}_4\text{N})\text{NH}_2$	94.12	22, 428			58.1	210.6	92	s aq, alc, bz, eth
a282	3-Aminopyridine	$(\text{C}_5\text{H}_4\text{N})\text{NH}_2$	94.12	22, 431			64	248		s aq, alc, bz, eth
a283	4-Aminopyridine	$(\text{C}_5\text{H}_4\text{N})\text{NH}_2$	94.12	22, 433			155–158	273		s aq, alc; sl s bz, eth
a284	2-Aminopyrimidine		95.11	24, 80			123–126	subl		v s aq
a285	4-Aminoquinaldine		158.20	22, 453			169	333		sl s aq; v s alc, eth, acet; s hot bz
a286	4-Aminosalicyclic acid	$\text{H}_2\text{NC}_6\text{H}_3(\text{OH})\text{COOH}$	153.14	14, 579			147 d			0.2 aq; 4.8 alc; s dil acid, alk
a287	5-Aminosalicyclic acid	$\text{H}_2\text{NC}_6\text{H}_3(\text{OH})\text{COOH}$	153.14	14, 579			280 d			sl s aq, alc; s acid
a288	2-Amino-3-sulfopropionic acid	$\text{HOOCCH}(\text{NH}_2)\text{CH}_2\text{SO}_3\text{H}$	187.17	4, 533			260 d			v s aq
a289	5-Amino-1,2,3,4-tetraazole hydrate		103.08	26, 403			204 d			
a290	5-Amino-1,3,4-thiadiazole-2-thiol		133.20	27, 674			235 d			
a291	2-Aminothiazole		100.14	27, 155			93			sl s aq, alc, eth
a292	2-Amino-2-thiazole		100.14	27, 136			91–93			
a293	2-Aminothiophenol	$\text{H}_2\text{NC}_6\text{H}_4\text{SH}$	125.19	13, 397		1.6405 ²⁰	26	234	79	
a294	6-Amino-3-toluene-sulfonic acid	$\text{H}_2\text{NC}_6\text{H}_3(\text{CH}_3)\text{SO}_3\text{H}$	187.22	14, 723			>300			1 aq ¹² ; v s hot aq
a295	3-Amino-1,2,4-triazole		84.08	26, 137			159			s aq, alc, chl

a296	5-Amino-2,2,4-trimethyl-1-cyclopent- anemethylamine		156.27		0.901	1.4733 ²⁰		221	97	
a297	11-Aminoundecanoic acid	H ₂ N(CH ₂) ₁₀ COOH	201.31					190–192		
a298	Aniline	C ₆ H ₅ NH ₂	93.13	12, 59	1.0217 ²⁰	1.5855 ²⁰	–5.98	184.40	70	3.5 aq ²⁵ ; s alc, CCl ₄ , eth, acids
a299	Aniline hydrochloride	C ₆ H ₄ NH ₂ ·HCl	129.59		1.222		198		193	100 aq; v s alc
a300	2-Anilinoethanol	C ₆ H ₅ NHCH ₂ CH ₂ OH	137.18	12, 182	1.085	1.5793 ²⁰		150– 152 ^{10mm}	>112	sl s aq; v s alc, chl, eth
a301	3-Anilinopropio- nitrile	C ₆ H ₅ NHCH ₂ CH ₂ CN	146.19				52–53			

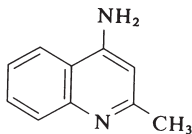
6-Aminopurine, a69
 2-Amino-3-pyridinol, a197
 Aminopyrimidinediols, a154, a155
 2-Aminosuccinamic acid, a313
 Aminosuccinic acid, a314
 6-Amino-2-thiouracil, a191
 α -Amino-*p*-toluenesulfonamide, a210
 2-Amino-1,1,3-tricyanopropene, a273
 1-Aminotricyclo[3.3.1.1^{3,7}]decane, a66

Aminouracil, a155
 2-Aminovaleric acid, a253
 5-Aminovaleric acid, a254
 Amyl compounds, *see* Pentyl
 Amyl alcohol, p37
act-Amyl alcohol, m153
sec-Amyl alcohol, p38
tert-Amyl alcohol, m154
tert-Amylamine, d601

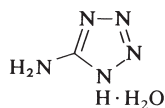
Amyl bromides, b322, b323
 Amyl chloride, c191
 Amyl iodide, i47
 Amyl mercaptan, p35
 Amyl methyl ketone, h15
 Anethole, m97
 Angelic acid, m162
 Anilinesulfonic acids, a118, a119, a120
 Aniline-2,5-disulfonic acid, a117



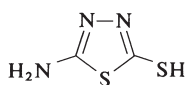
a284



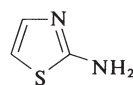
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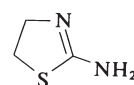
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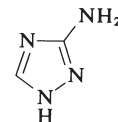
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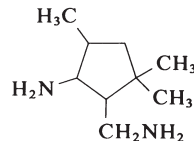
a291



a292



a295



a296

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

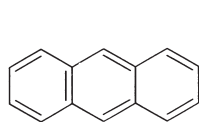
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a302	1-(<i>o</i> -Anisidino)-1,3-butanedione	$\text{CH}_3\text{OC}_6\text{H}_4\text{NHCOC}_2\text{H}_4\text{COCH}_3$	207.23	13 ¹ , 117			84–85			
a303	1-(<i>p</i> -Anisidino)-1,3-butanedione	$\text{CH}_3\text{OC}_6\text{H}_4\text{NHCOC}_2\text{H}_4\text{COCH}_3$	207.23	13 ¹ , 177			115–117			
a304	Anthracene		178.23	5, 657	1.25 ₄ ²⁷		216.3	340		i aq; 1.5 alc; 1.6 bz; 1.2 chl; 3.1 CS ₂
a305	9,10-Anthracene-dione		208.22	7, 781	1.43 ₄ ²⁰		286	377	185	i aq; 0.44 alc; 0.26 bz; 0.61 chl; 0.11 eth
a306	9,10-Anthraquinone-1,5-disulfonic acid disodium salt		412.31	11, 340			>300			s aq
a307	9,10-Anthraquinone-2,6-disulfonic acid disodium salt		412.31	11, 342			>325			s aq
a308	9,10-Anthraquinone-2-sulfonic acid Na salt		310.26							
a309	Antipyrine		188.23	24, 27	1.088 ₄ ¹¹³		114	319 ^{174mm}		100 aq; 77 alc; 100 chl; 2.3 eth
a310	L-(+)-Arabinose		150.13	31, 32			160–163			100 aq
a311	L-(+)-Arginine	$\text{H}_2\text{NC}(=\text{NH})\text{NH}(\text{CH}_2)_3\text{CH}(\text{NH}_2)\text{COOH}$	174.20	4, 420			223 d			17.6 aq; sl s alc
a312	L-(+)-Ascorbic acid		176.12				190–192 d			100 aq; 3.3 alc
a313	L-(+)-Asparagine hydrate	$\text{H}_2\text{NCOCH}_2\text{CH}(\text{NH}_2)\text{COOH} \cdot \text{H}_2\text{O}$	150.14	4, 484			233–235			3.6 aq ²⁸ ; s alk acids; i alc, bz, eth

a314	L-(+)-Aspartic acid	$\text{HOOCCH}_2\text{CH}(\text{NH}_2)\text{COOH}$	133.10	4, 472			270 sealed tube 114–116		0.45 aq; i alc, eth
a315	Atropine		289.38	21, 27					0.22 aq; s bz, dil acid

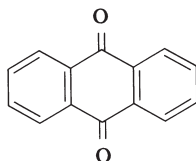
Anisaldehydes, m45, m46
 Anisamide, m47
 Anisic acids, m50, m51, m52
 Anisidines, m42, m43, m44
 Anisole, m48
p-Anisoyl chloride, m53

p-Anisyl alcohol, m54
 Anthraflavic acid, d374
 Anthranilamide, a114
 Anthranilic acid, a121
 Anthranionitrile, a124
 9,10-Anthraquinone, a305

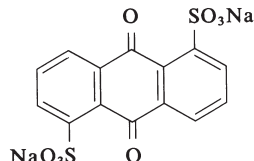
APDC, p271
 Araboascorbic acid, i59
 Aspirin, a56
 Arsanilic acids, a115, a116



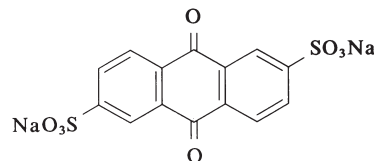
a304



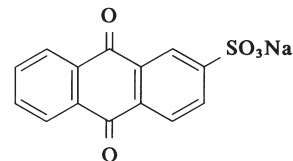
a305



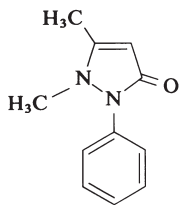
a306



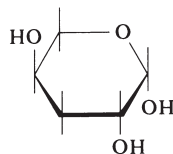
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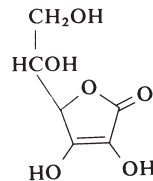
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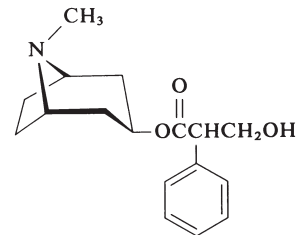
a309



a310



a312



a315

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
a316	Aurintricarboxylic acid, triammonium salt		473.44	10 ² , 775			225 d			v s aq
a317	2-Azacyclooctanone		127.19	21, 242			35–38	148 ^{10mm}		
a318	2-Azacyclotri-decanone		197.32				150–153			
a319	Azidotrimethylsilane	(CH ₃) ₃ SiN ₃	115.21		0.868	1.4142 ²⁰	–95	95–96	23	
a320	Azidotriphenylsilane	(C ₆ H ₅) ₃ SiN ₃	301.4				83–84	100 ^{0.01mm}		
a321	1-Aziridineethanol	(CH ₂) ₂ =NCH ₂ CH ₂ OH	87.12		1.088	1.4560 ²⁰		168	67	
a322	<i>cis</i> -Azobenzene	C ₆ H ₅ N=NC ₆ H ₅	182.23	16, 8	1.20		68.3	293		i aq; s alc, eth, HOAc
a323	2,2'-Azobis(2-methyl)-propionitrile	(CH ₃) ₂ C(CN)N=N-C(CN)(CH ₃) ₂	164.21	4, 563				107 d		2 EtOH; 5 MeOH; can explode in acetone
a324	Azodicarbonamide	H ₂ NCON=NCONH ₂	116.08	3, 123			225 d			
a325	4,4'-Azoxydianisole	CH ₃ OC ₆ H ₄ N=N(→O)-C ₆ H ₄ OCH ₃	258.28	16, 637			120			
a326	Azulene		128.17	5 ² , 432			100.5	250		
b1	Barbituric acid		128.09	24, 467			248–252 d			s hot aq, dil acid
b2	Basic fuchsin		337.86	13, 765	1.22		d 186			0.3 aq; s alc, acids
b3	Benzaldehyde	C ₆ H ₅ CHO	106.12	7, 174	1.0447 ²⁰	1.5455 ²⁰	–26	178.9	62	0.3 aq; misc alc, eth
b4	Benzamide	C ₆ H ₅ CONH ₂	121.14	9, 195	1.341 ⁴		127.2	288		1.3 aq; 17 alc; 30 pyr
b5	Benzanilide	C ₆ H ₅ CONHC ₆ H ₅	197.24	12, 262	1.315		163.1	117 ^{10mm}		i aq; 1.7 alc; sl s eth
b6	1,2-Benzanthracene		228.29	5, 718			155–157	437.6		sl s hot alc; s most other org solv

b7	2,3-Benzanthracene		228.29	5 ² , 628	1.35		341	subl		sl s most org solv
b8	7 <i>H</i> -Benz[<i>de</i>]-anthracen-7-one		230.27	7, 518			170			1.6 bz; 0.5 HOAc
b8a	Benzene	C ₆ H ₆	78.11	5, 179	0.8737 ²⁵	1.4979 ²⁵	5.53	80.10	−11	0.17 aq; s most org solv
b9	Benzene- <i>d</i>	C ₆ H ₅ D	79.12			1.4980 ²⁰		80	−11	
b10	Benzene- <i>d</i> ₆	C ₆ D ₆	84.16		0.95	1.4978 ²⁰		79.1	−11	

Azacyclopropane, e131

Azelaic acid, n95

Azelonitrile, n94

Aziridine, e131

Azobis(isobutyronitrile), a323

4,4'-Azoxyanisole, a325

Barbitol, d280

Behenic acid, d716

Behenyl alcohol, d717

Benzalacetone, p96

Benzal bromide, d102

Benzalpthalide, b101

Benzanthrone, b8

Benzeneacetaldehyde, p76a

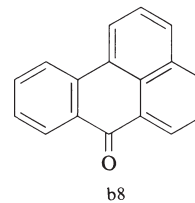
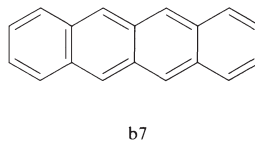
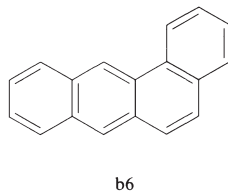
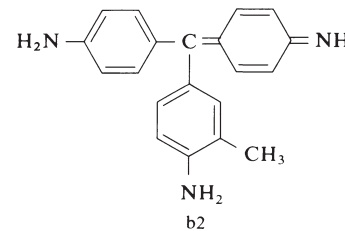
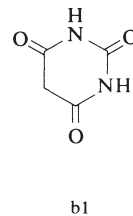
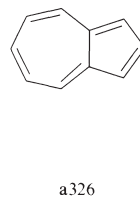
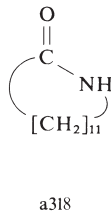
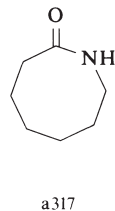
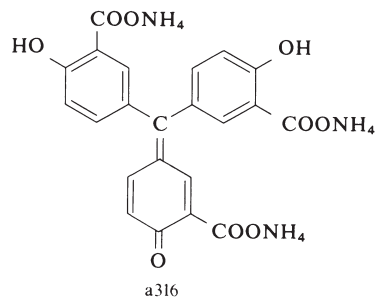


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

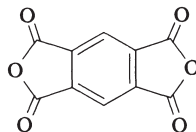
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b11	Benzenearsonic acid	$C_6H_5AsO(OH)_2$	202.04	16, 868	1.760 ²⁵		163 d	–H ₂ O on standing in air		2.5 aq; 2 alc 2.6 aq; 1.8 alc; 43 eth; s bz
b12	Benzeneboronic acid	$C_6H_5B(OH)_2$	121.93	16, 920			217 to the anhydride			
b13	1,4-Benzenedicarbaldehyde	$C_6H_4(CHO)_2$	134.13	7, 675			114	248	180	i aq; 6 bz; 17 acet; 2 eth; 14 diox; 46 MeOH 73 bz; 62 CCl ₄
b14	1,3-Benzendi-carbonyl dichloride	$C_6H_4(COCl)_2$	203.02	9, 834			43–44	276		
b15	1,4-Benzendi-carbonyl dichloride	$C_6H_4(COCl)_2$	203.02	9, 844			81	266	180	37 bz; 9 CCl ₄
b16	1,3-Benzenedicarboxylic acid	$C_6H_4(COOH)_2$	166.13	9, 832			345–348	subl		
b17	1,4-Benzendicarboxylic acid	$C_6H_4(COOH)_2$	166.13	9, 841			subl without melting		188	0.012 aq; v s alc, HOAc; i bz, PE v sl s aq, chl, eth; sl s alc; s alk
b18	1,4-Benzenedimethanol	$C_6H_4(CH_2OH)_2$	138.17	6, 919			115	143 ^{1mm}		
b19	Benzenehexacarboxylic acid	$C_6(COOH)_6$	342.17	9, 1008	1.100 ¹⁷		286 d			v s aq, alc
b20	Benzenesulfinic acid	$C_6H_5S(=O)OH$	142.16	11, 2			85	100 d		
b21	Benzenesulfonamide	$C_6H_5SO_2NH_2$	157.19	11, 39	1.3842 ¹⁵ ₁₅	1.5518	152	177 ^{100mm}	>112	i aq; sl s alc; s eth v s aq, alc; sl s bz i aq; s alc, eth
b22	Benzenesulfonic acid	$C_6H_5SO_2OH$	158.18	11, 26			50–51			
b23	Benzenesulfonyl chloride	$C_6H_5SO_2Cl$	176.62	11, 34	1.3286 ²⁰ ₄	1.4932 ¹⁸	14.5	203–204		s alc, eth
b24	Benzenesulfonyl fluoride	$C_6H_5SO_2F$	160.16	11 ² , 23						

b25	Benzenesulfonyl hydrazide	$C_6H_5SO_2NHNH_2$	172.21	11, 52			101–103		flammable solid
b26	1,2,4,5-Benzenetetracarboxylic acid	$C_6H_2(COOH)_4$	254.15	9, 997			276		1.5 aq; v s alc
b27	1,2,4,5-Benzenetetracarboxylic anhydride		218.12	19, 196			283–286	397–400	
b28	1,2,3-Benzenetricarboxylic acid dihydrate	$C_6H_3(COOH)_3 \cdot 2H_2O$	246.18	9, 976			192 d		sl s aq; v s eth
b29	1,2,4-Benzenetricarboxylic acid	$C_6H_3(COOH)_3$	210.14	9, 977			321 d		2.1 aq; 25.3 alc; 7.9 acet; v s eth
b30	1,3,5-Benzenetricarboxylic acid	$C_6H_3(COOH)_3$	210.14	9, 978			>330		sl s aq; v s alc; s eth
b31	1,2,4-Benzenetricarboxylic anhydride		192.13	18, 468			161–164	245 ^{14mm}	50 acet; 22 EtAc

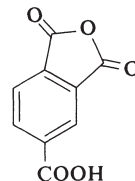
Benzenediazobenzene, a322
Benzenecarbonitrile, b51

Benzene-1,2-dicarboxylic acid, p167
Benzenemethanol, b78

Benzenethiol, t159



b27



b31

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b32	1,3,5-Benzenetricarboxylic trichloride	$C_6H_3(COCl)_3$	265.48				35–36			
b33	Benzethonium chloride	$(CH_3)_3CCH_2C(CH_3)_2C_6H_4OCH_2CH_2OCH_2CH_2N^+(CH_3)_2CH_2C_6H_5Cl^-$	448.10				164–166			v s aq; s alc, acet
b34	Benzil	$C_6H_5COCOC_6H_5$	210.23	7, 747	1.23 ₄ ¹⁵		94.9	346		i aq; s alc, eth
b35	Benzil- α -dioxime	$C_6H_5C(=NOH)C(=NOH)C_6H_5$								s alk
b36	Benzilic acid	$(C_6H_5)_2C(OH)COOH$	228.25	10, 342			153			sl s aq; v s alc, eth
b37	Benzil monohydrazone	$C_6H_5C(=NNH_2)COC_6H_5$	224.26	7 ¹ , 394			150–152			
b38	Benzimidazole		118.14	23, 131			170.5	>360		sl s aq, eth; v s alc
b39	Benzo-15-crown-5		268.3				76–78			
b40	7,8-Benzo-1,3-diazaspiro-[4,5]decane-2,4-dione		216.24				268–270			
b41	1,4-Benzodioxan		136.15		1.142	1.5485 ²⁰		103 ^{6mm}	87	
b42	2,3-Benzofuran		118.14	17, 54	1.072	1.5660 ²⁰	<–18	175		i aq; misc bz, eth, PE
b43	Benzofurazan-1-oxide		136.11	27 ¹ , 740			69–71			
b44	Benzoic acid	C_6H_5COOH	122.13	9, 92	1.080		122.4	132.5 ^{10mm}	121	0.29 aq; 43 alc; 10 bz; 22 chl; 33 eth; 33 acet
b45	Benzoic anhydride	$(C_6H_5CO)_2O$	226.23	9, 164	1.199		39–40	360		i aq; s alc, acet, chl, bz, HOAc
b46	DL-Benzoin	$C_6H_5COCHOHC_6H_5$	212.25	8, 165	1.3100 ₄ ²⁰		134–136	344		s acet; 20 pyr
b47	Benzoin ethyl ether	$C_6H_5CH(OC_2H_5)COC_6H_5$	240.30	8, 174	1.1016 ₄ ¹⁷	1.5727 ¹⁷	61	195 ^{20mm}		s alc, bz, eth

b48	Benzoin isobutyl ether	$C_6H_5CH[OCH_2CH(CH_3)_2]COC_6H_5$	268.36		0.985	1.5485 ²⁰		133 ^{0.5mm}	85	
b49	Benzoin methyl ether	$C_6H_5CH(OCH_3)COC_6H_5$	226.28	8, 174	1.1278 ¹⁴		48	189 ^{15mm}		v s alc, bz, eth
b50	α -Benzoinoxime	$C_6H_5CH(OH)C(=NOH)-C_6H_5$	227.26	8, 175			151–152			sl s aq; s alc, NH_4OH
b51	Benzonitrile	C_6H_5CN	103.12	9, 275	1.0006 ²⁵	1.5257 ²⁵	–12.75	191.1	71	0.2 aq; misc alc, bz, chl, eth
b52	Benzo[<i>def</i>]phenanthrene		202.26	5, 693	1.271 ²³			156	404	i aq; s alc, eth
b53	Benzophenone	$C_6H_5COC_6H_5$	182.22	7, 411	1.1108 ¹⁵		48.1	305		i aq; 13.3 alc; 17 eth
b54	Benzophenone hydrazone	$C_6H_5C(=NNH_2)C_6H_5$	196.25	7, 417			98	230 ^{55mm}		

Benzhydrazide, b72

Benzhydrol, d677

Benzhydramine, d678

Benzhydryl bromide, b274

Benzidine, b136

2-Benzimidazolethiol, m15

1,3-Benzodiazole, b38

1,3,2-Benzodioxaborole, c21

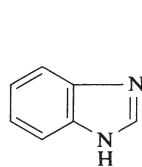
1,3-Benzodioxole, m240

Benzofuroxan, b43

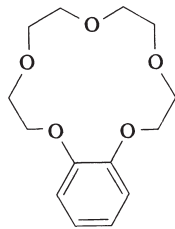
Benzoglyoxaline, b38

Benzoic acid hydrazide, b72

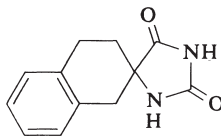
o-Benzoic sulfimide, s1



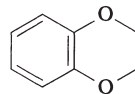
b38



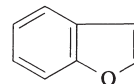
b39



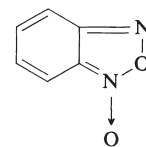
b40



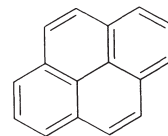
b41



b42



b43



b52

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

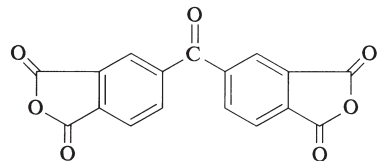
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b55	3,3',4,4'-Benzophenonetetracarboxylic dianhydride		322.23				215–217			
b56	1-Benzopyran-4(4 <i>H</i>)-one		146.15	17, 327			55–57			
b57	1,2-Benzo[<i>a</i>]pyrene		252.32				179.3	495		i aq; s bz; sl s alc
b58	4,5-Benzo[<i>e</i>]pyrene		252.32				182			i aq
b59	1,4-Benzoquinone	O=C ₆ H ₄ =O	108.10	7, 609	1.318 ₄ ²⁰		115.7			sl s aq; s alc, eth, hot bz, alk (with d)
b60	Benzothiazole		135.19		1.246 ₄ ²⁰	1.6379 ²⁰	2	231	>112	sl s aq; v s alc, CS ₂
b61	Benzo[<i>b</i>]thiophene		134.20	17, 59	1.1937 ⁴⁰	1.6302 ⁴⁰	31.32	221		s alc, bz, chl, eth
b62	1,2,3-Benzotriazole		119.13	26, 38	1.238	1.6420 ²⁰	98.5	204 ^{15mm}		sl s aq; s alc, bz, chl
b63	Benzoxazole		119.12	27, 42		1.5594	30	182	58	sl s aq
b64	1-Benzoylacetone	C ₆ H ₅ COCH ₂ COCH ₃	162.19	7, 680	1.090 ₆₀ ⁶⁰		60	260 sl d		sl s aq; v s alc, eth
b65	2-Benzoylbenzoic acid	C ₆ H ₅ COC ₆ H ₄ COOH	226.23	10, 747			129	265		sl s aq; v s alc, eth
b66	Benzoyl bromide	C ₆ H ₅ COBr	185.03	9, 195	1.5467 ²⁰			218–219	90	d aq, alc; misc eth
b67	Benzoyl chloride	C ₆ H ₅ COCl	140.57	9, 182	1.211 ₄ ²⁰	1.5525 ²⁰	–1.0	197.2	68	d aq, alc; misc bz, CS ₂ , eth
b68	Benzoyl cyanide	C ₆ H ₅ COCN	131.13	10, 659			32	206		i aq
b69	Benzoyl fluoride	C ₆ H ₅ COF	124.11	9, 181	1.140	1.4960 ²⁰	–28	161	48	d hot aq; v s alc, eth
b70	Benzoylformic acid	C ₆ H ₅ COCOOH	150.13	10, 654			69			
b71	<i>N</i> -Benzoylglycine	C ₆ H ₅ CONHCH ₂ COOH	179.18	9, 225			178–179			0.4 aq; 0.1 chl; 0.25 eth; sl s alc; i bz, PE
b72	Benzoylhydrazine	C ₆ H ₅ CONHNH ₂	136.15	9, 319			117			

b73	3-Benzoylpropionic acid	$C_6H_5COCH_2CH_2COOH$	178.19	10, 696			116			sl s aq; s alc
b74	2-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 330			44	317	150	
b75	3-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 331			40	307	150	s alc, bz, eth
b76	4-Benzoylpyridine	$C_6H_5CO(C_5H_4N)$	183.21	21, 331			71	315	150	s alc, bz, eth
b77	Benzyl acetate	$CH_3COOCH_2C_6H_5$	150.18	6, 435	1.0515 ²⁵	1.5232 ²⁰	-51.5	215.5	102	sl s aq; misc alc, eth
b78	Benzyl alcohol	$C_6H_5CH_2OH$	108.13	6, 428	1.0413 ²⁵	1.5371 ²⁵	-15.3	205.45	100	0.08 aq; misc alc, eth
b79	Benzylamine	$C_6H_5CH_2NH_2$	107.16	12, 1013	0.981 ¹⁹ ₄	1.5424 ²⁰	10	185	60	misc aq, alc, eth
b80	2-Benzylaminoethanol	$C_6H_5CH_2NHCH_2CH_2OH$	151.21	12, 1040	1.065	1.5435 ²⁰		156 ^{12mm}	>112	
b81	(3-Benzylamino)-propionitrile	$C_6H_5CH_2NHCH_2CH_2CN$	160.22			1.5308 ²⁰				

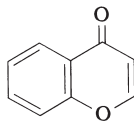
Benzoresorcinol, d386
2-Benzothiazolethiol, m17
Benzotrichloride, t248

Benzotrifluoride, t300
Benzoylamide, b4
Benzoylbenzene, b53

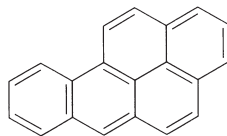
Benzoyl peroxide, d54
1,2-Benzphenanthrene, b6
Benzylaniline, p92



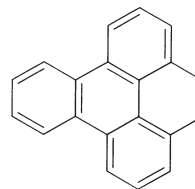
b55



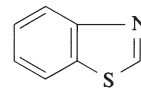
b56



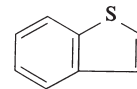
b57



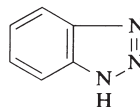
b58



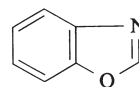
b60



b61



b62



b63

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b82	<i>N</i> -Benzylbenzamide	$C_6H_5CONHCH_2C_6H_5$	211.26				106			
b83	Benzyl benzoate	$C_6H_5COOCH_2C_6H_5$	212.25	9, 121	1.118_4^{25}	1.5681^{21}	19.4	323.5	147	i aq; misc alc, chl, eth
b84	2-Benzylbenzoic acid	$C_6H_5CH_2C_6H_4COOH$	212.24	9 ² , 471			110–113			sl s aq; s alc, bz, chl, eth
b85	Benzyl bromide	$C_6H_5CH_2Br$	171.04	5, 306	1.438_0^{22}	1.5752^{20}	−3.9	198–199	86	sl d aq
b86	Benzyl- <i>tert</i> -butanol	$C_6H_5CH_2CH_2-C(CH_3)_3OH$	164.25	6, 548		1.5090^{20}	33	144 ^{85mm}	>112	
b87	Benzyl butyl-1,2-phthalate	$C_6H_5CH_2OOC C_6H_4COOC_4H_9$	312.37		1.119_{25}^{25}				218	
b88	Benzyl carbamate	$C_6H_5CH_2OCONH_2$	151.17	6, 437			87–89	220 d		i aq; v s alc; sl s eth
b89	Benzyl chloride	$C_6H_5CH_2Cl$	126.59	5, 292	1.0993^{20}	1.5391^{20}	−43 to −48	179	73	i aq; misc alc, chl, eth
b90	Benzyl chloroformate	$C_6H_5CH_2OC(O)Cl$	170.60	6, 437	1.195	1.5190^{20}		103 ^{20mm}	91	d aq; s eth
b91	Benzyl chlorothiolfomate	$C_6H_5CH_2S(COCl)$	186.5		1.237_4^{30}	1.5711^{30}		80 ^{0.13mm}	118	
b92	<i>S</i> -Benzyl-L-cysteine	$C_6H_5CH_2SCH_2-CH(NH_2)COOH$	211.28	6, 465			214 d			
b93	Benzyl diethyl phosphite	$C_6H_5CH_2P(O)(OC_2H_5)_2$	228.23		1.076	1.4930^{20}		110 ^{2mm}	>112	
b94	Benzyltrimethylstearylammonium chloride	$C_6H_5CH_2N[(CH_2)_{17}CH_3](CH_3)_2Cl \cdot H_2O$	442.18	12 ³ , 2212			67–69			
b95	Benzyl ethyl ether	$C_6H_5CH_2OC_2H_5$	136.20		0.9478^{20}	1.4958^{20}		185.0		i aq; misc alc, eth
b96	<i>N</i> -Benzylformamide	$C_6H_5CH_2NHCHO$	135.17	12, 1043			60–61			
b97	Benzyl formate	$C_6H_5CH_2OOCH$	136.15		1.081_4^{20}			203		i aq; s alc; misc eth
b98	<i>O</i> -Benzylhydroxylamine	$C_6H_5CH_2ONH_2$	123.16	6, 440				119 ^{30mm}		

b99	Benzylidenemalononitrile	$C_6H_5CH=C(CN)_2$	154.17	9, 895			83–85		
b100	<i>N</i> -Benzylidenemethylamine	$C_6H_5CH=NCH_3$	119.17	7, 213	0.967	1.5526 ²⁰		80 ^{18mm}	>112
b101	3-Benzylidene-phthalide		222.24	17, 376			102		
b102	2-Benzyl-2-imidazoline HCl		196.68				174		v s aq, alc; s chl; v sl s eth, EtAc
b103	Benzylmethylamine	$C_6H_5CH_2NHCH_3$	138.23	12, 1019	0.939	1.5224 ²⁰		184.189	77
b104	3-(<i>N</i> -Benzyl- <i>N</i> -methylamino)-1,2-propanediol	$C_6H_5CH_2N(CH_3)-CH_2CH(OH)CH_2OH$	195.26		1.084	1.5341 ²⁰		206 ^{30mm}	>112
b105	Benzyl methyl sulfide	$C_6H_5CH_2SCH_3$	138.23	6, 453	1.015	1.5620 ²⁰		195–198	73
b106	3-Benzzyloxyaniline	$C_6H_5CH_2OC_6H_4NH_2$	199.25	13, 404			63–67		
b107	3-Benzzyloxybenzaldehyde	$C_6H_5CH_2OC_6H_4CHO$	212.25	8, 73			56–58		
b108	4-Benzzyloxybenzaldehyde	$C_6H_5CH_2OC_6H_4CHO$	212.25	8, 73			73–74		

Benzyl cyanide, p80

Benzyl disulfide, d57

N-Benzylethanolamine, b20

Benzyl ether, d58

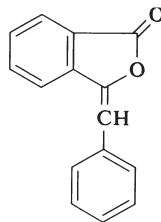
Benzylideneacetone, p96

Benzylideneacetophenone, d686

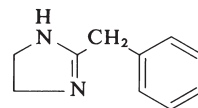
Benzyl mercaptan, p128

Benzyl methyl ketone, p144

Benzzyloxyamine, b98



b101



• HCl

b102

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b109	4-Benzyloxybenzyl alcohol	$C_6H_5CH_2OC_6H_4CH_2OH$	214.26				86–87			
b110	2-Benzyloxyethanol	$C_6H_5CH_2OCH_2CH_2OH$	152.19		1.07 ²⁰ ₂₀			255.9	129	0.4 aq
b111	4-Benzyloxy-3-methoxybenzaldehyde	$C_6H_5CH_2OC_6H_3(OCH_3)CHO$	242.27				63–65			
b112	4'-Benzyloxypropio-phenone	$C_6H_5CH_2OC_6H_4COC_2H_5$	240.30				100–102			
b113	Benzyl phenyl sulfide	$C_6H_5CH_2SC_6H_5$	200.30	6, 454			43	197 ^{27mm}		i aq; sl s alc; s eth
b114	1-Benzylpiperazine		176.26		1.014	1.5467 ²⁰			>112	s aq, alc, eth
b115	4-Benzylpiperidine		175.28	20, 296	0.997	1.5379 ²⁰	7	279	>112	
b116	1-Benzyl-4-piperidone		189.26		1.021	1.5399 ²⁰		134 ^{7mm}	>112	
b117	2-Benzylpyridine	$C_6H_5CH_2(C_5H_4N)$	169.23	20, 425	1.054	1.5785 ²⁰	10	276	125	i aq; v s alc, eth
b118	4-Benzylpyridine	$C_6H_5CH_2(C_5H_4N)$	169.23	20, 426	1.061 ²⁰ ₀	1.5818 ²⁰		287	115	s alc; v s eth
b119	1-Benzyl-2-pyrrolidinone		175.23		1.095	1.5525 ²⁰			>112	
b120	(Benzylthio)acetic acid	$C_6H_5CH_2SCH_2COOH$	182.24				59–63			
b121	Benzyl thiocyanate	$C_6H_5CH_2SCN$	149.22	6, 460			43	235		i aq; s alc; v s eth
b122	Benzyltributylammonium chloride	$C_6H_5CH_2N(C_4H_9)_3^+Cl^-$	312.94				155 d			
b123	Benzyltrichlorosilane	$C_6H_5CH_2SiCl_3$	225.57		1.288 ²⁰ ₄	1.526 ²⁰		140–142 ^{100mm}		
b124	Benzyltriethoxysilane	$C_6H_5CH_2Si(OC_2H_5)_3$	254.40		0.986 ²⁰ ₄			170–175 ^{70mm}		
b125	Benzyltriethylammonium chloride	$C_6H_5CH_2N(C_2H_5)_3^+Cl^-$	227.78				185 d			
b126	Benzyltrimethylammonium chloride	$C_6H_5CH_2N(CH_3)_3^+Cl^-$	185.70	12, 1020						

b127	Benzyltrimethylsilane	$C_6H_5CH_2Si(CH_3)_3$	164.32		0.8933 ²⁰	1.4941 ²⁰		190–191		
b128	Betaine	$(CH_3)_3N^+CH_2COO^-$	117.15	4, 347			d > 310			160 aq; 55 MeOH; 6 alc
b129	Bicyclo[2.2.1]hepta-2,5-diene		92.14		0.909 ²⁰	1.4707 ²⁰	–20	89	–21	i aq; s PE
b130	Bicyclo[2.2.1]-2-heptene		94.16				46	96	–15	s eth
b131	Bicyclo[2.2.1]-5-heptene-2-carbaldehyde		122.16		1.018	1.4883 ²⁰		67– 70 ^{12mm}	51	

Benzylphenol, h113
 BES, b180
 Betahistine, m121

o,o-Bibenzoic acid, b137
 Bibenzyl, d666
 Bicine, b182

Bicyclo[4.4.0]decane, d1, d2

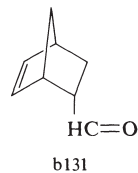
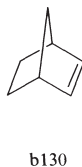
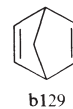
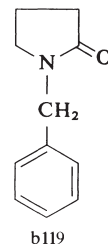
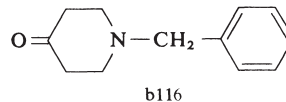
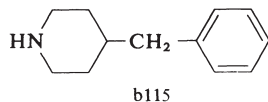
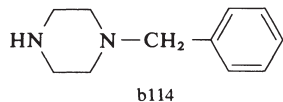


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b132	Bicyclo[2.2.2]oct-7-ene-2,3,5,6-tetracarboxylic-2,3,5,6-dianhydride		248.19				>300			
b133	Biguanide	$\text{H}_2\text{NC}(=\text{NH})\text{NHC}(=\text{NH})\text{NH}_2$	101.11	3, 93			130	d 142		s aq, alc; i bz, eth
b134	Biphenyl	$\text{C}_6\text{H}_5-\text{C}_6\text{H}_5$	154.20	5, 578	0.9939 ⁷⁰	1.588 ⁷⁷	68.8	255.0		i aq; s alc, eth
b135	4-Biphenylcarboxylic acid	$\text{C}_6\text{H}_5\text{C}_6\text{H}_4\text{COOH}$	198.22	9, 671			226	subl		i aq; v s alc, eth; s bz
b136	(1,1'-Biphenyl)-4,4'-diamine	$\text{H}_2\text{NC}_6\text{H}_4\text{C}_6\text{H}_4\text{NH}_2$	184.23	13, 214			128	400 ^{740mm}		0.04 aq; s alc; 2 eth
b137	(1,1'-Biphenyl)-2,2'-dicarboxylic acid	$\text{HOOC}\text{C}_6\text{H}_4\text{C}_6\text{H}_4\text{COOH}$	242.23	9, 922			228–229			0.06 aq; s org solv
b138	4-Biphenylmethanol	$\text{C}_6\text{H}_5\text{C}_6\text{H}_4\text{CH}_2\text{OH}$	184.24	6 ² , 636			101			
b139	4-Biphenylsulfonic acid	$\text{C}_6\text{H}_5\text{C}_6\text{H}_4\text{SO}_3\text{H}$	234.26				138			
b140	2-(4-Biphenyl)-5-(4- <i>tert</i> -butylphenyl)-1,3,4-oxadiazole		354.46				138			
b141	<i>o</i> -Biphenyl glycidyl ether		226.28				30–32	120 ^{0.1mm}		
b142	2-(4-Biphenyl)-5-phenyloxazole		197.36				118			
b143	2,2'-Bipyridinium chlorochromate	$\text{C}_5\text{H}_4\text{N}-\text{C}_5\text{H}_4\text{NH}^+\text{CrClO}_3^-$	292.64							
b144	2,2-Bis[<i>p</i> -(allyloxy)phenyl]propane	$\text{H}_2\text{C}=\text{CHCH}_2\text{OC}_6\text{H}_4\text{C}(\text{CH}_3)_2\text{C}_6\text{H}_4\text{OCH}_2\text{CH}=\text{CH}_2$	308.42		1.022	1.5636 ²⁰			>112	

b145	<i>N,N'</i> -Bis(3-amino-propyl)-ethylenedi-amine	$\text{H}_2\text{N}(\text{CH}_2)_3\text{NHCH}_2\text{CH}_2\text{-NH}(\text{CH}_2)_3\text{NH}_2$	174.29					118 ^{0.2mm}	
b146	<i>N,N'</i> -Bis(3-amino-propyl)piperazine		200.33	23 ² , 12	0.973	1.5015 ²⁰	15	152 ^{2mm}	
b147	<i>N,N'</i> -Bis(3-amino-propyl)-1,3-propanediamine	$\text{H}_2\text{N}(\text{CH}_2)_3\text{NHCH}_2\text{CH}_2\text{-CH}_2\text{NH}(\text{CH}_2)_3\text{NH}_2$	188.32					98–103 ^{1mm}	
b148	2,5-Bis(4-biphenyl)-oxazole		373.46				240		

Bicyclo[4.3.0]nonane, h46

Biphenol, d387

Biphenylamines, a134, a135

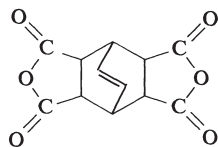
3-(*o*-Biphenyloxy)-1,2-epoxypropane, b142

2,2'-Bipyridine, d705

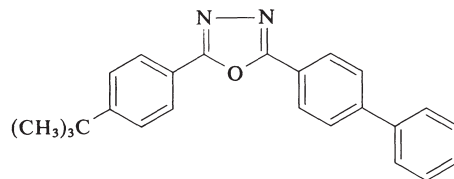
Bis(4-aminophenyl)ether, o61

1,3-Bis(aminomethyl)cyclohexane, c314

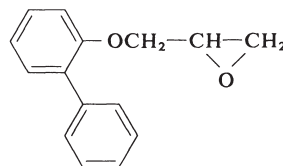
1,2-Bis(benzylamino)ethane, d59



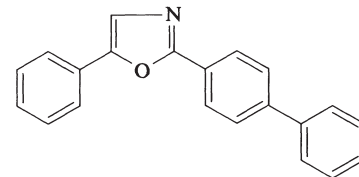
b132



b140



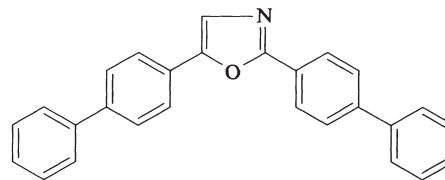
b141



142



b146



b148

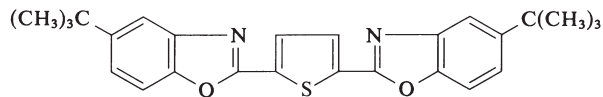
TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b149	Bis(2-bromoethyl) ether	$\text{BrCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{Br}$	231.92					103–107 ²⁰		
b150	1,3-Bis(bromoethyl)-tetramethyldi-siloxane	$[\text{BrCH}_2\text{Si}(\text{CH}_3)_2]_2\text{O}$	320.17		1.3918 ₄ ²⁰	1.4719 ²⁰		103–104 ^{15mm}		
b151	Bis(2-butoxyethyl) ether	$(\text{C}_4\text{H}_9\text{OCH}_2\text{CH}_2)_2\text{O}$	218.33		0.8853 ₂₀ ²⁰	1.4233 ²⁰	–60.2	254.6	47	0.3 aq; misc alc, eth, ketones, esters, CCl_4
b152	2,5-Bis(5- <i>tert</i> -butyl-2'-benzoxazolyl)-thiophene		430.57				201			
b153	Bis(<i>sec</i> -butyl) disulfide	$[\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)]_2\text{S}_2$	178.36	1 ³ , 1549	0.957	1.4920 ²⁰		164 ^{739mm}	>112	
b154	Bis(<i>tert</i> -butyl) disulfide	$(\text{CH}_3)_3\text{CSSC}(\text{CH}_3)_3$	178.36	1, 379	0.909	1.4930 ²⁰		204	79	
b155	Bis(carboxymethyl) trithiocarbonate	$\text{HOOCCH}_2\text{SC}(=\text{S})\text{SCH}_2\text{COOH}$	226.29	3, 252			172–175			
b156	1,2-Bis(2-chloroethoxy)ethane	$(\text{ClCH}_2\text{CH}_2\text{OCH}_2\text{—})_2$	187.07		1.197 ₄ ²⁰	1.4617		108 ^{8mm}		
b157	Bis(2-chloroethoxy)-methylsilane	$\text{H}(\text{CH}_3)\text{Si}(\text{OCH}_2\text{CH}_2\text{Cl})_2$	203.1		1.1643 ₄ ²⁰	1.4431 ²⁰		95–97 ^{18mm}		
b158	Bis(2-chloroethyl) ether	$\text{ClCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{Cl}$	143.01	1 ² , 335	1.2192 ²⁰	1.4575 ²⁰	–51.7	178.8	55	i aq; s most org solv
b159	Bis(2-chloroethyl)- <i>N</i> -methylamine	$\text{CH}_3\text{N}(\text{CH}_2\text{CH}_2\text{Cl})_2$	156.07		1.118 ₄ ²⁵		–60	75 ^{10mm}		v sl s aq; misc most org solv
b160	Bis(chloromethyl)-dimethylsilane	$(\text{CH}_3)_2\text{Si}(\text{CH}_2\text{Cl})_2$	157.12	4 ³ , 1845	1.075 ₄ ²⁰	1.4600 ²⁰		160		

b161	Bis(2-chloro-1-methyl)ethyl ether	$\text{ClCH}_2\text{CH}(\text{CH}_3)\text{OCH}(\text{CH}_3)\text{CH}_2\text{Cl}$	171.07		1.1122 ²⁰ ₂₀		187.3	85	
b162	Bis(4-chlorophenoxy)-acetic acid	$(\text{ClC}_6\text{H}_4\text{O})_2\text{CHCOOH}$	313.14			142			
b163	2,2-Bis(<i>p</i> -chlorophenyl)-1,1-dichloroethane	$(\text{ClC}_6\text{H}_4)_2\text{CHCHCl}_2$	320.05			111			
b164	1,1-Bis(4'-chlorophenyl)ethanol	$(\text{ClC}_6\text{H}_4)_2\text{C}(\text{OH})\text{CH}_3$	267.16	6 ³ , 3396		69			v sl s aq; s org solv
b165	Bis(4-chlorophenyl)sulfone	$\text{ClC}_6\text{H}_4\text{SO}_2\text{C}_6\text{H}_4\text{Cl}$	287.16	6, 327			250 ^{10mm}		
b166	Bis(4-chlorophenyl)sulfoxide	$\text{ClC}_6\text{H}_4\text{S}(\text{O})\text{C}_6\text{H}_4\text{Cl}$	271.17	6 ¹ , 149		144			
b167	1,1-Bis(<i>p</i> -chlorophenyl)-2,2,2-trichloroethane	$(\text{ClC}_6\text{H}_4)_2\text{CHCCl}_3$	354.49			109			i aq; 58 acet; 78 bz; 45 CCl ₄ ; v s pyr, diox
b168	1,3-Bis(dichloromethyl)tetramethyldisiloxane	$[\text{Cl}_2\text{CH}(\text{CH}_3)_2\text{Si}]_2\text{O}$	300.16		1.2213 ²⁰ ₄	1.4660 ²⁰	149 ^{40mm}		
b169	<i>N,N</i> -Bis(2,2-diethoxyethyl)-methylamine	$[(\text{C}_2\text{H}_5\text{O})_2\text{CHCH}_2]_2\text{-NCH}_3$	263.38	4, 311	0.945	1.4259 ²⁰	222 ^{244mm}	60	

Bis(3-*tert*-butyl-4-hydroxy-5-methylphenyl)sulfide, t144

Bis(2-cyanoethyl) ether, o63



b152

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b170	4,4'-Bis(diethyl-amino)benzo-phenone	$[(C_2H_5)_2NC_6H_4]_2C=O$	324.47	14, 98			95			
b171	4,4'-Bis(dimethyl-amino)benzo-phenone	$[(CH_3)_2NC_6H_4]_2C(=O)$	268.36	14, 89			172–176	d 360		i aq; s alc, warm bz
b172	Bis(dimethylamino)-dimethylsilane	$[(CH_3)_2N]_2Si(CH_3)_2$	146.3		0.810 ²²	1.432 ²²	–98	128–129		
b173	1,3-Bis(dimethyl-amino)-2-propanol	$[(CH_3)_2NCH_2]_2CHOH$	146.23	4, 290	0.897	1.4422 ²⁰			>112	
b174	Bis(dimethylthiocarbamyl) disulfide	$[(CH_3)_2NC(=S)S-]_2$	240.43	4, 76	1.29		155–156			s alc, eth; sl s bz, acet; i aq
b175	1,4-Bis(2,3-epoxy-propoxy)butane	$H_2C \begin{array}{c} \diagup \quad \diagdown \\ \quad O \end{array} CHCH_2- \\ OCH_2CH_2-]_2$	202.25		1.049	1.4535 ²⁰		160 ^{11mm}	>112	
b176	Bis(2-ethoxyethyl) ether	$(C_2H_5OCH_2CH_2)_2O$	162.23	1 ² , 519	0.907 ²⁰ ₄	1.4110 ²⁰	–44.3	188.4	54	v s aq, alc, org solv
b177	Bis(2-ethylhexyl) decanedioate	$CH_3(CH_2)_3CH(C_2H_5)-CH_2OOC(CH_2)_8COOCH_2-CH(C_2H_5)(CH_2)_3CH_3$	426.66		1.9119 ²⁵ ₂₅	1.4496 ²⁵				
b178	Bis(2-ethylhexyl) hydrogen phosphate	$[CH_3(CH_2)_3CH(C_2H_5)-CH_2O]_2P(O)OH$	322.43	1 ⁴ , 1786	0.965	1.4450 ²⁰	–60	209 ^{10mm}		
b179	Bis(2-ethylhexyl) <i>o</i> -phthalate	$[CH_3(CH_2)_3CH(C_2H_5)-CH_2OOC]_2C_6H_4$	390.57		0.9843 ²⁰	1.4859 ²⁰	–50	384	207	0.01 aq
b180	<i>N,N</i> -Bis(2-hydroxy-ethyl)-2-amino-ethanesulfonic acid	$(HOC_2H_5)_2-NCH_2CH_2SO_3H$	213.25				152–154			
b181	Bis(2-hydroxyethyl) ether	$HOCH_2CH_2OCH_2CH_2OH$	106.12	1, 468	1.118 ²⁰ ₂₀	1.4460 ²⁰	–10.45	245	143	misc aq, alc, acet, eth

b182	<i>N,N</i> -Bis(2-hydroxyethyl)glycine	(HOCH ₂ CH ₂) ₂ NCH ₂ COOH	163.17				192 sl d		sl s aq
b183	Bis(2-hydroxyethyl)-iminotris(hydroxymethyl)methane	(HOCH ₂ CH ₂) ₂ -NC(CH ₂ OH) ₃	209.24				104		
b184	2,2-Bis(hydroxymethyl)propionic acid	(HOCH ₂) ₂ C(CH ₃)COOH	134.13	3, 401			189–191		
b185	4,8-Bis(hydroxymethyl)tricyclo[5.2.0 ²⁻⁶]decane		196.29			1.5280 ²⁰		>112	
b186	Bis(2-mercaptoethyl) ether	(HSCH ₂ CH ₂) ₂ O	138.25		1.114		–80	217	
b187	Bis(2-mercaptoethyl) sulfide	(HSCH ₂ CH ₂) ₂ S	154.32		1.183	1.5982 ²⁰		136 ^{10mm}	90
b188	1,4-Bis(methanesulfonyl)butane	(CH ₃ SO ₂ OCH ₂ CH ₂ —) ₂	246.30				115–117		sl hyd aq; 0.1 alc; 1.4 acet
b189	1,2-Bis(methoxyethoxy)ethane	(CH ₃ OCH ₂ CH ₂ OCH ₂ —) ₂	178.23		0.990 ²⁰ ₄	1.4224 ²⁰	–45	216	110 misc aq
b190	Bis[2,(2-methoxyethoxy)ethyl] ether	(CH ₃ OCH ₂ CH ₂ OCH ₂ -CH ₂ —) ₂ O	222.28	1 ³ , 2107	1.0087 ²⁰ ₄	1.4330 ²⁰	–27	275.3	140 s aq
b191	Bis(2-methoxyethyl) ether	(CH ₃ OCH ₂ CH ₂ —) ₂ O	134.18		0.9440 ²⁵	1.4043 ²⁵	–68	162	70 misc aq

Bis(2-ethylhexyl) sebacate, b177
Bis(2-hydroxyethyl) sulfide, t149

2,2-Bis(hydroxymethyl)-2,2',2''-nitrilotriethanol,
b183

Bis(4-hydroxyphenyl) sulfide, t150

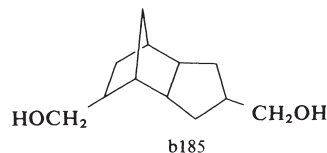


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

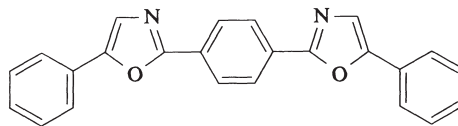
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b192	Bis(2-methylallyl) carbonate	$[\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{CH}_2\text{O}]_2\text{C}(=\text{O})$	170.21		0.943 ²⁰	1.4371		202	72	
b193	Bis(4-nitrophenyl) carbonate	$(\text{O}_2\text{NC}_6\text{H}_4\text{O})_2\text{C}(=\text{O})$	304.21	6 ¹ , 120			141			
b194	Bis(3-nitrophenyl) disulfide	$\text{O}_2\text{NC}_6\text{H}_4\text{SSC}_6\text{H}_4\text{NO}_2$	308.22	6, 339			83			i aq; s alc, eth
b195	Bis(4-nitrophenyl) disulfide	$\text{O}_2\text{NC}_6\text{H}_4\text{SSC}_6\text{H}_4\text{NO}_2$	308.33	6, 340			181			sl s alc
b196	Bis(octadecyl)pentaerythritol diphosphite	$[\text{C}_{18}\text{H}_{37}\text{OP}(\text{OCH}_2)_2]_2$	721.01		0.925	1.457	40		261	
b197	Bis(pentabromophenyl) ether	$\text{C}_6\text{Br}_5\text{OC}_6\text{Br}_5$	969.22	6 ¹ , 108			>300			
b198	1,4-Bis(5-phenyloxazol-2-yl)benzene		364.40				244			
b199	Bis(<i>p</i> -tolyl) disulfide	$\text{CH}_3\text{C}_6\text{H}_4\text{SSC}_6\text{H}_4\text{CH}_3$	246.39	6, 425			43–46			i aq; s alc; v s eth
b200	Bis(<i>p</i> -tolyl) sulfoxide	$\text{CH}_3\text{C}_6\text{H}_4\text{S}(\text{O})\text{C}_6\text{H}_4\text{CH}_3$	230.33	6, 419			94–96			v s alc, bz, chl, eth
b201	Bis(tributyltin) oxide	$(\text{C}_4\text{H}_9)_3\text{SnOSn}(\text{C}_4\text{H}_9)_3$	596.08		1.170	1.4864 ²⁰		180 ^{2mm}	>112	
b202	1,4-Bis(trichloromethyl)benzene	$\text{Cl}_3\text{CC}_6\text{H}_4\text{CCl}_3$	312.84	5, 385			108–110			i aq; 26 acet; 38 bz; 22 CCl_4 ; 33 eth; 3 MeOH
b203	Bis(2,4,5-trichlorophenyl) disulfide	$\text{Cl}_3\text{C}_6\text{H}_4\text{SSC}_6\text{H}_4\text{Cl}_3$	425.01				140–144			
b204	1,2-Bis(trichlorosilyl)ethane	$\text{Cl}_3\text{SiCH}_2\text{CH}_2\text{SiCl}_3$	296.64		1.483 ²⁰	1.473 ²⁰	24.5	201–202		
b205	3,5-Bis(trifluoromethyl)aniline	$(\text{F}_3\text{C})_2\text{C}_6\text{H}_3\text{NH}_2$	229.13		1.467	1.4335 ²⁰		85 ^{15mm}	83	

b206	1,3-Bis(trifluoromethyl)benzene	$F_3CC_6H_4CF_3$	214.0		1.3790 ²⁵	1.3916 ²⁵		116	
b207	<i>N,O</i> -Bis(trimethylsilyl)acetamide	$CH_3C \equiv N - Si(CH_3)_3$ $ $ $O - Si(CH_3)_3$	203.43		0.832 ²⁰ ₄	1.4170 ²⁰		73 ^{35mm}	11
b208	Bis(trimethylsilyl)acetylene	$(CH_3)_3SiC \equiv CSi(CH_3)_3$	170.41		0.770 ²⁰ ₄	1.413 ²⁰		137	2
b209	Bis(trimethylsilyl)formamide	$HC = NSi(CH_3)_3$ $ $ $O - Si(CH_3)_3$	189.41		0.885	1.4381 ²⁰		54– 55 ^{13mm}	
b210	<i>N,O</i> -Bis(trimethylsilyl)hydroxylamine	$(CH_3)_3SiONHSi(CH_3)_3$	177.40		0.830	1.4112 ²⁰		78– 80 ^{100mm}	28
b211	1,2-Bis(trimethylsilyloxy)ethane	$(CH_3)_3SiOCH_2CH_2OSi(CH_3)_3$	206.43		0.842	1.4034 ²⁰		165–166	46
b212	<i>N,O</i> -Bis(trimethylsilyl)trifluoroacetamide	$CF_3C[=NSi(CH_3)_3]OSi(CH_3)_3$	257.40		0.969	1.3939 ²⁰	–10	50 ^{14mm}	23
b213	Bis(triphenylphosphine)dicarbonylnickel	$[(C_6H_5)_3P]_2Ni(CO)_2$	639.32				209		

Bis(phenylmethyl) disulfide, d57

“Bis-tris,” b183

“Bis-tris” propane, b214



b198

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b214	1,3-Bis[tris(hydroxymethyl)methylamino]propane	$\text{CH}_2[\text{CH}_2\text{NHC}(\text{CH}_2\text{OH})_3]_2$	282.34	4 ³ , 859			170			
b215	Biuret	$\text{H}_2\text{NCONHCONH}_2$	103.08	3, 70	1.467_4^{-5}		110	d 190		v s alc; 2 aq
b216	1-Borneol		154.25	6, 72	1.011_4^{20}		204	212	65	i aq; 176 alc; s eth, bz, PE
b217	1-Bornyl acetate		196.29	6, 82	0.982	1.4626	27	224	84	sl s aq; s alc, eth
b218	<i>N</i> -Bromoacetamide	CH_3CONBrH	137.97	2, 181			102–105			sl s aq; v s eth
b219	<i>p</i> -Bromoacetanilide	$\text{BrC}_6\text{H}_4\text{NHCOCCH}_3$	214.07	12, 642	1.717		168			i aq; s bz, chl, EtAc
b220	Bromoacetic acid	BrCH_2COOH	138.95	2, 213	1.934_4^{50}	1.4804 ⁵⁰	50	208		v s aq, alc, eth
b221	α -Bromoacetophenone	$\text{C}_6\text{H}_5\text{COCH}_2\text{Br}$	199.05	7, 283	1.647_4^{20}		50	135 ^{18mm}		i aq; v s alc, bz, chl, eth
b222	<i>p</i> -Bromoacetophenone	$\text{BrC}_6\text{H}_4\text{COCH}_3$	199.05	7, 283	1.647		54	255		s alc, bz, eth, HOAc
b223	Bromoacetyl bromide	BrCH_2COBr	201.86	2, 215	2.317_{22}^{22}	1.5480 ²⁰		150	none	d aq, alc
b224	Bromoacetyl chloride	BrCH_2COCl	157.40	2, 215	1.908	1.4960 ²⁰		128	none	d aq, alc
b225	2-Bromoaniline	$\text{BrC}_6\text{H}_4\text{NH}_2$	172.03	12, 631	1.578_4^{20}	1.6113^{20}	31	229		i aq; s alc, eth
b226	3-Bromoaniline	$\text{BrC}_6\text{H}_4\text{NH}_2$	172.03	12, 633	1.580_4^{20}	1.6250^{20}	16.8	251	> 112	sl s aq; s alc, eth
b227	4-Bromoaniline	$\text{BrC}_6\text{H}_4\text{NH}_2$	172.03	12, 636	1.4970_4^{100}		66.3			i aq; v s alc, eth
b228	3-Bromobenzaldehyde	$\text{BrC}_6\text{H}_4\text{CHO}$	185.03	7, 238	1.587	1.5935 ²⁰		230	96	i aq; v s alc, eth
b229	Bromobenzene	$\text{C}_6\text{H}_5\text{Br}$	157.02	5, 206	1.4952_4^{20}	1.5580 ²⁰	−30.72	156.2	51	0.044 aq; 10.4 alc; misc bz, chl, PE; 71.6 eth
b230	Bromobenzene- <i>d</i> ₅	$\text{C}_6\text{D}_5\text{Br}$	162.06					53 ^{23mm}	65	
b231	4-Bromobenzene-sulfonyl chloride	$\text{BrC}_6\text{H}_4\text{SO}_2\text{Cl}$	255.52	11, 57			74.5	153 ^{15mm}		i aq; d alc; v s eth
b232	4-Bromobenzophenone	$\text{BrC}_6\text{H}_4\text{COC}_6\text{H}_5$	261.12	7, 422				82	350	i alc; sl s bz, eth

b233	2-Bromobenzotri- fluoride	$\text{BrC}_6\text{H}_4\text{CF}_3$	225.01		1.652 ²⁰	1.4817 ²⁰		168	51	
b234	3-Bromobenzotri- fluoride	$\text{BrC}_6\text{H}_4\text{CF}_3$	225.01		1.613	1.4749 ²⁰		152	43	
b235	2-Bromobenzyl alcohol	$\text{BrC}_6\text{H}_4\text{CH}_2\text{OH}$	187.04	6, 445			82			s hot aq; v s alc, eth
b236	2-Bromobenzyl bromide	$\text{BrC}_6\text{H}_4\text{CH}_2\text{Br}$	249.94	5, 308		1.6193 ²⁰	31	129 ^{19mm}		d hot aq; s alc, eth
b237	4-Bromobiphenyl	$\text{BrC}_6\text{H}_4\text{C}_6\text{H}_5$	233.11	5, 580	9.9327 ²⁵ ₄		87	310		i aq; s alc, bz, eth
b238	1-Bromobutane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$	137.02	1, 119	1.2686 ²⁵ ₄	1.4374 ²⁵	−112.4	101.6	23	i aq; s alc, bz, eth
b239	2-Bromobutane	$\text{CH}_3\text{CH}_2\text{CHBrCH}_3$	137.03	1, 119	1.2530 ²⁵ ₄	1.4360 ²⁰	−112.4	21		<0.1 aq; v s alc, eth
b240	1-Bromo-2-butene	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{Br}$	135.01	1, 205	1.312	1.4765 ²⁰		99	11	
b241	2-Bromo-2-butene	$\text{CH}_3\text{CH}=\text{C}(\text{Br})\text{CH}_3$	135.01	1, 205	1.328	1.4613 ²⁰		90 ^{740mm}	<1	
b242	4-Bromo-1-butene	$\text{BrCH}_2\text{CH}_2\text{CH}=\text{CH}_2$	135.01	1 ¹ , 84	1.3230 ²⁰ ₄	1.4608 ³⁰		100	<1	i aq; s alc, eth

2-Bornanone, c3

Bromal, t201

Bromoacetaldehyde diethyl acetal, b267

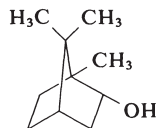
Bromoanisoles, b301, b302, b303

p-Bromobenzenethiol, b354

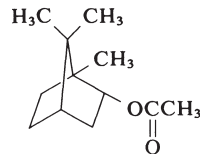
4-Bromobenzyl cyanide, b329

exo-2-Bromobicyclo[2.2.1]heptane, b318

Bromobutanedioic acid, b350



b216



b217

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

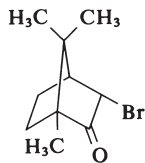
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b243	4-Bromobutyl phenyl ether	$C_6H_5OCH_2CH_2CH_2CH_2Br$	229.12	6 ² , 82			41–42	153–156 ^{18mm}		
b244	2-Bromobutyric acid	$CH_3CH_2CH(Br)COOH$	167.01	2, 281	1.5669 ²⁰ ₂₀	1.4720 ²⁰	–4	103 ^{10mm}	>112	6.7 aq; s alc, eth
b245	<i>endo</i> -3-Bromo-D-camphor		231.14	7 ² , 101	1.449		76–78	244		i aq; 15 alc; 200 chl; 62 eth
b246	α -Bromo- <i>p</i> -chloroacetophenone	$ClC_6H_4COCH_2Br$	233.50	7, 285			96.5			
b247	2-Bromochlorobenzene	BrC_6H_4Cl	191.46	5, 209	1.6382 ²⁵ ₄	1.5789 ²⁵		204	79	i aq; v s bz
b248	3-Bromochlorobenzene	BrC_6H_4Cl	191.46	5, 209	1.6302 ²⁰ ₄	1.5771 ²⁰	–21	196	80	i aq; v s alc, eth
b249	4-Bromochlorobenzene	BrC_6H_4Cl	191.46	5, 209	1.576 ⁷¹ ₄	1.5531 ⁷⁰	64.5	196		0.1 aq; misc MeOH, eth
b250	3-Bromo-4-chlorobenzotrifluoride	$Br(Cl)C_6H_3CF_3$	259.47		1.743 ²⁵	1.4973 ²⁵	–22	191–192		
b251	1-Bromo-4-chlorobutane	$ClCH_2CH_2CH_2CH_2Br$	171.47	5 ³ , 294	1.488	1.4875 ²⁰		82 ^{30mm}	60	i aq; s alc, chl, eth
b252	4-Bromo-6-chloro- <i>o</i> -cresol	$Br(Cl)C_6H_2(OH)CH_3$	221.49	6, 360			47			
b253	Bromochlorodifluoromethane	$Br(Cl)CF_2$	165.4		1.83 ²¹		–160.5	–4.01		
b254	1-Bromo-2-chloroethane	$ClCH_2CH_2Br$	143.43	1, 89	1.7392 ²⁰ ₄	1.4917 ²⁰	–18.4	106.6	none	0.7 aq; misc org solv
b255	7-Bromo-5-chloro-8-hydroxyquinoline		258.51	21 ¹ , 222			177–179			
b256	Bromochloromethane	$ClCH_2Br$	129.39	1, 67	1.923 ²⁵ ₄	1.480 ²⁵	–88	67.8	none	0.9 aq; misc MeOH, eth

b257	1-Bromo-3-chloropropane	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{Br}$	157.44	1, 109	1.472	1.486 ²⁰	< -50	143.5	none	0.1 aq; misc org solv
b258	2-Bromo-2-chloro-1,1,1-trifluoroethane	$\text{HC}(\text{Br})\text{ClCF}_3$	197.4		1.8636 ²⁵	1.3738 ²⁵		50		
b259	α -Bromocinnamaldehyde	$\text{C}_6\text{H}_5\text{CH}=\text{C}(\text{Br})\text{CHO}$	211.06	7, 358			66-68			
b260	Bromocycloheptane	$\text{BrC}_7\text{H}_{13}$	177.09	5, 29	1.2887 ²² ₄	1.5052 ²⁰		72 ^{10mm}	68	i aq; v s chl, eth
b261	Bromocyclohexane	$\text{BrC}_6\text{H}_{11}$	163.06	5, 24	1.3264 ¹⁵ ₄	1.4956 ¹⁵		165.8	62	0.1 aq; 10 MeOH; 71 eth
b262	3-Bromocyclohexene		161.04	5 ² , 40	1.3890 ²⁰ ₄	1.5292 ²⁰		64-65 ^{15mm}		
b263	Bromocyclopentane	BrC_5H_9	149.04	5, 19	1.3900 ²⁰ ₄	1.4881 ²⁰		137-139	35	
b264	Bromocyclopropane	BrC_3H_5	120.98			1.4605 ²⁰		69	2	
b265	1-Bromodecane	$\text{CH}_3(\text{CH}_2)_9\text{Br}$	221.19	1 ² , 130	1.0658 ²⁰ ₄	1.4560 ²⁰	-30	238	94	i aq; v s chl, eth
b266	Bromodichloromethane	HCBBrCl_2	163.83	1, 67	1.980 ²⁰	1.4964 ²⁰	-55	89.2	none	sl s aq; misc org solv
b267	2-Bromo-1,1-diethoxyethane	$\text{BrCH}_2\text{CH}(\text{OC}_2\text{H}_5)_2$	197.08	1, 625	1.310	1.4385 ²⁰		67 ^{18mm} 180 d	51	s hot alc

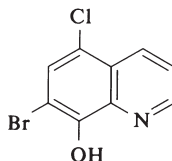
2-Bromo-*p*-cumene, b298
 β -Bromocumene, b297

4-Bromodiphenyl ether, b330

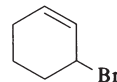
Bromoethene, b284



b245



b255



b262

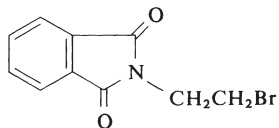
TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b268	4-Bromo-1,2-dimethoxybenzene	$\text{BrC}_6\text{H}_3(\text{OCH}_3)_2$	217.07	6, 784	1.702	1.5743 ²⁰		256	109	
b269	1-Bromo-2,2-dimethoxypropane	$\text{CH}_3\text{C}(\text{OCH}_3)_2\text{CH}_2\text{Br}$	183.05		1.355	1.4475 ²⁰		87 ^{80mm}	40	
b270	4-Bromo-2,6-dimethylphenol	$\text{BrC}_6\text{H}_2(\text{CH}_3)_2\text{OH}$	201.07	6, 485			78			
b271	2-Bromo-4,6-dinitroaniline	$\text{BrC}_6\text{H}_2(\text{NO}_2)_2\text{NH}_2$	262.02	12, 761			154	subl		v s hot alc, hot acet
b272	3-Bromo-4,6-dinitrofluorobenzene	$\text{BrC}_6\text{H}_2(\text{NO}_2)_2\text{F}$	264.9				90–91			
b273	2-Bromo-2,2-diphenylacetyl bromide	$\text{BrC}(\text{C}_6\text{H}_5)_2\text{COBr}$	354.05	9 ¹ , 283			63–65			
b274	α -Bromodiphenylmethane	$\text{C}_6\text{H}_5\text{CH}(\text{Br})\text{C}_6\text{H}_5$	247.14	5, 592			40	184 ^{20mm}		
b275	1-Bromododecane	$\text{CH}_3(\text{CH}_2)_{11}\text{Br}$	249.24	1 ² , 133	1.038	1.4580 ²⁰	–9	135 ^{6mm}	110	0.1 aq; s alc, eth
b276	1-Bromo-2,3-epoxypropane	$\text{H}_2\text{C}-\text{CHCH}_2\text{Br}$ O O	136.98	17, 9	1.601 ²⁰	1.4820 ²⁰	–40	134–136	56	i aq; sl s alc; s eth
b277	Bromoethane	$\text{CH}_3\text{CH}_2\text{Br}$	108.97	1, 88	1.4708 ¹⁵	1.4276 ¹⁵	–118.6	38.4	none	0.91 aq
b278	2-Bromoethanesulfonic acid, sodium salt	$\text{BrCH}_2\text{CH}_2\text{SO}_3^-\text{Na}^+$	211.02	4, 7			283–285 d			
b279	2-Bromoethanol	$\text{BrCH}_2\text{CH}_2\text{OH}$	124.97	1, 338	1.7629 ²⁰ ₄	1.4920 ²⁰		150	40	misc aq; s org solv
b280	2-Bromoethyl acetate	$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{Br}$	167.01	2 ¹ , 57	1.514 ²⁰ ₄	1.4547 ²⁰	–13.8	159	71	v s aq; misc alc, eth
b281	2-Bromoethylamine HBr	$\text{BrCH}_2\text{CH}_2\text{NH}_2\cdot\text{HBr}$	204.90	4, 134			172–174			v s aq, alc

b282	<i>o</i> -Bromo(ethyl)-benzene	$\text{CH}_3\text{CH}_2\text{C}_6\text{H}_4\text{Br}$	185.07	5, 355	1.3566 ²⁵ ₂₅	1.5603 ²⁰		199		0.1 aq; misc org solv
b283	(2-Bromoethyl)-benzene	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{Br}$	185.07	5, 356	1.355	1.5563 ²⁰		221	89	i aq; s bz, eth
b284	Bromoethylene	$\text{H}_2\text{C}=\text{CHBr}$	106.96	1, 188	1.493 ²⁰	1.4350 ²⁰	−139.5	15.8		i aq; misc alc, eth
b285	2-Bromoethyl ethyl ether	$\text{BrCH}_2\text{CH}_2\text{OCH}_2\text{CH}_3$	153.02	1, 338	1.3572 ²⁰ ₄	1.4450 ²⁰		150	21	sl s aq; misc alc, eth
b286	2-Bromoethyl phenyl ether	$\text{BrCH}_2\text{CH}_2\text{OC}_6\text{H}_5$	201.07	6, 142			34	144 ^{40mm}	65	i aq; v s alc, eth
b287	<i>N</i> -(2-Bromoethyl)-phthalimide		254.09	21, 461			81–84			s hot aq; v s eth
b288	2-Bromofluorobenzene	$\text{BrC}_6\text{H}_4\text{F}$	175.01		1.601	1.5337 ²⁰		156	43	
b289	3-Bromofluorobenzene	$\text{BrC}_6\text{H}_4\text{F}$	175.01		1.567	1.5257 ²⁰		150	38	
b290	4-Bromofluorobenzene	$\text{BrC}_6\text{H}_4\text{F}$	175.01	5, 209	1.593 ¹⁵	1.5310 ¹⁵	−17.4	151–152	60	
b291	1-Bromoheptane	$\text{H}(\text{CH}_2)_7\text{Br}$	179.11	1, 155	1.1384 ²⁰ ₄	1.4505 ²⁰	−58	180	60	i aq; v s alc, eth
b292	2-Bromoheptane	$\text{H}(\text{CH}_2)_5\text{CH}(\text{Br})\text{CH}_3$	179.11	1, 155	1.142	1.4470 ²⁰		66 ^{21mm}	47	
b293	1-Bromohexadecane	$\text{H}(\text{CH}_2)_{16}\text{Br}$	305.35	1 ² , 138	0.9991	1.4618	17.8	336	87	i aq; misc org solv
b294	1-Bromohexane	$\text{H}(\text{CH}_2)_6\text{Br}$	165.08	1, 144	1.1763 ²⁰ ₀	1.4475	−85	154–158	57	i aq; misc alc, eth

(Bromomethyl)benzene, b85

Bromoform, t206



b287

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

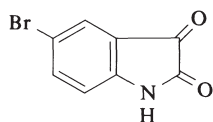
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b295	DL-2-Bromohexanoic acid	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{Br})\text{COOH}$	195.06	2, 325	1.370	1.4720 ²⁰		136–138 ^{18mm}		
b296	5-Bromoisatin		226.03	21, 453			251–253			
b297	(2-Bromoisopropyl)-benzene	$\text{C}_6\text{H}_5\text{CH}(\text{CH}_3)\text{CH}_2\text{Br}$	199.10	5 ¹ , 191	1.316	1.5480 ²⁰		108 ^{18mm}	91	
b298	2-Bromo-4-isopropyl-1-methylbenzene	$\text{CH}_3(\text{Br})\text{C}_6\text{H}_3\text{CH}(\text{CH}_3)_2$	213.0		1.253 ²⁵ ₂₅	1.535 ²⁵	–20	120		i aq; 50 MeOH; misc org solv
b299	Bromomaleic anhydride		176.96	17, 435	1.905	1.5400 ²⁰		215	>112	
b300	Bromomethane	CH_3Br	94.94	1, 67	1.732 ⁰ ₀	1.4234 ¹⁰	–84	3.56	none	0.1 aq; s alc, chl, eth
b301	2-Bromo-1-methoxybenzene	$\text{BrC}_6\text{H}_4\text{OCH}_3$	187.04	6, 197	1.5018 ²⁵ ₄	1.5737 ²⁰	2	223	96	i aq; v s alc, eth
b302	3-Bromo-1-methoxybenzene	$\text{BrC}_6\text{H}_4\text{OCH}_3$	187.04	6, 198	1.477	1.5635 ²⁰	211	93		i aq; s alc, eth
b303	4-Bromo-1-methoxybenzene	$\text{BrC}_6\text{H}_4\text{OCH}_3$	187.04	6, 199	1.4564 ²⁰ ₄	1.5630 ²⁰	10	223	94	sl s aq; v s alc, eth
b304	4-Bromo-2-methylaniline	$\text{CH}_3(\text{Br})\text{C}_6\text{H}_3\text{NH}_2$	186.06	12, 838			56	240		sl s aq; v s alc
b305	1-Bromo-3-methylbutane	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{Br}$	151.05	1, 136	1.210 ¹⁵ ₄	1.4409 ²⁰	–112	119.7	32	0.02 aq; misc alc, eth
b306	(Bromomethyl)cyclohexane	$\text{C}_6\text{H}_{11}\text{CH}_2\text{Br}$	177.09	5 ² , 18	1.269	1.4907 ²⁰		76–77 ^{26mm}	57	
b307	2-Bromomethyl-1,3-dioxalane		167.01	19 ² , 8	1.613	1.4817 ²⁰		80–82 ^{27mm}	62	
b308	Bromomethyl methyl ether	$\text{BrCH}_2\text{OCH}_3$	124.97	1, 582	1.531	1.4550 ²⁰		87	26	

b309	1-Bromo-2-methyl-naphthalene	$\text{BrC}_{10}\text{H}_6\text{CH}_3$	221.10	5, 568	1.418	1.6484 ²⁰		296	>112	
b310	1-Bromo-2-methyl-propane	$(\text{CH}_3)_2\text{CHCH}_2\text{Br}$	137.03	1, 126	1.2641 ²⁰	1.4362 ²⁰	-119	91.5	18	0.06 aq; misc alc, eth
b311	2-Bromo-2-methyl-propane	$(\text{CH}_3)_3\text{CBr}$	137.03	1, 127	1.215 ²⁵ ₂₅	1.425 ²⁵	-16.2	73.1	18	i aq; misc org solv
b311a	α -Bromo- α -methyl-propiophenone	$\text{C}_6\text{H}_5\text{COC}(\text{CH}_3)_2\text{Br}$	227.11	7, 316	1.350	1.5561 ²⁰		148 ^{30mm}	>112	
b312	1-Bromonaphthalene	$\text{C}_{10}\text{H}_7\text{Br}$	207.08	5, 547	1.4834 ²⁰ ₄	1.6580 ²⁰	-1	281.1	>112	misc alc, bz, chl, eth
b313	1-Bromo-1-naphthol	$\text{BrC}_{10}\text{H}_6\text{OH}$	223.07	6, 650			78	130 d		i aq; s alc, bz, eth
b314	1-Bromo-2-nitro-benzene	$\text{BrC}_6\text{H}_4\text{NO}_2$	202.01	5 ¹ , 247	09.9327 ²⁵ ₄		43	261		v s alc; s bz, eth
b315	5-Bromo-2-nitro-benzotrifluoride	$\text{O}_2\text{N}(\text{Br})\text{C}_6\text{H}_3\text{CF}_3$	270.02		1.7992 ²⁵	1.5180 ²⁵	40-44	99-100		
b316	2-Bromo-2-nitro-1,3-propanediol	$(\text{HOCH}_2)_2\text{C}(\text{Br})\text{NO}_2$	199.99	1, 476			133			
b317	1-Bromononane	$\text{H}(\text{CH}_2)_9\text{Br}$	207.16	1 ¹ , 63	1.084	1.4540 ²⁰		201	51	i aq; s chl, eth
b318	<i>exo</i> -2-Bromo-norbornane		175.07		1.363	1.5148 ²⁰		82 ^{29mm}	60	
b319	1-Bromooctadecane	$\text{H}(\text{CH}_2)_{18}\text{Br}$	333.41	1 ¹ , 69			23	216 ^{12mm}		i aq; s alc, eth

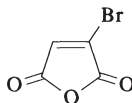
α -Bromoisobutyrophenone, b311a
2-Bromomesitylene, b362

α -Bromo-4-nitro-*o*-cresol, h155

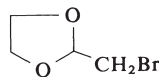
α -Bromo-*p*-nitrotoluene, n46



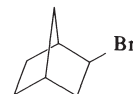
b296



b299



b307



b318

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

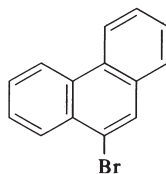
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b320	1-Bromooctane	$\text{H}(\text{CH}_2)_8\text{Br}$	193.13	1, 160	1.108 ₄ ²⁵	1.4503 ²⁵	−55	201	78	i aq; misc alc, eth
b321	Bromopentafluorobenzene	BrC_6F_5	246.97		1.947 ²⁰	1.4490 ²⁰	−31	137	87	
b322	1-Bromopentane	$\text{H}(\text{CH}_2)_5\text{Br}$	151.05	1, 131	1.2337 ₄ ¹⁵	1.4444 ²⁰	−88	129.6	31	i aq; s alc; misc eth
b323	2-Bromopentane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{Br})\text{CH}_3$	151.05	1, 131	1.2039 ₄ ²⁰	1.4403 ²⁰		117	20	
b324	9-Bromophenanthrene		257.14	5, 671	1.409 ₄ ¹⁰¹		54–58	190 ^{2mm}		i aq; s alc, eth
b325	2-Bromophenol	$\text{BrC}_6\text{H}_4\text{OH}$	173.01	6, 197	1.492	1.5892 ²⁰	6	194	42	s aq; misc chl, eth
b326	4-Bromophenol	$\text{BrC}_6\text{H}_4\text{OH}$	173.01	6, 198	1.5875 ⁸⁰		68	238		14 aq; v s alc, chl
b327	2-Bromo-2-phenylacetic acid	$\text{C}_6\text{H}_5\text{CH}(\text{Br})\text{COOH}$	215.05	9, 451			83			
b328	<i>p</i> -Bromophenylacetic acid	$\text{BrC}_6\text{H}_4\text{CH}_2\text{COOH}$	215.05	9, 451			119			sl s aq; v s alc, eth
b329	<i>p</i> -Bromophenylacetonitrile	$\text{BrC}_6\text{H}_4\text{CH}_2\text{CN}$	196.05	9, 451			47–49			i aq; sl s alc; v s bz
b330	4-Bromophenyl phenyl ether	$\text{BrC}_6\text{H}_4\text{OC}_6\text{H}_5$	249.11	6 ¹ , 105	1.423	1.6070 ²⁰	18	305	>112	
b331	1-Bromo-3-phenylpropane	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$	199.10	5, 391	1.310	1.5450 ²⁰		220	101	
b332	1-Bromopropane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$	123.00	1, 108	1.3597 ¹⁵	1.4370 ¹⁵	−110.1	71.0	25	0.23 aq ³⁰ ; misc alc
b333	2-Bromopropane	$\text{CH}_3\text{CH}(\text{Br})\text{CH}_3$	123.00	1, 108	1.3222 ¹⁵	1.4285 ¹⁵	−89.0	59.5	19	0.3 aq ¹⁸ ; misc alc, bz, chl, eth
b334	3-Bromo-1-propanol	$\text{BrCH}_2\text{CH}_2\text{CH}_2\text{OH}$	139.00	1, 356	1.5374 ₄ ²⁰	1.4858 ²⁰		62 ^{5mm}		s aq; misc alc, eth
b335	1-Bromo-1-propene	$\text{CH}_3\text{CH}=\text{CHBr}$	120.98	1, 200	1.4133 ₄ ²⁰	1.4538 ²⁰	−116	63	4	i aq
b336	2-Bromo-1-propene	$\text{CH}_3\text{C}(\text{Br})=\text{CH}_2$	120.98	1, 200	1.362 ₄ ²⁰	1.4425 ²⁰	−125	49	4	
b337	2-Bromopropionic acid	$\text{CH}_3\text{CH}(\text{Br})\text{COOH}$	152.98	2, 254	1.7000 ²⁰	1.4750 ²⁰	25.7	203	100	v s aq, alc, eth
b338	3-Bromopropionic acid	$\text{BrCH}_2\text{CH}_2\text{COOH}$	152.98	2, 256	1.480		62.5		65	s aq, alc, bz, chl, eth

b339	3-Bromopropionitrile	$\text{BrCH}_2\text{CH}_2\text{CN}$	133.98	2 ² , 231	1.6152 ²⁰ ₄	1.4800 ²⁰		78 ^{10mm}	98	v s alc, eth
b340	2-Bromopropionyl chloride	$\text{CH}_3\text{CH}(\text{Br})\text{COCl}$	171.43	2, 256	1.700 ¹¹	1.4800 ²⁰		133	51	d aq; s chl, eth
b341	3-Bromopropionyl chloride	$\text{BrCH}_2\text{CH}_2\text{COCl}$	171.43	2 ² , 231	1.701	1.4968 ²⁰		57 ^{17mm}	79	
b342	α -Bromopropiophenone	$\text{C}_6\text{H}_5\text{COCHBrCH}_3$	213.08	7, 302	1.430 ²⁰ ₄	1.5715 ²⁰		250	>112	s alc, bz, eth, acet
b343	3-Bromopropyl phenyl ether	$\text{C}_6\text{H}_5\text{OCH}_2\text{CH}_2\text{CH}_2\text{Br}$	215.10	6, 142	1.365	1.5464 ²⁰	10–11	130–134 ^{14mm}	96	
b344	3-Bromopropyne	$\text{BrCH}_2\text{C}\equiv\text{CH}$	118.97	1, 248	1.335	1.4905 ²⁰		88–90	18	
b345	2-Bromopyridine	$\text{BrC}_5\text{H}_4\text{N}$	158.00	20, 233	1.657 ¹⁸	1.5720 ²⁰		194	54	i aq; s org solv
b346	3-Bromopyridine	$\text{BrC}_5\text{H}_4\text{N}$	158.00	20, 233	1.645 ⁰ ₄	1.5695 ²⁰	142–143	173	51	s aq; v s alc, eth
b347	3-Bromoquinoline		208.06	20, 363	1.533	1.6640 ²⁰	15	276	>112	s HOAc
b348	5-Bromosalicylic acid	$\text{Br}(\text{HO})\text{C}_6\text{H}_3\text{COOH}$	217.02	10, 107			166			0.3 aq ⁸⁰ ; 85 alc ²⁵ ; 70 eth ²⁵
b349	β -Bromostyrene	$\text{C}_6\text{H}_5\text{CH}=\text{CHBr}$	183.05	5, 477	1.422 ²⁰ ₄	1.6066 ²⁰	7	112 ^{20mm}	79	i aq; misc alc, eth
b350	Bromosuccinic acid	$\text{HOOCCH}_2\text{CH}(\text{Br})\text{COOH}$	196.99	2, 621	2.073		172 d			18 aq; s alc

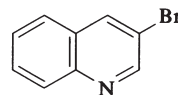
β -Bromophenetole, b286
3-Bromopropene, a85

3-(Bromopropyl)benzene, b330

5-Bromopseudocumene, b361



b324



b347

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b351	<i>N</i> -Bromosuccinimide		177.99	21, 380	2.098		173 sl d			1.5 aq; 14.4 acet; 3.1 HOAc; 0.02 CCl ₄
b352	1-Bromotetradecane	H(CH ₂) ₁₄ Br	277.30	1 ² , 136	1.0124 ₄ ²⁵	1.4600 ²⁰	6	178 ^{20mm}	>112	s alc; v s chl; misc bz, acet
b353	2-Bromothiophene	Br(C ₄ H ₃ S)	163.04	17, 33	1.684 ₄ ²⁰	1.5860 ²⁰		151	60	v s acet, eth
b354	4-Bromothiophenol	BrC ₆ H ₄ SH	189.08	6, 330			76	239		
b355	2-Bromotoluene	BrC ₆ H ₄ CH ₃	171.04	5, 304	1.422 ₂₅ ²⁵	1.552 ²⁵	−26	181	78	0.1 aq; misc alc, bz, chl, eth
b356	3-Bromotoluene	BrC ₆ H ₄ CH ₃	171.04	5, 305	1.4099 ₄ ²⁰	1.5517 ²⁰	−39.8	183.7	60	s alc, bz, eth
b357	4-Bromotoluene	BrC ₆ H ₄ CH ₃	171.04	5, 305	1.3959 ₃₅ ³⁵	1.5490	28.5	184.5	85	s alc, bz, eth
b358	Bromotri-chloromethane	BrCCl ₃	198.28	1, 67	1.997 ₂₅ ²⁵	1.5063	−21	103.8	none	misc org solv
b359	1-Bromotridecane	H(CH ₂) ₁₃ Br	263.27	1 ² , 134	1.0262 ₄ ²⁰	1.4592 ²⁰	7	150 ^{10mm}	>112	v s chl
b360	Bromotri-fluoromethane	BrCF ₃	148.92	1 ³ , 83	1.5800 ₄ ²⁰			−57.8		v s chl
b361	5-Bromo-1,2,4-trimethylbenzene	BrC ₆ H ₂ (CH ₃) ₃	199.10	5, 403			73	235		i aq; s alc
b362	2-Bromo-1,3,5-trimethylbenzene	BrC ₆ H ₂ (CH ₃) ₃	199.10	5, 408	1.301	1.5511 ²⁰	2	225	96	i aq; s bz; v s eth
b363	Bromotrimethyl-germane	(CH ₃) ₃ GeBr	197.60		1.544 ¹⁸	1.4705 ²⁰	−25	113.7		
b364	Bromotrimethylsilane	(CH ₃) ₃ SiBr	153.10		1.160	1.4145 ²⁰		79	1	
b365	Bromotriphenyl-ethylene	(C ₆ H ₅) ₂ C=C(Br)C ₆ H ₅	335.22				114–115			
b366	Bromotriphenyl-methane	(C ₆ H ₅) ₃ CBr	323.24	5, 704			152–154	230 ^{15mm}		
b367	11-Bromoundecanoic acid	Br(CH ₂) ₁₀ COOH	265.20	2 ² , 315			51	174 ^{2mm}		i aq; v s alc

b368	α -Bromo- <i>o</i> -xylene	$\text{BrCH}_2\text{C}_6\text{H}_4\text{CH}_3$	185.07	5, 365	1.381^{23}	1.5742^{20}	21	223–224	82	s alc, eth
b369	α -Bromo- <i>m</i> -xylene	$\text{BrCH}_2\text{C}_6\text{H}_4\text{CH}_3$	185.07	5, 374	1.370^{23}	1.5560^{20}		$185^{340\text{mm}}$	82	s alc, eth
b370	2-Bromo- <i>p</i> -xylene	$\text{BrC}_6\text{H}_3(\text{CH}_3)_2$	185.07	5, 385	1.340	1.5505^{20}	9–10	199–201	79	
b371	4-Bromo- <i>o</i> -xylene	$\text{BrC}_6\text{H}_3(\text{CH}_3)_2$	185.07	5, 365	1.370^{15}_{15}	1.5560^{20}		215	80	v s alc, eth
b372	Brucine		394.45	$27^2, 797$			178			77 alc; 1 bz; 20 chl
b373	1,2-Butadiene	$\text{CH}_3\text{CH}=\text{C}=\text{CH}_2$	54.09	1, 249	0.676^{10}_4	1.4205^1	–136.2	10.9		misc alc, eth
b374	1,3-Butadiene	$\text{CH}_2=\text{CHCH}=\text{CH}_2$	54.09	1, 249	0.650^{6}_4	1.4293^{-25}	–108.9	–4.4		misc alc, eth
b375	1,3-Butadienyl acetate	$\text{CH}_3\text{C}(=\text{O})\text{OCH}=\text{CH}-\text{CH}=\text{CH}_2$	112.13	$2^3, 295$	0.945	1.4690^{20}		$60^{40\text{mm}}$	33	
b376	1,3-Butadiyne	$\text{HC}\equiv\text{CC}\equiv\text{CH}$	50.06	$1^3, 1056$	0.7364^{10}_4	1.4189^5	–36	10.3		v s eth; s bz, acet
b377	2-Butanamine	$\text{CH}_3\text{CH}_2\text{CH}(\text{NH}_2)\text{CH}_3$	73.14	4, 160	0.7308^{15}_4	1.3963^{15}	–104.5	66	–19	misc aq, alc
b378	Butane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	58.12		0.6011^{10}	1.3562^{-13}	–138.3	–0.50		
b379	1,4-Butanediamine	$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$	88.15	4, 264	0.877^{25}_4	1.4569^{20}	27–28	158–160	51	s aq
b380	Butanedinitrile	$\text{NCCH}_2\text{CH}_2\text{CN}$	80.09	2, 615	0.9867^{60}_4	1.4173^{60}	57.9	265–267		11.5 aq; s acet, chl, diox; sl s bz, eth
b381	1,2-Butanediol	$\text{CH}_3\text{CH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$	90.12	1, 477	1.006^{18}_0	1.4380^{20}		207.5	93	s aq, alc, acet
b382	1,3-Butanediol	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_2\text{OH}$	90.12	1, 477	1.0053^{20}_{20}	1.441^{20}	<–50	207.5	121	s aq, alc, acet; 9 eth

α -Bromotoluene, b85

Bromo- α, α, α -trifluorotoluenes, b233, b234

3-Bromo-1,7,7-trimethylbicyclo[2.2.1]heptane-2-one, b245

4-Bromoveratrole, b268

4-Bromo-2,6-xyleneol, b270

BSA, b207

BSTFA, b212

BTMSA, b208

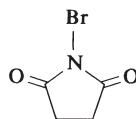
Busulfan, b188

α -Butadiene sulfone, d368

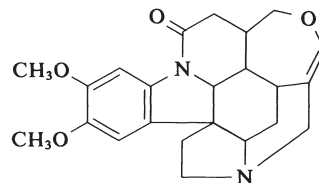
Butanedioic acid, s14

1,4-Butanediol diglycidyl ether, b175

1,4-Butanediol dimethanesulfonate, b188



b351



b372

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b383	1,4-Butanediol	HOCH ₂ CH ₂ CH ₂ CH ₂ OH	90.12	1, 478	1.016 ₄ ²⁵	1.4452 ²⁰	120.9	230	>112	misc aq, alc, acet; 0.3 bz; 3.1 eth; 0.9 PE
b384	<i>meso</i> -2,3-Butanediol	CH ₃ CH(OH)CH(OH)CH ₃	90.12	1, 479	0.9939 ₄ ²⁵	1.4324 ³⁵	34.4	182	85	misc aq, alc
b385	<i>D</i> -(−)-2,3-Butanediol	CH ₃ CH(OH)CH(OH)CH ₃	90.12	1 ² , 546	0.9869 ₄ ²⁵	1.4315 ²⁵	19.7	180 ^{715mm}	85	misc aq, alc; s eth
b386	2,3-Butanedione	CH ₃ C(O)C(O)CH ₃	86.09	1, 769	0.990 ₁₅ ¹⁵	1.3951 ²⁰		88	26	25 aq; misc alc, eth
b387	1,4-Butanedithiol	HSCH ₂ CH ₂ CH ₂ CH ₂ SH	122.25	1, 479	1.042	1.5290 ²⁰		106 ^{30mm}	70	i aq; v s alc
b388	1-Butanethiol	CH ₃ CH ₂ CH ₂ CH ₂ SH	90.19	1, 370	0.8367 ₄ ²⁵	1.4403 ²⁵	−115.7	98.5	12	0.06 aq; v s alc, eth
b389	2-Butanethiol	CH ₃ CH ₂ CH(SH)CH ₃	90.19	1, 373	0.8246 ₄ ²⁵	1.4338 ²⁵	−165	85.0	21	sl s aq; v s alc, eth
b390	1,2,4-Butanetriol	HOCH ₂ CH ₂ CH(OH)-CH ₂ OH	106.12	1, 519	1.018 ²⁰	1.4748 ²⁰		191 ^{18mm}	167	v s aq, alc
b391	1-Butanol	CH ₃ CH ₂ CH ₂ CH ₂ OH	74.12	1, 367	0.8097 ₄ ²⁰	1.3993 ²⁰	−88.6	117.7	35	7.4 aq; misc alc, eth
b392	2-Butanol	CH ₃ CH ₂ CH(OH)CH ₃	74.12	1, 371	0.8069 ₄ ²⁰	1.3972 ²⁰	−114.7	99.5	26	12.5 aq; misc alc, eth
b393	2-Butanone	CH ₃ CH ₂ COCH ₃	72.11	1 ² , 726	0.8049 ₄ ²⁰	1.3788 ²⁰	−86.7	79.6	−3	24 aq; misc alc, bz, eth
b394	2-Butanone oxime	CH ₃ CH ₂ C(=NOH)CH ₃	87.12	1 ² , 730	0.9232 ₄ ²⁰	1.4428	−29.5	72 ^{25mm}		s aq; misc alc, eth
b395	1-Butene	CH ₃ CH ₂ CH=CH ₂	56.10	1 ³ , 715	0.6255 ₄ ¹⁸⁵	1.3962 ²⁰	−185.3	−6.3		i aq; v s alc, eth
b396	<i>cis</i> -2-Butene	CH ₃ CH=CHCH ₃	56.10	1 ³ , 728	0.6213 ₄ ²⁰	1.3931 ^{−25}	−138.9	3.7		i aq; v s alc, eth
b397	<i>trans</i> -2-Butene	CH ₃ CH=CHCH ₃	56.10	1 ³ , 730	0.6041 ₄ ²⁰	1.3848 ^{−25}	−105.6	0.88		i aq; v s alc, eth
b398	<i>cis</i> -2-Butene-1,4-diol	HOCH ₂ CH=CHCH ₂ OH	88.11	1 ² , 567	0.0700 ₄ ²⁰	1.4793 ²⁰	12.5	234	128	s aq; v s alc
b399	<i>trans</i> -2-Butene-1,4-diol	HOCH ₂ CH=CHCH ₂ OH	88.11	1 ³ , 2252	0.070 ₄ ²⁰	1.4779 ²⁰	27.3	132		v s aq, alc
b400	3-Butenenitrile	H ₂ C=CHCH ₂ CN	67.09	2, 408	0.8341 ₄ ²⁰	1.4060 ²⁰	−87	119	21	sl s aq; misc alc, eth
b401	<i>cis</i> -2-Butenoic acid	CH ₃ CH=CHCOOH	86.09	2, 412	1.0267 ₄ ²⁰	1.4482 ¹⁴	14	168–169		v s aq; s alc

b402	<i>trans</i> -2-Butenoic acid	$\text{CH}_3\text{CH}=\text{CHCOOH}$	86.09	2, 408	0.964^{80}_4	1.4228^{77}	71.4	185.0	87	54.6 aq; v s EtOH, bz, acet
b403	3-Butenoic acid	$\text{H}_2\text{C}=\text{CHCH}_2\text{COOH}$	86.09	2, 407	1.0091^{20}_4	1.4249^{20}	−39	163	65	s aq; misc alc, eth
b404	<i>cis</i> -2-Buten-1-ol	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{OH}$	72.11	1, 442	0.8662^{20}_4	1.4342^{20}	−89.4	123.6	56	16.6 aq; misc alc
b405	<i>trans</i> -2-Buten-1-ol	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{OH}$	72.11	1, 442	0.8454^{20}_4	1.4289^{20}		121.2	56	16.6 aq; misc alc
b406	3-Buten-2-one	$\text{H}_2\text{C}=\text{CHCOCH}_3$	70.09	1, 728	0.8636^{20}_4	1.4086^{20}		81.4	−6	v s aq, alc, acet, eth
b407	1-Buten-3-yne	$\text{HC}\equiv\text{CCH}=\text{CH}_2$	52.07	1^3 , 1032	0.7095^1_4	1.4161^1		5.1		
b408	4-Butoxylaniline	$\text{CH}_3(\text{CH}_2)_3\text{OC}_6\text{H}_4\text{NH}_2$	165.24	13^2 , 226	0.992	1.5343^{20}		148– 149 ^{13mm}		
b409	4-Butoxybenzoic acid	$\text{CH}_3(\text{CH}_2)_3\text{OC}_6\text{H}_4\text{COOH}$	194.23	10^2 , 93			150			
b410	2-Butoxyethanol	$\text{CH}_3(\text{CH}_2)_3\text{OCH}_2\text{CH}_2\text{OH}$	118.18	1^2 , 519	0.9012^{20}_4	1.4198^{20}	−40	170.2	60	5 aq; s most org solv
b411	2-(2-Butoxyethoxy)-ethanol	$\text{HOCH}_2\text{CH}_2\text{OCH}_2\text{-CH}_2\text{OC}_4\text{H}_9$	162.23	1^2 , 521	0.9536^{20}_{20}	1.4306^{20}	−68.1	230.4	110	misc aq, alc, bz, acet, PE, CCl_4
b412	Butyl acetate	$\text{C}_4\text{H}_9\text{OOCCH}_3$	116.16	2, 130	0.8813^{20}_4	1.3941^{20}	−73.5	126.1	37	0.43 aq; misc alc, eth; s most org solv
b413	DL- <i>sec</i> -Butyl acetate	$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{C}_2\text{H}_5$	116.16	2^2 , 141	0.865^{25}_4	1.3840^{25}		112.3	32	0.62 aq; s alc, eth
b414	<i>tert</i> -Butyl acetate	$(\text{CH}_3)_3\text{COOCCH}_3$	116.16	2, 131	0.8665^{20}_4	1.3853^{20}		97.8	15	i aq; misc alc, eth
b415	<i>tert</i> -Butyl acetoacetate	$(\text{CH}_3)_3\text{COC}(=\text{O})\text{CH}_2\text{-C}(=\text{O})\text{CH}_3$	158.20		0.954	1.4180^{20}			60	
b416	Butyl acrylate	$\text{H}_2\text{C}=\text{CHCOOC}_4\text{H}_9$	128.17	2^2 , 388	0.894^{25}_{16}	1.4160		148	38	i aq; s alc, eth
b417	Butylamine	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$	73.14	4, 156	0.7327^{25}_4	1.3992^{25}	−50.5	77.9	−1	misc aq, alc, eth, PE
b418	<i>tert</i> -Butylamine	$(\text{CH}_3)_3\text{CNH}_2$	73.14	4, 173	0.6951^{20}_4	1.3788^{20}	−67.5	44.4	−8	misc aq, alc
b419	2-(<i>tert</i> -Butylamino)-ethanol	$(\text{CH}_3)_3\text{CNHCH}_2\text{CH}_2\text{OH}$	117.19				42–45	90–92 ^{25mm}	68	

(*E*)-2-Butenal, c282
 Buten-4-carboxylic acid, p50
 Butopyronoxyl, b445

Butoxybenzene, b477
 1-Butoxybutane, d115
 Butyl alcohols, b393, b392, m382

sec-Butylamine, b377

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b420	3-(<i>tert</i> -Butylamino)-1,2-propanediol	$(\text{CH}_3)_3\text{CNHCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$	147.22				70	92 ^{1mm}		
b421	4-Butylaniline	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{-C}_6\text{H}_4\text{NH}_2$	149.24	12 ¹ , 503	0.945	1.5350 ²⁰		120 ^{15mm}	101	
b422	2- <i>tert</i> -Butylantraquinone		264.32				100			
b423	Butylbenzene	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}_6\text{H}_5$	134.22	5, 413	0.8604 ²⁰ ₄	1.4898 ²⁰	−88	183.3	59	misc alc, bz, eth
b424	<i>sec</i> -Butylbenzene	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}_6\text{H}_5$	134.22	5, 414	0.8608 ²⁰ ₄	1.4902 ²⁰	−82.7	173.3	45	misc alc, bz, eth
b425	<i>tert</i> -Butylbenzene	$(\text{CH}_3)_3\text{CC}_6\text{H}_5$	134.22	5, 415	0.8669 ²⁰ ₄	1.4927 ²⁰	−57.9	169.1	34	misc alc, bz, eth
b426	Butyl benzoate	$\text{C}_6\text{H}_5\text{COOC}_4\text{H}_9$	178.23	9, 112	1.000 ²⁰	1.496	−22	250		i aq; s alc, eth
b427	4- <i>tert</i> -Butylbenzoic acid	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{COOH}$	178.23	9, 560			167			i aq; v s alc, bz
b428	4- <i>tert</i> -Butylbenzoyl chloride	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{COCl}$	196.68		1.007	1.5364 ²⁰		135 ^{20mm}	87	
b429	<i>N</i> -(<i>tert</i> -Butyl)benzylamine	$\text{C}_6\text{H}_5\text{CH}_2\text{NHC}(\text{CH}_3)_3$	163.27	12, 1022	0.881	1.4968 ²⁰		80 ^{5mm}	80	
b430	Butyl butyrate	$\text{CH}_3\text{CH}_2\text{CH}_2\text{COOC}_4\text{H}_9$	144.21	2, 271	0.8717 ²⁰ ₂₀	1.4035		156.9	51	i aq; misc alc, eth
b431	<i>tert</i> -Butyl carbazate	$\text{H}_2\text{NNHCOOC}(\text{CH}_3)_3$	132.16				42	65 ^{0.03mm}		
b432	4- <i>tert</i> -Butylcatechol	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{OH})_2$	166.22		1.049 ⁶⁰ ₂₅		55	285	151	0.2 aq ⁸⁰ ; 240 eth ²⁵ ; s alc; v s acet
b433	<i>tert</i> -Butyl chloroacetate	$\text{ClCH}_2\text{COOC}(\text{CH}_3)_3$	150.61	2 ³ , 444	1.053	1.4230 ²⁰		48–49 ^{11mm}	41	
b434	4- <i>tert</i> -Butyl-1-chlorobenzene	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{Cl}$	168.67	5, 416	1.006	1.5108 ²⁰	23–25	217		
b435	<i>tert</i> -Butylchlorodiphenylsilane	$(\text{CH}_3)_3\text{CSi}(\text{C}_6\text{H}_5)_2\text{Cl}$	274.87		1.057	1.5675 ²⁰		90 ^{0.02mm}	>112	
b436	Butyl chloroformate	$\text{ClCOOC}_4\text{H}_9$	136.58	3 ² , 11	1.074 ²⁵ ₄	1.4114 ²⁰		142	25	d aq, alc; misc eth

b437	S- <i>tert</i> -Butyl chloro- thioformate	$\text{ClC(=O)SC(CH}_3)_3$	152.6		1.081 ₄ ³⁰	1.4691 ³⁰		42.0 ^{10mm}	46	
b438	<i>tert</i> -Butyl cyano- acetate	$\text{NCCOOC(CH}_3)_3$	141.17			1.4200 ²⁰		108		
b439	2- <i>tert</i> -Butylcyclo- hexanol	$(\text{CH}_3)_3\text{CC}_6\text{H}_{10}\text{OH}$	156.27		0.902		46			i aq
b440	4- <i>tert</i> -Butylcyclo- hexanol	$(\text{CH}_3)_3\text{CC}_6\text{H}_{10}\text{OH}$	156.27	6 ¹ , 18			70	115 ^{15mm}	105	i aq
b441	2- <i>tert</i> -Butylcyclo- hexanone	$(\text{CH}_3)_3\text{CC}_6\text{H}_9(\text{=O})$	154.25	7 ³ , 143	0.896	1.4565 ²⁰		62.5 ^{4mm}		
b442	4- <i>tert</i> -Butylcyclo- hexanone	$(\text{CH}_3)_3\text{CC}_6\text{H}_9(\text{=O})$	154.25	7 ¹ , 29			50	116 ^{20mm}	96	i aq
b443	Butyl decyl- <i>o</i> -phthalate	$\text{C}_4\text{H}_9\text{OOC C}_6\text{H}_4\text{COO-}$ $\text{C}_{10}\text{H}_{21}$	362.51		0.994 ²⁵ ₂₅				202	
b444	<i>N</i> -Butyldiethanol- amine	$\text{C}_4\text{H}_9\text{N(CH}_2\text{CH}_2\text{OH})_2$	161.25	4, 285	0.986 ²⁰ ₂₀	1.4625 ²⁰	< - 70	276	126	
b445	Butyl 3,4-dihydro-2,2- dimethyl-4-oxo-2 <i>H</i> - pyran-6-carboxylate		226.27		1.054 ²⁵ ₂₅	1.4767 ²⁰		256-270	> 112	misc alc, chl, eth

Butyl bromides, b238, b239, b311
N-Butyl-1-butanamine, d107
 Butyl carbitol, b411

Butyl Cellosolve, b410
 Butyl chlorides, c64, c65, c162
 2-*tert*-Butyl-*o*-cresol, b462

2-*tert*-Butyl-*p*-cresol, b461
tert-Butyldihydroxybenzene, b432

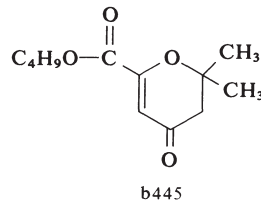
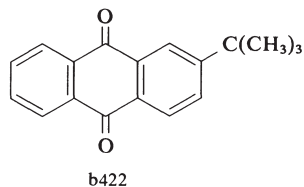


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b446	<i>tert</i> -Butyldimethylchlorosilane	$(\text{CH}_3)_3\text{CSi}(\text{CH}_3)_2\text{Cl}$	150.7				91.5	124–126		
b447	1,3-Butylene diacetate	$\text{CH}_3\text{CH}(\text{OOCCH}_3)\text{CH}_2\text{CH}_2\text{OOCCH}_3$	174.20	2, 143	1.028	1.4199 ²⁰		99 ^{8mm}	85	v s aq; s alc
b448	<i>N</i> -Butylethanolamine	$\text{HOCH}_2\text{CH}_2\text{NHC}_4\text{H}_9$	117.19		0.89 ²⁰	1.444 ²⁰	−3.5	192	77	
b449	Butyl ethyl ether	$\text{C}_4\text{H}_9\text{OC}_2\text{H}_5$	102.18	1 ³ , 1502	0.7495 ²⁰ ₄	1.3818 ²⁰	−103	92.5		i aq; misc alc, eth
b450	2-Butyl-2-ethyl-1,3-propanediol	$\text{HOCH}_2\text{C}(\text{C}_2\text{H}_5)(\text{C}_4\text{H}_9)\text{CH}_2\text{OH}$	160.25		0.931 ⁵⁰ ₂₀	1.4587 ²⁵	41.4	195 ^{100mm}		0.8 aq
b451	Butyl ethyl sulfide	$\text{C}_4\text{H}_9\text{SC}_2\text{H}_5$	118.24	1 ³ , 1522	0.8376 ²⁰ ₄	1.4491 ²⁰	−95.1	144.2		s chl
b452	<i>tert</i> -Butylhydrazine HCl	$(\text{CH}_3)_3\text{CNHNH}_2 \cdot \text{HCl}$	124.61	4 ³ , 1734			191–174			
b453	<i>tert</i> -Butylhydroperoxide	$(\text{CH}_3)_3\text{C—O—OH}$	90.12		0.896 ²⁰ ₄	1.4007 ²⁰	4–5	33–4 ^{17mm}	62	s aq, alc, chl, eth
b454	<i>tert</i> -Butylhydroquinone	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{OH})_2$	166.22				129			
b455	Butyl isocyanate	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NCO}$	99.13		0.880	1.4061 ²⁰		115	26	
b456	<i>tert</i> -Butyl isocyanate	$(\text{CH}_3)_3\text{CNCO}$	99.13	4, 175	0.868	1.3865 ²⁰		86	26	
b457	Butyllithium	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Li}$	64.06					80 ^{0.0001mm}	pyrophoric	
b458	<i>tert</i> -Butyllithium	$(\text{CH}_3)_3\text{CLi}$	64.06					subl 70 ^{0.1mm}	pyrophoric	
b459	Butyl methacrylate	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COOC}_4\text{H}_9$	142.19		0.889 ²⁵ ₁₅	1.4220 ²⁵		170	49	i aq; misc alc, eth
b460	<i>tert</i> -Butyl methyl ether	$(\text{CH}_3)_3\text{COCH}_3$	88.15	1, 381	0.758	1.3685 ²⁰	−109	56	−10	s aq; v s alc, eth
b461	2- <i>tert</i> -Butyl-4-methylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{CH}_3)\text{OH}$	164.25		0.9247 ⁷⁵ ₄	1.4969 ⁷⁵	51.7	237		i aq; s org solv

b462	2- <i>tert</i> -Butyl-6-methylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{CH}_3)\text{OH}$	164.25			1.5195 ²⁰	32	230	107	
b463	Butyl methyl sulfide	$\text{C}_4\text{H}_9\text{SCH}_3$	104.21	1 ³ , 1521	0.8426 ²⁰ ₄	1.4477 ²⁰	−97.8	123.4		v s alc
b464	Butyl nitrite	$\text{C}_4\text{H}_9\text{ONO}$	103.12	1, 369	0.9114 ⁰ ₄	1.3768		78	4	misc alc, eth
b465	<i>tert</i> -Butyl nitrite	$(\text{CH}_3)_3\text{CONO}$	103.12	1 ² , 415	0.8671 ²⁰ ₄	1.3687 ²⁰		63		sl s aq; v s alc, chl, eth, CS ₂
b466	Butyl octadecanoate	$\text{CH}_3(\text{CH}_2)_{16}\text{COOC}_4\text{H}_9$	340.60	2 ² , 352	0.8551 ²⁰ ₄	1.4422 ²⁵	26.3	343	160	s alc, v s acet
b467	Butyl 4-oxopentanoate	$\text{CH}_3\text{C}(=\text{O})\text{CH}_2\text{CH}_2\text{COOC}_4\text{H}_9$	172.22		0.9735 ²⁰ ₄	1.4270 ²⁰		107 ^{6mm}	91	s alc, eth, acet
b468	<i>tert</i> -Butyl peroxybenzoate	$\text{C}_6\text{H}_5(\text{=O})\text{O—OC}(\text{CH}_3)_3$	194.23		1.021	1.4990 ²⁰		76 ^{0.2mm}	93	
b469	2- <i>sec</i> -Butylphenol	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{—C}_6\text{H}_4\text{OH}$	150.22		0.982	1.5222 ²⁰	12	228	112	i aq; s alc; v s eth
b470	2- <i>tert</i> -Butylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{OH}$	150.22	6 ² , 489	0.9783 ²⁰ ₄	1.5228 ²⁰	−7	221–224	110	
b471	3- <i>tert</i> -Butylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{OH}$	150.22				40–41	240		
b472	4- <i>sec</i> -Butylphenol	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{—C}_6\text{H}_4\text{OH}$	150.22	6, 522	0.969 ²⁰ ₄	1.5150	62	136 ^{25mm}	115	s hot aq, alc, eth
b473	4- <i>tert</i> -Butylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{OH}$	150.22	6, 524	0.908 ¹¹⁴ ₄	1.4787 ¹¹⁴	100–101	237		i aq; s alc, eth
b474	2-(4- <i>sec</i> -Butylphenoxy)ethanol	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}_6\text{H}_4\text{—OCH}_2\text{CH}_2\text{OH}$	194.2		1.008 ²⁵		< −20	158 ^{10mm}	149	0.1 aq
b475	2-(4- <i>tert</i> -Butylphenoxy)ethanol	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{—OCH}_2\text{CH}_2\text{OH}$	194.3		1.016 ²⁵		54	167 ^{10mm}	157	0.1 aq
b476	<i>tert</i> -Butyl phenyl carbonate	$\text{C}_6\text{H}_5\text{OC}(=\text{O})\text{OC}(\text{CH}_3)_3$	194.23		1.047	1.4805 ²⁰		79 ^{0.8mm}		
b477	Butyl phenyl ether	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OC}_6\text{H}_5$	150.22	6, 143	0.9351 ²⁰ ₄	1.4970 ²⁰	−19	210.3	82	

Butyl disulfides, d113, d114

1,4-Butylene bis(2,3-epoxypropyl) ether, b175

1,3-Butylene glycol methyl ether, m57

1,2-Butylene oxide, e3

Butyl ether, d115

Butyl ethyl ketone, h16

tert-Butyl fluoride, f20

Butyl glycol, b410

2,2'-(Butylimino)diethanol, b444

Butyl iodides, i30, i31, i44

Butyl levulinate, b467

Butyl mercaptans, b388, m378, m379, m380

Butyl methyl ketone, d497

tert-Butyl perbenzoate, b468

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

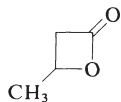
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
b478	4- <i>tert</i> -Butylphenyl salicylate	$\text{HOC}_6\text{H}_4\text{COOC}_6\text{H}_4\text{-C}(\text{CH}_3)_3$	270.31				62–64			0.1 aq; 79 alc; 153 EtAc; 158 toluene
b479	Butyl propionate	$\text{CH}_3\text{CH}_2\text{COOC}_4\text{H}_9$	130.19	2, 241	0.8818 ¹⁵	1.3982 ²⁵	–89.6	145.5		misc alc, eth
b480	4- <i>tert</i> -Butylpyridine	$(\text{CH}_3)_3\text{C}(\text{C}_5\text{H}_4\text{N})$	135.21	20, 252	0.915	1.4952 ²⁰		197	63	
b481	Butyltin chloride	$\text{C}_4\text{H}_9\text{SnCl}_3$	282.17		1.693	1.5229 ²⁰		93 ^{10mm}	81	
b482	4- <i>tert</i> -Butyltoluene	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{CH}_3$	148.25	5, 439	0.853	1.4897 ²⁰		192	54	d aq, hot alc; s eth
b483	Butyltrichlorosilane	$\text{C}_4\text{H}_9\text{SiCl}_3$	191.5	4 ¹ , 582	1.1614 ²⁰	1.436 ²⁰		142–143		
b484	Butyl trifluoroacetate	$\text{CF}_3\text{COOC}_4\text{H}_9$	170.1		1.0268 ²²	1.353 ²²		100.2		
b485	Butyltrimethoxysilane	$\text{C}_4\text{H}_9\text{Si}(\text{OCH}_3)_3$	178.3		0.9312 ²⁰	1.3979 ²⁰		164–165		
b486	<i>tert</i> -Butyl trimethylsilyl peroxide	$(\text{CH}_3)_3\text{C—O—O—Si}(\text{CH}_3)_3$	162.3		0.8219 ²⁰	1.3935 ²⁵	d 135	41 ^{41mm}		
b487	Butyl urea	$\text{C}_4\text{H}_9\text{NHCONH}_2$	116.16	4 ¹ , 371			93–95			s aq, alc, eth
b488	Butyl vinyl ether	$\text{C}_4\text{H}_9\text{OCH=CH}_2$	100.16		0.7792 ²⁰	1.4007 ²⁰	–112.7	94.2	–9	0.3 aq
b489	5- <i>tert</i> -Butyl- <i>m</i> -xylene	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{CH}_3)_2$	162.28	5, 447	0.867	1.4946 ²⁰		205–206	72	
b490	1-Butyne	$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CH}$	54.09	1, 249	0.7110 ²⁰	1.3962 ²⁰	–125.7	8.1		i aq; s alc, eth
b491	2-Butyne	$\text{CH}_3\text{C}\equiv\text{CCH}_3$	54.09	1, 249	0.6910 ²⁰	1.3920 ²⁰	–32.3	17.0		i aq; s alc, eth
b492	2-Butyne-1,4-diol	$\text{HOCH}_2\text{C}\equiv\text{CCH}_2\text{OH}$	86.09	1 ¹ , 261		1.450 ²⁵	54–58	238	152	374 aq; 83 alc; 0.04 bz; 2.6 eth; 70 acet
b493	Butyraldehyde	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$	72.11	1, 662	0.8016 ²⁰	1.3791 ²⁰	–96.4	74.8	–6.7	7.1 aq; misc alc, eth, acet, EtAc
b494	Butyramide	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CONH}_2$	87.12	2, 275			116	216		16 aq; s alc
b495	Butyric acid	$\text{CH}_3\text{CH}_2\text{CH}_2\text{COOH}$	88.11	2, 264	0.9582 ²⁰	1.3980 ²⁰	–5.3	163.3	77	misc aq, alc, eth
b496	Butyric anhydride	$[\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})]_2\text{O}$	158.20	2, 274	0.9668 ²⁰	1.4130 ²⁰	–65.7	199.5	87	s aq, alc(d), eth

b497	3-Butyrolactone		86.09	17 ¹ , 130	1.056	1.4109	20	73 ^{29mm}	60	
b498	4-Butyrolactone		86.09	17, 234	1.124 ²⁵ ₄	1.4348 ²⁵	−43.5	204	98	misc aq, alc, acet, bz, eth, CCl ₄
b499	Butyronitrile	CH ₃ CH ₂ CH ₂ CN	69.11	2 ² , 252	0.7954 ¹⁵ ₄	1.3860 ¹⁵	−111.9	117.9	16	3.3 aq; misc alc, eth
b500	Butyrophenone	C ₆ H ₅ C(O)C ₃ H ₇	148.21	7, 313	1.021	1.5195 ²⁰	13	222	88	
b501	Butyryl chloride	CH ₃ CH ₂ CH ₂ COCl	106.55	2, 274	1.0263 ²¹ ₄	1.4122 ²⁰	−89	102	21	s aq, alc(d); misc eth
c1	Caffeine		194.19	26, 461	1.23 ¹⁸ ₄		238	subl 178		2.1 aq; 1.5 alc; 18 chl; 0.19 eth; 1 bz
c2	DL-Camphene		136.24	5, 156	0.8422 ⁵⁴ ₄	1.4551 ⁵⁴	51–52	159	36	i aq; s alc, chl, eth
c3	D-(+)-Camphor		152.23	7, 101	0.9920 ²⁵ ₄		178.8	207.4		100 alc; 100 eth; 200 chl; 250 acet
c4	DL-Camphor		152.24	7, 135			177	204	64	
c5	D-Camphoric acid		200.23	9, 745	1.186 ²⁰ ₄		186–188			4 aq; 100 alc; s chl, eth

Butyl *o*-phthalate, d128
 Butyl propyl ketone, 036
 Butyl stearate, b466
 Butyl sulfate, d131

Butyl sulfides, d132, d133
 Butyl sulfite, d134
 Butyl sulfone, d135
 Butyrolactam, p275

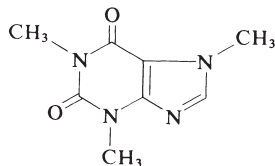
Cadaverine, p29
 2-Camphanone, c3



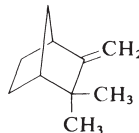
b497



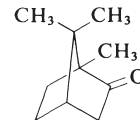
b498



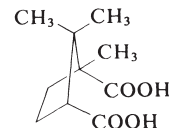
c1



c2



c3, c4



c5

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c6	DL-Camphoric anhydride		182.22	17, 455	1.194 ₄ ²⁰		225	270		s bz; sl s aq, alc, eth
c7	D-10-Camphor-sulfonic acid hydrate		250.32	11, 316			194 d			deliq moist air; sl s HOAc, EtAc; i eth
c8	Carbazole		167.21	20, 433			245–246	355		
c9	4-Carboethoxy-3-methyl-3-cyclohexen-1-one		182.22	10, 631	1.078	1.4880 ²⁰		268–272	>112	
c10	Carbobenzyloxy-glycine	C ₆ H ₅ CH ₂ OC(=O)NH-CH ₂ COOH	209.20				122			
c11	Carbohydrazide	H ₂ NNHC(=O)NHNH ₂	90.09	3, 121			d 153			v s aq; i alc, bz, eth
c12	2-(Carbomethoxy)-ethylmethyl-dichlorosilane	CH ₃ OC(=O)CH ₂ CH ₂ Si-(CH ₃)Cl ₂	201.1		1.187 ₄ ²⁵	1.4439 ²⁵		98–99 ^{25mm}		
c13	2-Carbomethoxyethyl-trichlorosilane	CH ₃ OC(=O)CH ₂ CH ₂ -SiCl ₃	221.6		1.325 ₄ ²⁰	1.448 ²⁰		88–89 ^{2mm}		
c14	2-Carboxybenzaldehyde	HC(=O)C ₆ H ₄ COOH	150.13	10, 666			96–98			
c15	4-Carboxy-1,2-benzenedicarboxylic anhydride		192.13	18, 468			161–164	240–245 ^{14mm}		15.5 DMF; 49.6 acet; 21.6 EtAc
c16	4-Carboxybenzenesulfonamide	HOCC ₆ H ₄ SO ₂ NH ₂	201.20	11, 390			d 280			i aq, bz, eth; v s alc
c17	2-Carboxyethyl-phosphonic acid	HOCCCH ₂ CH ₂ -P(O)(OH) ₂	154.06	4 ² , 976						
c18	DL-Carnitine HCl	(CH ₃) ₃ NCH ₂ CHOH-CH ₂ COOH · HCl	197.66				197 d			v s aq; i acet, eth

c19	<i>trans</i> - β -Carotene	536.89	30, 87	1.000 ₂₀ ²⁰		183			i aq; s bz, chl, CS ₂
c20	D-(+)-Carvone	150.22	7, 153	0.965 ₄ ²⁰	1.4989 ²⁰		230		i aq; misc alc
c21	Catecholborane	119.92			1.5070 ²⁰	12	50 ^{50mm}	88	

Capric acid, d14

Caproaldehyde, h54

Caproic acid, h66

Caproic anhydride, h67

ϵ -Caprolactam, o57

ϵ -Caprolactone, h71

Capronitrile, h63

Caproyl chloride, h73

Caprylic acid, o29

Capryl alcohol, o30

Caprylaldehyde, o40

Caprylonitrile, o27

Capryloyl chloride, o37

CAPS, c337

N-(Carbamoylmethyl)iminodiacetic acid, a14

Carbamylurea, b215

Carbanilide, d693

Carbazole, d665

Carbitol, e35

Carbitol acetate, e36

Carbomethoxy chloride, b90

4,4'-Carboxyldiphthalic anhydride, b55

N-Carbonylsulfamyl chloride, c240

Carboxybenzaldehyde, f33

(3-Carboxy-2-hydroxypropyl)

trimethylammonium hydroxide, c18

3-Carbomethoxypropionyl chloride, m188

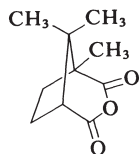
(Carboxymethylimino)bis(ethylenenitrilo)-

tetraacetic acid, d299

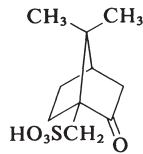
(Carboxymethyl)trimethylammonium

hydroxide, b128

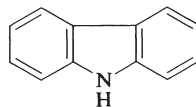
3-Carboxypropyl disulfide, d708



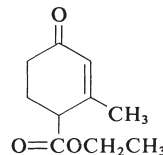
c6



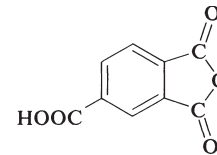
c7



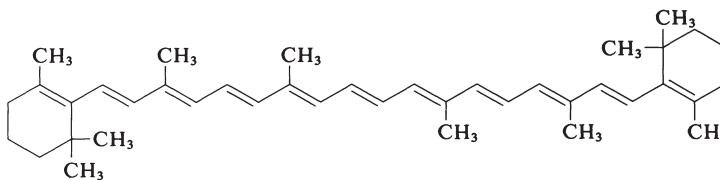
c8



c9

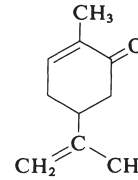


c15

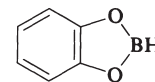


c19

[Note: 9 successive
(\searrow) units]



c20



c21

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c22	2-Chloroacetamide	$\text{ClCH}_2\text{CONH}_2$	93.51	2, 199			118	225 d		10 aq; 10 alc; sl s eth
c23	<i>p</i> -Chloroacetanilide	$\text{ClC}_6\text{H}_4\text{NHCOCH}_3$	169.61	12, 611	1.385 ₄ ²⁰		179			i aq; v s alc, eth, CS ₂
c24	Chloroacetic acid	ClCH_2COOH	94.50	2, 194	1.580(<i>c</i>)	1.4297 ⁶⁵	63(α)	189		v s aq; s alc, bz, eth
c25	Chloroacetic anhydride	$[\text{ClCH}_2\text{C(O)}]_2\text{O}$	170.98	2, 199	1.5494 ₄ ²⁰		46	203		d aq; v s chl, eth
c26	<i>p</i> -Chloroacetoacetanilide	$\text{CH}_3\text{COCH}_2\text{CONHC}_6\text{H}_4\text{Cl}$	211.65				134			
c27	Chloroacetonitrile	ClCH_2CN	75.50	2, 201	1.193	1.4225 ²⁰		126	47	
c28	α -Chloroacetophenone	$\text{C}_6\text{H}_5\text{COCH}_2\text{Cl}$	154.60	7, 282	1.324 ¹⁵		54	245		i aq; v s alc, bz, eth
c29	<i>o</i> -Chloroacetophenone	$\text{ClC}_6\text{H}_4\text{COCH}_3$	154.60	7 ¹ , 151	1.188	1.5438 ²⁰		228 ^{738mm}	88	sl s aq; s eth
c30	<i>p</i> -Chloroacetophenone	$\text{ClC}_6\text{H}_4\text{COCH}_3$	154.60	7, 281	1.192 ₄ ²⁰	1.5549	20–21	237	90	i aq; misc alc, eth
c31	Chloroacetyl chloride	ClCH_2COCl	112.94	2, 199	1.418 ₂₅ ²⁵	1.4530 ²⁰	–22.5	106	none	d aq, MeOH
c32	2-Chloroacrylonitrile	$\text{H}_2\text{C}=\text{C}(\text{Cl})\text{CN}$	87.51		1.096	1.4290 ²⁰	–65	89	6	
c33	2-Chloroaniline	$\text{ClC}_6\text{H}_4\text{NH}_2$	127.57	12, 597	1.2125 ₄ ²⁰	1.5881 ²⁰	–1.94	208.8	97	0.88 aq; s alc, bz, eth
c34	3-Chloroaniline	$\text{ClC}_6\text{H}_4\text{NH}_2$	127.57	12, 602	1.2150 ₄ ²²	1.5931 ²⁰	–10.4	230.5	123	i aq; s alc, bz, eth
c35	<i>p</i> -Chloroaniline	$\text{ClC}_6\text{H}_4\text{NH}_2$	127.57	12, 607	1.169 ₇₄ ⁷⁷	1.5546 ⁸⁵	72.5	232		s hot aq; v s alc, acet, eth, CS ₂
c36	1-Chloroanthraquinone		242.66	7, 787			160	subl		sl s alc; misc eth; s hot bz
c37	2-Chloroanthraquinone		242.66	7, 787			211	subl		sl s alc, bz; i eth

c38	2-Chlorobenzaldehyde	$\text{ClC}_6\text{H}_4\text{CHO}$	140.57	7, 233	1.2483 ₄ ²⁰	1.5658	11	215	87	sl s aq; s alc, bz, eth
c39	4-Chlorobenzaldehyde	$\text{ClC}_6\text{H}_4\text{CHO}$	140.57	7, 235	1.196 ₄ ⁶¹	1.552 ⁶¹	47	214	87	s aq; v s alc, bz, eth
c40	2-Chlorobenzamide	$\text{ClC}_6\text{H}_4\text{CONH}_2$	155.58	9, 336			142–144			
c41	Chlorobenzene	$\text{C}_6\text{H}_5\text{Cl}$	112.56	5, 199	1.1063 ²⁰	1.5248 ²⁰	–45.3	131.7	23	0.049 aq ³⁰ ; v s alc, bz, chl, eth
c42	4-Chlorobenzene-sulfonamide	$\text{ClC}_6\text{H}_4\text{SO}_2\text{NH}_2$	191.64	11, 55			146			s hot aq, hot alc, hot eth
c43	4-Chlorobenzene-sulfonyl chloride	$\text{ClC}_6\text{H}_4\text{SO}_2\text{Cl}$	211.07	11, 55			55	141 ^{15mm}		d aq, alc; v s bz, eth
c44	4-Chlorobenzhydrol	$\text{ClC}_6\text{H}_4\text{CH}(\text{OH})\text{C}_6\text{H}_5$	218.68	6, 680			58–60			
c45	2-Chlorobenzoic acid	$\text{ClC}_6\text{H}_4\text{COOH}$	156.57	9, 334	1.544 ₄ ²⁵		142			0.11 aq; v s alc, eth

Cellosolve, c34
 Cellosolve acetate, e37
 Cetyl alcohol, h36
 Cetyl bromide, b294
 Chalcone, d686
 CHES, c335

Chloramine T, c247
 Chloranils, t24, t25
 Chloranilic acid, d172
 Chlorendic anhydride, h30
 Chloroacetaldehyde diethyl acetal, c81
 Chloroacetaldehyde dimethyl acetal, c89

Chloroacetone, c215
 4-(Chloroacetyl)catechol, c86
 Chloroanthranilic acid, a140
 5-Chloroanthranilonitrile, a141
p-Chlorobenzenethiol, c243

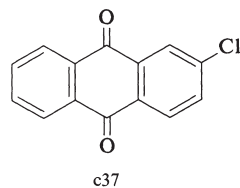
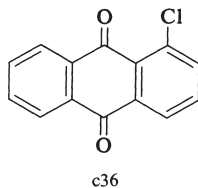


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c46	3-Chlorobenzoic acid	$\text{ClC}_6\text{H}_4\text{COOH}$	156.57	9, 337	1.496 ₄ ²⁵		157–158			0.04 aq; v s alc, eth
c46a	4-Chlorobenzoic acid	$\text{ClC}_6\text{H}_4\text{COOH}$	156.57	9, 340			241–243			0.02 aq; v s alc, eth
c47	2-Chlorobenzonitrile	$\text{ClC}_6\text{H}_4\text{CN}$	137.57	9, 336			46	232		s alc, eth
c48	4-Chlorobenzonitrile	$\text{ClC}_6\text{H}_4\text{CN}$	137.57	9, 341			93	22		s alc, bz, chl, eth
c49	2-Chlorobenzophenone	$\text{ClC}_6\text{H}_4\text{COC}_6\text{H}_5$	216.67	7, 419			44–47	300		
c50	4-Chlorobenzophenone	$\text{ClC}_6\text{H}_4\text{COC}_6\text{H}_5$	216.67	7, 419			77	196 ^{17mm}		s alc, acet, bz, eth
c51	2-Chlorobenzotrifluoride	$\text{ClC}_6\text{H}_4\text{CF}_3$	180.56		1.3540 ²⁵	1.4513 ²⁵	–6.4	152.3		
c52	3-Chlorobenzotrifluoride	$\text{ClC}_6\text{H}_4\text{CF}_3$	180.56		1.3311 ²⁵	1.4438 ²⁵	–56.7	137.7	36	
c53	4-Chlorobenzotrifluoride	$\text{ClC}_6\text{H}_4\text{CF}_3$	180.56		1.353 ²⁰	1.4463	–33.2	138.7	47	
c54	2-(4-Chlorobenzoyl)-benzoic acid	$\text{ClC}_6\text{H}_4\text{COC}_6\text{H}_4\text{COCH}$	260.68	10, 750			150			s alc, bz, eth
c55	2-Chlorobenzoyl chloride	$\text{ClC}_6\text{H}_4\text{COCl}$	175.01	9, 336	1.382	1.5718 ²⁰	–3	238	110	d aq, alc
c56	4-Chlorobenzoyl chloride	$\text{ClC}_6\text{H}_4\text{COCl}$	175.01	9, 341	1.377	1.5780 ²⁰	14	222	105	d aq, alc
c57	4-Chlorobenzyl alcohol	$\text{ClC}_6\text{H}_4\text{CH}_2\text{OH}$	142.59	6, 444			72	234		v s alc, eth
c58	4-Chlorobenzylamine	$\text{ClC}_6\text{H}_4\text{CH}_2\text{NH}_2$	141.60	12, 1074	1.164	1.5586 ²⁰		215	90	
c59	2-Chlorobenzyl chloride	$\text{ClC}_6\text{H}_4\text{CH}_2\text{Cl}$	161.03	5, 297	1.274	1.5591 ²⁰	–17	214	82	
c60	4-Chlorobenzyl chloride	$\text{ClC}_6\text{H}_4\text{CH}_2\text{Cl}$	161.03	5, 308			30	214	97	s alc; v s eth

c61	2(<i>p</i> -Chlorobenzyl)-pyridine	$\text{ClC}_6\text{H}_4\text{CH}_2-\text{C}_5\text{H}_4\text{N}$	203.67		1.390	1.5868 ²⁰		183 ^{20mm}	>112	
c62	4-(<i>p</i> -Chlorobenzyl)-pyridine	$\text{ClC}_6\text{H}_4\text{CH}_2-\text{C}_5\text{H}_4\text{N}$	203.67		1.167	1.5900 ²⁰			>112	
c63	1-Chloro-1,3-butadiene	$\text{H}_2\text{C}=\text{CHCH}=\text{CHCl}$	88.54	1 ³ , 949	0.9601 ²⁰ ₄	1.4712 ²⁰		68		v s chl
c64	1-Chlorobutane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$	92.57	1, 118	0.8864 ²⁰ ₄	1.4021 ²⁰	−123.1	78.44	−6	0.11 aq; misc alc, eth
c65	2-Chlorobutane	$\text{CH}_3\text{CH}_2\text{CH}(\text{Cl})\text{CH}_3$	92.57	1, 119	0.8732 ²⁰ ₄	1.3971 ²⁰	−113.3	68.25	−15	0.1 aq; misc alc, eth
c66	4-Chloro-1-butanol	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$	108.56	1 ² , 398	1.0883 ²⁰ ₄	1.4518 ²⁰		86–89 ^{20mm}	32	s alc, eth
c67	3-Chloro-2-butanone	$\text{CH}_3\text{CH}(\text{Cl})\text{COCH}_3$	106.55	1, 669	1.055	1.4172 ²⁰		117	21	v s alc, eth
c68	<i>cis</i> -1-Chloro-2-butene	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{Cl}$	90.55	1 ² , 176	0.9426 ²⁰ ₄	1.4390 ²⁰		84.1	−15	s alc, acet
c69	3-Chloro-1-butene	$\text{CH}_3\text{CH}(\text{Cl})\text{CH}=\text{CH}_2$	90.55	1 ² , 174	0.90001 ²⁰ ₄	1.4155 ²⁰		62–65	−20	v s acet
c70	3-Chloro-1-butyne	$\text{CH}_3\text{CH}(\text{Cl})\text{C}\equiv\text{CH}$	88.54	1 ⁴ , 970	0.961	1.4280 ²⁰		68–70	1	
c71	3-Chlorobutyric acid	$\text{CH}_3\text{CH}(\text{Cl})\text{CH}_2\text{COOH}$	122.55	2, 277	1.186 ²⁰ ₄	1.4421 ²⁰	16.3	109 ^{17mm}		s alc, eth
c72	4-Chlorobutyric acid	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{COOH}$	122.55	2, 278	1.2336 ²⁰ ₄	1.4510 ²⁰	12–16	196 ^{22mm}	>112	sl s aq; v s eth
c73	4-Chlorobutyronitrile	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{CN}$	103.55	2, 278	1.158	1.4413 ²⁰		197	85	s alc, eth
c74	4-Chlorobutyryl chloride	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{COCl}$	141.00	2, 278	1.258	1.4609 ²⁰		174	72	d aq, alc; s eth
c75	Chloro(chloromethyl)-dimethylsilane	$\text{ClCH}_2\text{Si}(\text{CH}_3)_2\text{Cl}$	143.09		1.086	1.4373 ²⁰		114 ^{752mm}	21	
c76	<i>trans-p</i> -Chlorocinnamic acid	$\text{ClC}_6\text{H}_4\text{CH}=\text{CHCOOH}$	182.61	9, 594			248–250			
c77	Chlorocyclohexane	$\text{ClC}_6\text{H}_{11}$	118.61	5, 21	1.000 ²⁰ ₄	1.4620 ²⁰	−44	142	28	i aq; s alc, eth
c78	2-Chlorocyclohexanone	$\text{ClC}_6\text{H}_9(=\text{O})$	132.59	7, 10	1.161	1.4835 ²⁰	23	83 ^{10mm}	82	s bz, eth, diox

4-Chlorobenzyl mercaptan, c248

Chlorocresols, c158, c159

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c79	Chlorocyclopentane	ClC_5H_9	104.58	5, 19	1.0051_4^{20}	1.4512^{20}		114	15	i aq
c80	1-Chlorodecane	$\text{CH}_3(\text{CH}_2)_9\text{Cl}$	176.73	1, 168	0.868	1.4362^{20}	−34	223	83	i aq
c81	2-Chloro-1,1-diethoxyethane	$\text{ClCH}_2\text{CH}(\text{OC}_2\text{H}_5)_2$	152.62	1, 611	1.018	1.4157^{20}		157	29	
c82	3-Chloro-1,1-diethoxypropane	$\text{ClCH}_2\text{CH}_2\text{CH}(\text{OC}_2\text{H}_5)_2$	166.65	1, 632	0.995	1.4240^{20}		$84^{25\text{mm}}$	36	
c83	Chlorodifluoroacetic acid	$\text{F}_2\text{C}(\text{Cl})\text{COOH}$	130.48	2, 201		1.3559^{20}	22.9	121.5		
c84	1-Chloro-1,1-difluoroethane	$\text{CH}_3\text{C}(\text{Cl})\text{F}_2$	100.50		1.118^{21}		−131	−9		0.19 aq
c85	Chlorodifluoromethane	HCClF_2	86.47		1.209^{21}		−160	−40.8		0.30 aq
c86	α -Chloro-3',4'-dihydroxyacetophenone	$(\text{HO})_2\text{C}_6\text{H}_3\text{C}(=\text{O})\text{CH}_2\text{Cl}$	186.59	8, 273			176			
c87	1-Chloro-2,4-dihydroxybenzene	$\text{ClC}_6\text{H}_3(\text{OH})_2$	144.56	6 ² , 818			107	$147^{18\text{mm}}$		v s aq, alc, chl, eth
c88	2-Chloro-1,4-dihydroxybenzene	$\text{ClC}_6\text{H}_3(\text{OH})_2$	144.56	6, 849			101–102	263		v s aq; i alc; s eth
c89	2-Chloro-1,1-dimethoxyethane	$\text{ClCH}_2\text{CH}(\text{OCH}_3)_2$	124.57		1.094_{20}^{20}	1.4148^{20}		130	28	
c90	4-Chloro-3,5-dimethylphenol	$\text{Cl}(\text{CH}_3)_2\text{C}_6\text{H}_2\text{OH}$	156.61	6 ² , 463			115.5	246		0.1 aq; 1 alc; s bz, eth, alk
c91	1-Chloro-2,2-dimethylpropane	$(\text{CH}_3)_3\text{CCH}_2\text{Cl}$	106.59		0.866_4^{20}	1.4042^{20}	−20	84.4		
c92	Chlorodimethylsilane	$(\text{CH}_3)_2\text{Si}(\text{Cl})\text{H}$	94.62		0.852_4^{20}	1.3827^{20}	−111	36	−28	
c93	Chlorodimethylvinylsilane	$(\text{CH}_3)_2\text{Si}(\text{Cl})\text{CH}=\text{CH}_2$	120.7		0.884_4^{25}	1.414^{25}		82.5		

c94	1-Chloro-2,4-di-nitrobenzene	$\text{ClC}_6\text{H}_3(\text{NO}_2)_2$	202.55	5, 263	1.4982 ⁷⁵ ₄	1.5857 ⁶⁰	52–54	315	186	sl s alc; s hot alc, bz, eth
c95	1-Chloro-3,4-di-nitrobenzene	$\text{ClC}_6\text{H}_3(\text{NO}_2)_2$	202.55	5, 262	1.6867 ¹⁶	1.5870 ²⁰			>112	v s eth; s alc
c96	2-Chloro-3,5-di-nitrobenzoic acid	$\text{ClC}_6\text{H}_2(\text{NO}_2)_2\text{COOH}$	246.56	9, 415			198	241 ex-plodes		0.3 aq
c97	α -Chlorodiphenyl-methane	$\text{C}_6\text{H}_5\text{CH}(\text{Cl})\text{C}_6\text{H}_5$	202.68	5 ² , 600	1.140 ²⁰ ₄	1.5951 ²⁰	17	140 ^{3mm}	>112	
c98	Chlorodiphenyl-methylsilane	$(\text{C}_6\text{H}_5)_2\text{Si}(\text{Cl})\text{CH}_3$	232.8		1.1277 ²⁰ ₄	1.5742 ²⁰		295		
c99	Chlorodiphenyl-phosphine	$(\text{C}_6\text{H}_5)_2\text{PCl}$	220.64	16, 763	1.229	1.6338 ²⁰		320	>112	
c100	1-Chlorododecane	$\text{CH}_3(\text{CH}_2)_{11}\text{Cl}$	204.79		0.8673 ²⁰ ₄	1.4426	–9	116	93	v s alc; s bz
c101	1-Chloro-2,3-epoxy-propane	$\text{H}_2\text{C}-\text{CHCH}_2\text{Cl}$ $\diagup \quad \diagdown$ O	92.53	17, 6	1.1812 ²⁰ ₄	1.4381 ²⁰	–57.2	116.1	33	5.9 aq; misc alc, chl,
c102	Chloroethane	$\text{CH}_3\text{CH}_2\text{Cl}$	64.52	1, 82	0.9214 ⁰ ₄	1.3742 ¹⁰	–136 to –138	12.3	–43	0.45 aq ⁰ ; 48 alc; misc eth
c103	2-Chloroethanol	$\text{ClCH}_2\text{CH}_2\text{OH}$	80.52	1, 337	1.197 ²⁰ ₄	1.4422 ²⁰	–67.5	128.6	60	misc aq, alc
c104	2-(2-Chloroethoxy)-ethanol	$\text{ClCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{OH}$	124.57	1, 467	1.180	1.4529 ²⁰		81 ^{5mm}	90	
c105	2-[2-(2-Chloroethoxy)ethoxy]ethanol	$\text{ClCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{-OCH}_2\text{CH}_2\text{OH}$	168.62	1, 468	1.160	1.4580 ²⁰		120 ^{5mm}	107	
c106	2-Chloroethylamine HCl	$\text{ClCH}_2\text{CH}_2\text{NH}_2 \text{HCl}$	115.99	4, 133			146			
c107	1-Chloro-2-ethylbenzene	$\text{ClC}_6\text{H}_4\text{C}_2\text{H}_5$	140.61		1.055 ²⁵ ₂₃		–81	179.2		i aq; misc alc, eth
c108	(2-Chloroethyl)-benzene	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{Cl}$	140.61	5, 354	1.069	1.5300 ²⁰		84 ^{16mm}	66	s alc, bz, eth

Chlorodibromomethane, d71
2-Chloro-*N,N*-diethylethylamine, d272

Chlorodimethyl ether, c155
2-Chloro-*N,N*-dimethylethylamine, d467

4'-Chlorodiphenylmethanol, c44
2-Chloroethyl alcohol, c103

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

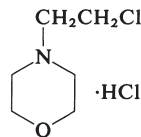
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c109	Chloroethylene	$\text{H}_2\text{C}=\text{CHCl}$	62.50	1, 186	0.97^{-14}		-159.7	-13.9		sl s aq; s alc
c110	2-Chloroethyl ethyl ether	$\text{ClCH}_2\text{CH}_2\text{OCH}_2\text{CH}_3$	108.57	1, 337	0.989	1.4125 ²⁰		107	15	
c111	2-Chloroethyl methyl ether	$\text{ClCH}_2\text{CH}_2\text{OCH}_3$	94.54	1, 337	1.035	1.4111 ²⁰		89-90	15	
c112	<i>N</i> -(2-Chloroethyl)-morpholine HCl		186.08				186			
c113	<i>N</i> -(2-Chloroethyl)-piperidine HCl		184.11	20, 17			236			
c114	2-Chloroethyl <i>p</i> -toluenesulfonate	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_3\text{CH}_2\text{CH}_2\text{Cl}$	234.70	11 ² , 45	1.294	1.5290 ²⁰		153 ^{0.3mm}	>112	
c115	2-Chloroethyl vinyl ether	$\text{H}_2\text{C}=\text{CHOCH}_2\text{CH}_2\text{Cl}$	106.55	1 ² , 473	1.048	1.4370 ²⁰	-69.7	110	16	0.6 aq
c116	1-Chloro-2-fluorobenzene	$\text{ClC}_6\text{H}_4\text{F}$	130.55	5 ¹ , 110	1.244	1.5010 ²⁰	-42.5	138.5	31	s alc, eth
c117	1-Chloro-3-fluorobenzene	$\text{ClC}_6\text{H}_4\text{F}$	130.55		1.219	1.4944 ²⁰		126	20	s alc, eth
c118	1-Chloro-4-fluorobenzene	$\text{ClC}_6\text{H}_4\text{F}$	130.55	5, 201	1.226 ²⁰ ₄	1.4967 ²⁰	-21.5	130-131		s alc, eth
c119	2-Chloro-6-fluorobenzyl chloride	$\text{Cl(F)C}_6\text{H}_3\text{CH}_2\text{Cl}$	179.02		1.401	1.5372 ²⁰				
c120	4-Chloro-4'-fluorobutyrophenone	$\text{FC}_6\text{H}_4\text{C(=O)CH}_2\text{CH}_2\text{CH}_2\text{Cl}$	200.64		1.220	1.5255 ²⁰			110	
c121	3-Chloro-4-fluoronitrobenzene	$\text{Cl(F)C}_6\text{H}_3\text{NO}_2$	175.5		1.6028 ¹⁷	1.5674 ¹⁷	41.5	127 ^{17mm}		
c122	2-Chloro-4-fluorophenol	$\text{Cl(F)C}_6\text{H}_3\text{OH}$	146.5				23	88 ^{4mm}		
c123	2-Chloro-4-fluorotoluene	$\text{Cl(F)C}_6\text{H}_3\text{CH}_3$	144.58		1.1972 ²⁰	1.4985 ²⁵		152-153		

c124	2-Chloro-6-fluoro-toluene	Cl(F)C ₆ H ₃ CH ₃	144.58		1.191	1.5026 ²⁰		156	46	
c125	4-Chloro-2-fluoro-toluene	Cl(F)C ₆ H ₃ CH ₃	144.58			1.4998 ²⁰		158		
c126	Chloroform	CHCl ₃	119.39	1, 61	1.4985 ¹⁵	1.4486 ¹⁵	−63.59	61.7	none	0.82 aq
c127	Chloroform- <i>d</i>	CDCl ₃	120.39		1.50	1.4445 ²⁰		60.9	none	
c128	1-Chloroheptane	CH ₃ (CH ₂) ₆ Cl	134.65	1, 154	0.881 ₀ ¹⁶	1.4250 ²⁰	−69	159–161	41	misc alc, eth
c129	1-Chlorohexane	CH ₃ (CH ₂) ₅ Cl	120.62		0.8780 ₄ ²⁰	1.4236 ²⁰		134	38	i aq
c130	6-Chloro-1-hexanol	Cl(CH ₂) ₆ OH	136.62		1.204	1.4557 ²⁰		108 ^{14mm}	98	sl s aq; v s alc, eth
c131	4-Chloro-4'-hydroxy-benzophenone	ClC ₆ H ₄ C(=O)C ₆ H ₄ OH	232.67	8 ² , 187			175–178	257 ^{14mm}		
c132	5-Chloro-8-hydroxy-7-iodoquinoline		305.50				d 172			i alc, eth; 0.8 chl; 0.6 HOAc
c133	3-Chloro-4-hydroxy-mandelic acid	ClC ₆ H ₃ (OH)-CH(OH)COOH	202.60				145–147			
c134	5-Chloro-8-hydroxy-quinoline		179.61	21, 95			130			sl s aq HCl
c135	1-Chloro-4-iodo-benzene	ClC ₆ H ₄ I	238.46	5, 221	1.186 ₄ ⁵⁷		53–54	226–227		s alc

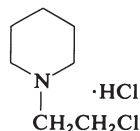
2-Chloroethyl ether, b158
2-Chloro-6-fluorobenzal chloride, t233

α-Chloro-4-fluorotoluene, f16
2375-Chloro-2-hydroxyaniline, a148

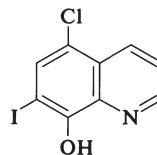
Chlorohydroxybenzoic acids, c237, c238
1-Chloro-3-hydroxypropane, c214



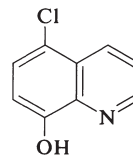
c112



c113



c132



c134

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

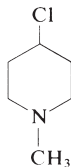
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c136	1-Chloro-3-mercapto-2-propanol	$\text{HSCH}_2\text{CH}(\text{OH})\text{CH}_2\text{Cl}$	126.61	1 ³ , 2156	1.277	1.5276 ²⁰		57 ^{1.3mm}	97	
c137	Chloromethane	CH_3Cl	50.49	1, 59	0.92 ²⁰	1.3712 ⁻²⁴	-97.7	-24.22		0.48 aq ²⁵ ; s alc; misc chl, eth, HOAc
c137a	3-Chloro-4-methoxyaniline	$\text{ClC}_6\text{H}_3(\text{OCH}_3)\text{NH}_2$	157.60	13, 511			50-55			
c138	5-Chloro-2-methoxyaniline	$\text{ClC}_6\text{H}_3(\text{OCH}_3)\text{NH}_2$	157.60	13, 383			83-85			
c139	1-Chloro-2-methoxybenzene	$\text{ClC}_6\text{H}_4\text{OCH}_3$	142.59	6, 184	1.123	1.5445 ²⁰		196	76	i aq; s alc, eth
c140	1-Chloro-4-methoxy-2-nitrobenzene	$\text{CH}_3\text{O}(\text{Cl})\text{C}_6\text{H}_3\text{NO}_2$	187.58				45			s hot alc
c141	2-Chloro-6-methoxypyridine	$\text{CH}_3\text{O}(\text{Cl})(\text{C}_5\text{H}_3\text{N})$	143.57		1.207	1.5263 ²⁰		186		
c142	2-Chloro-6-methylaniline	$\text{CH}_3(\text{Cl})\text{C}_6\text{H}_3\text{NH}_2$	141.60	12 ¹ , 388	1.152	1.5761 ²⁰	2	215	98	s alc
c143	3-Chloro-2-methylaniline	$\text{CH}_3(\text{Cl})\text{C}_6\text{H}_3\text{NH}_2$	141.60	12, 836		1.5874 ²⁰	2	115-117 ^{10mm}	>112	
c144	3-Chloro-4-methylaniline	$\text{CH}_3(\text{Cl})\text{C}_6\text{H}_3\text{NH}_2$	141.60	12, 988		1.5830 ²⁰	25	238	100	
c145	4-Chloro-2-methylaniline	$\text{CH}_3(\text{Cl})\text{C}_6\text{H}_3\text{NH}_2$	141.60	12, 835		1.5848 ²⁰	27	241	99	s hot alc
c146	5-Chloro-2-methylaniline	$\text{CH}_3(\text{Cl})\text{C}_6\text{H}_3\text{NH}_2$	141.60	12, 835		1.5840 ²⁰	22	237	160	
c147	DL-4-Chloro-2-(α -methylbenzyl)-phenol	$\text{C}_6\text{H}_5\text{CH}(\text{CH}_3)\text{C}_6\text{H}_3(\text{Cl})\text{OH}$	232.71	6 ⁴ , 4710				155 ^{2mm}		
c148	1-Chloro-3-methylbutane	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{Cl}$	106.59	1, 135	0.8704 ²⁰ ₄	1.4084 ²⁰	-104	99	16	sl s aq; misc alc, eth

c149	2-Chloro-2-methylbutane	$\text{CH}_3\text{CH}_2\text{CCl}(\text{CH}_3)_2$	106.59	1, 134	0.8650^{20}_4	1.4052^{20}	-73.7	85	16	i aq; s alc, eth
c150	Chloromethyldimethylchlorosilane	$(\text{CH}_3)_2\text{Si}(\text{Cl})\text{CH}_2\text{Cl}$	143.1		1.0865^{20}_4	1.4360^{20}		115-116		
c151	Chloromethyl 2,2-dimethylpropionate	$(\text{CH}_3)_3\text{CCOOCH}_2\text{Cl}$	150.61		1.045	1.4170^{20}			40	
c152	Chloromethyl ethyl ether	$\text{ClCH}_2\text{OCH}_2\text{CH}_3$	94.54	1 ² , 645	1.04^{20}_4	1.4040^{20}		79-83		s alc; v s eth
c153	Chloromethylmethyl-dichlorosilane	$\text{ClCH}_2\text{Si}(\text{CH}_3)\text{Cl}_2$	163.5		1.2858^{20}_4	1.4500^{20}		121-122		
c154	Chloromethylmethyl-diethoxysilane	$\text{ClCH}_2\text{Si}(\text{OC}_2\text{H}_5)_2\text{CH}_3$	182.7		1.000^{20}_4	1.407^{25}		160-161		
c155	Chloromethyl methyl ether	$\text{ClCH}_2\text{OCH}_3$	80.51	1, 580	1.0703^{20}_4	1.3961^{20}	-103.5	57-59	15	d aq; s acet, CS_2
c156	Chloromethyl methyl sulfide	$\text{ClCH}_2\text{SCH}_3$	95.48		1.153	1.4963^{20}		105		
c157	1-(Chloromethyl)-naphthalene	$\text{C}_{10}\text{H}_7\text{CH}_2\text{Cl}$	176.65	5, 566		1.6380^{20}	32	$169^{25\text{mm}}$	>112	
c158	4-Chloro-2-methylphenol	$\text{CH}_3(\text{Cl})\text{C}_6\text{H}_3\text{OH}$	142.59	6, 359			48	225		sl s aq
c159	4-Chloro-3-methylphenol	$\text{CH}_3(\text{Cl})\text{C}_6\text{H}_3\text{OH}$	142.59	6, 381			68	235		i aq; s alc, bz, chl, eth, acet
c160	4-Chloro-N-methylpiperidine HCl		170.08				164			

Chloromethylbenzenes, c244, c245, c246

(Chloromethyl)oxirane, c101

Chloromethyl pivalate, c151



c160

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

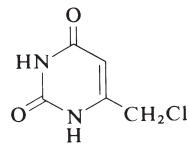
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c161	1-Chloro-2-methylpropane	$(\text{CH}_3)_2\text{CHCH}_2\text{Cl}$	92.57	1, 124	0.8829 ¹⁵	1.4010 ¹⁵	−130.3	68.9	21	0.09 aq; misc alc, eth
c162	2-Chloro-2-methylpropane	$(\text{CH}_3)_3\text{CCl}$	92.57	1, 125	0.8474 ¹⁵ ₄	1.3856 ²⁰	−25.4	50.8	18	sl s aq; misc alc, eth
c163	1-Chloro-2-methylpropene	$(\text{CH}_3)_2\text{C}=\text{CHCl}$	90.55	1, 209	0.9186 ²⁰ ₄	1.4225 ²⁰		68.1	−1	misc alc, eth
c164	3-Chloro-2-methylpropene	$\text{ClCH}_2\text{C}(\text{CH}_3)=\text{CH}_2$	90.55	1, 209	0.9210 ¹⁵ ₄	1.4272 ²⁰	−80	72	−10	misc alc, eth
c165	Chloromethyltrichlorosilane	$\text{ClCH}_2\text{SiCl}_3$	183.9		1.465 ²⁰ ₄	1.4555 ²⁰		117–118		
c166	Chloromethyltrimethylsilane	$\text{ClCH}_2\text{Si}(\text{CH}_3)_3$	122.7	4 ³ , 1844	0.8861 ²⁰ ₄	1.4180 ²⁰		99	<1	
c167	6-(Chloromethyl)uracil		160.56	23 ¹ , 328			257 d			
c168	1-Chloronaphthalene	$\text{C}_{10}\text{H}_7\text{Cl}$	162.62	5, 541	1.1938 ²⁰ ₄	1.6332 ²⁰	−2.3	259.3	121	s alc, bz, PE
c169	2-Chloronaphthalene	$\text{C}_{10}\text{H}_7\text{Cl}$	162.62		1.1377 ⁷¹	1.6079 ⁷¹	59.5	256		s alc, bz, chl, eth
c170	4-Chloro-1,8-naphthalic anhydride		232.63	17, 522			210			
c171	4'-Chloro-3'-nitroacetophenone	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{C}(=\text{O})\text{CH}_3$	199.60	7 ³ , 995			101			
c172	2-Chloro-4-nitroaniline	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{NH}_2$	172.57	12, 733			109			sl s aq; v s alc, eth
c172a	2-Chloro-5-nitroaniline	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{NH}_2$	172.57	12, 732			114			
c173	4-Chloro-2-nitroaniline	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{NH}_2$	172.57	12, 729			119			v s alc, eth
c174	4-Chloro-3-nitroaniline	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{NH}_2$	172.57	12, 731			101			v s alc; s eth

c175	1-Chloro-2-nitro-benzene	$\text{ClC}_6\text{H}_4\text{NO}_2$	157.56	5, 241	1.348		32–33	246	123	s alc, bz, eth
c176	1-Chloro-3-nitro-benzene	$\text{ClC}_6\text{H}_4\text{NO}_2$	157.56	5, 243	1.534 ²⁰		46	236	103	sl s alc; v s eth, chl
c177	1-Chloro-4-nitro-benzene	$\text{ClC}_6\text{H}_4\text{NO}_2$	157.56	5, 243	1.520		82–84	242	110	sl s alc; v s eth, CS_2 s hot aq, hot bz
c178	2-Chloro-4-nitro-benzoic acid	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{COOH}$	201.57	9, 404			141			
c179	2-Chloro-5-nitro-benzoic acid	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{COOH}$	201.57	9, 403	1.608 ¹⁸		168			sl s aq; s alc, bz, eth
c180	4-Chloro-3-nitro-benzoic acid	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{COOH}$	201.57	9, 402	1.645 ¹⁸		183			sl s alc; s hot aq
c181	4-Chloro-3-nitro-benzophenone	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{-C(=O)C}_6\text{H}_5$	261.66	7 ¹ , 230			104–105	235 ^{13mm}		
c182	2-Chloro-5-nitro-benzotrifluoride	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{CF}_3$	225.55		1.527	1.5083 ²⁰		231	98	
c183	4-Chloro-3-nitro-benzotrifluoride	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{CF}_3$	225.55		1.511	1.4893 ²⁰	–2.5	222	101	
c184	5-Chloro-2-nitro-benzotrifluoride	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{CF}_3$	225.55		1.526	1.4980 ²⁰	21–22	222–224	102	

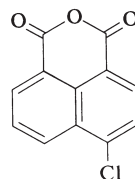
Chloronicotinic acids, c234, c235

α -Chloronitrotoluene, n47

Chloronitro- α,α,α -trifluorotoluenes, c182, c183, c184



c167



c170

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c185	<i>o</i> -(4-Chloro-3-nitro-benzoyl)benzoic acid	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{COC}_6\text{H}_4\text{-COOH}$	305.68	10, 752			201			
c186	2-Chloro-4-nitro-phenol	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{OH}$	173.56	6, 240			106			
c187	2-Chloro-4-nitro-toluene	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{CH}_3$	171.58	5, 329		1.5470 ⁷⁰	61	260		i aq; s alc, eth
c188	2-Chloro-6-nitro-toluene	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{CH}_3$	171.58	5, 327		1.5377 ⁷⁰	36	238	125	i aq
c189	4-Chloro-3-nitro-toluene	$\text{ClC}_6\text{H}_3(\text{NO}_2)\text{CH}_3$	171.58	5, 329	1.297	1.5580 ²⁰	7	260 ^{745mm}	>112	i aq
c190	1-Chlorooctane	$\text{CH}_3(\text{CH}_2)_7\text{Cl}$	148.68	1, 159	0.875 ²⁰ ₄	1.4298 ²⁰	−61	183	54	i aq; v s alc, eth
c191	1-Chloropentane	$\text{CH}_3(\text{CH}_2)_4\text{Cl}$	106.60	1, 130	0.8824 ²⁰ ₄	1.4118 ²⁰	−99.0	98.3	12	0.02 aq; misc alc, eth
c192	5-Chloro-2-pentanone	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{COCH}_3$	120.58	1 ² , 738	1.0571 ¹⁸ ₄	1.4375 ²⁰		72 ^{20mm}	62	s acet, eth
c193	3-Chloroperoxy-benzoic acid	$\text{ClC}_6\text{H}_4\text{C(O)OOH}$	172.57				94 d			
c194	2-Chlorophenol	$\text{ClC}_6\text{H}_4\text{OH}$	128.56	6, 183	1.2573 ²⁵ ₄	1.5579 ²⁰	9.3	175–176	63	sl s aq; v s alc, eth
c195	3-Chlorophenol	$\text{ClC}_6\text{H}_4\text{OH}$	128.56	6, 185	1.245 ²⁵ ₄	1.5565 ⁴⁰	33.5	214	>112	sl s aq; s alc, eth
c196	4-Chlorophenol	$\text{ClC}_6\text{H}_4\text{OH}$	128.56	6, 186	1.2238 ⁷⁸ ₄	1.5419 ⁴⁵	43.5	220	115	sl s aq; v s alc, chl, eth
c197	4-Chlorophenoxy-acetic acid	$\text{ClC}_6\text{H}_4\text{OCH}_2\text{COOH}$	186.59	6, 187			159			
c198	2-(4-Chlorophenoxy)-2-methylpropionic acid	$\text{ClC}_6\text{H}_4\text{OC}(\text{CH}_3)_2\text{COOH}$	214.65				122			
c199	DL-2-(4-Chlorophenoxy)propionic acid	$\text{ClC}_6\text{H}_4\text{OCH}(\text{CH}_3)\text{COOH}$	200.62	6 ³ , 695			117			

c200	4-Chlorophenylacetic acid	$\text{ClC}_6\text{H}_4\text{CH}_2\text{COOH}$	170.60	9, 448			105			v s aq, alc, eth; s bz
c201	<i>p</i> -Chlorophenylacetonitrile	$\text{ClC}_6\text{H}_4\text{CH}_2\text{CN}$	151.60	9, 448			30.5	267		
c202	2-Chloro- <i>p</i> -phenylenediamine sulfate	$\text{H}_2\text{NC}_6\text{H}_3(\text{Cl})\text{NH}_2 \cdot \text{H}_2\text{SO}_4$	240.67	13, 117			253			
c202	4-Chloro-1,2-phenylenediamine	$\text{ClC}_6\text{H}_3(\text{NH}_2)_2$	142.59	13, 25			70			
c204	4-Chloro-1,3-phenylenediamine	$\text{H}_2\text{N}(\text{Cl})\text{C}_6\text{H}_3\text{NH}_2$	142.59	13, 53			90			
c205	3-Chlorophenylhydrazine HCl	$\text{ClC}_6\text{H}_4\text{NHNH}_2 \cdot \text{HCl}$	179.05	15, 424			242 d			
c206	4-Chlorophenyl isocyanate	$\text{ClC}_6\text{H}_4\text{NCO}$	153.57	12, 616		1.5618 ²⁰	31	204	110	
c207	4-Chlorophenyl phenyl sulfone	$\text{ClC}_6\text{H}_4\text{SO}_2\text{C}_6\text{H}_5$	252.72	6 ¹ , 149			94			74 acet; 44 bz; 5 CCl_4 ; 65 diox; 21 i-PrOH
c208	4-Chlorophenyltrichlorosilane	$\text{ClC}_6\text{H}_4\text{SiCl}_3$	246.0		1.4316 ²⁰ ₄	1.5418 ²⁰		115–117 ^{20mm}		
c209	4-Chloro- <i>o</i> -phthalic acid	$\text{ClC}_6\text{H}_3(\text{COOH})_2$	200.58	9, 816			148			
c210	1-Chloropropane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$	78.54	1, 104	0.8985 ¹⁵	1.3880 ²⁰	–122.8	46.6	18	0.27 aq; misc alc, eth
c211	2-Chloropropane	$\text{CH}_3\text{CHClCH}_3$	78.54	1, 105	0.8563 ²⁰	1.3777 ²⁰	–117.2	35	–35	0.34 aq; misc alc, eth
c212	3-Chloro-1,2-propanediol	$\text{ClCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$	110.54		1.3218 ²⁰ ₄	1.4805 ²⁰		213	58	s aq, alc, eth
c213	1-Chloro-2-propanol	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{Cl}$	94.54	1, 363	1.115 ²⁰	1.4375 ²⁰		126–127	51	misc aq; s alc
c214	3-Chloro-1-propanol	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{OH}$	94.54	1, 356	1.1309 ²⁰ ₄	1.4460 ²⁰		160–162	73	

p-Chlorophenacyl bromide, b246
Chlorophenylamines, c33, c34, c35

4-Chlorophenyl sulfone, b165
4-Chlorophenyl sulfoxide, b166

Chloropicrin, t239
Chloroprene, c216

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c215	Chloro-2-propanone	$\text{ClCH}_2\text{COCH}_3$	92.53	1, 653	1.135 ₄ ¹⁵	1.4350 ²⁰	−44.5	119.7	7	10 aq; misc alc, chl
c216	3-Chloro-1-propene	$\text{ClCH}_2\text{CH}=\text{CH}_2$	76.53	1, 198	0.939 ²⁰	1.4151 ²⁰	−134.5	45.2	−28	0.36 aq; misc alc, chl
c217	(3-Chloropropenyl)-benzene	$\text{C}_6\text{H}_5\text{CH}=\text{CHCH}_2\text{Cl}$	152.62	5 ² , 372		1.5845 ²⁰	−19	108 ^{12mm}	79	
c218	2-Chloropropionic acid	$\text{CH}_3\text{CH}(\text{Cl})\text{COOH}$	108.52	2, 248	1.182	1.4345 ²⁰		186	101	misc aq, alc, eth
c219	3-Chloropropionic acid	$\text{ClCH}_2\text{CH}_2\text{COOH}$	108.52	2, 249			41	205	>112	v s aq, alc, chl
c220	3-Chloropropionitrile	$\text{ClCH}_2\text{CH}_2\text{CN}$	89.53	2, 250	1.1443 ¹⁸	1.4379 ²⁰	−50	176	75	
c221	2-Chloropropionyl chloride	$\text{CH}_3\text{CH}(\text{Cl})\text{COCl}$	126.97	2, 248	1.308	1.4400 ²⁰		111	31	d aq, alc
c222	3-Chloropropionyl chloride	$\text{ClCH}_2\text{CH}_2\text{COCl}$	126.97	2, 250	1.3307 ¹³	1.4570 ²⁰		145	61	i aq; d hot aq, hot alc; s alc; v s eth
c223	<i>p</i> -Chloropropiophenone	$\text{ClC}_6\text{H}_4\text{C}(=\text{O})\text{CH}_2\text{CH}_3$	168.62	7, 301			37	97 ^{1mm}		
c224	3-Chloropropylamine HCl	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{NH}_2\cdot\text{HCl}$	130.02	4, 148			150			
c225	3-Chloropropylmethylchlorosilane	$\text{Cl}(\text{CH}_2)_3\text{Si}(\text{CH}_3)\text{Cl}_2$	191.6		1.2045 ₄ ²⁰	1.4580 ²⁰		70 ^{15mm}		
c226	2-Chloropropyl(phenyl)dichlorosilane	$\text{Cl}(\text{CH}_2)_3\text{SiCl}_2(\text{C}_6\text{H}_5)$	253.6		1.241 ₄ ²⁰	1.5332 ²⁰		141 ^{10mm}		
c227	<i>N</i> -(3-Chloropropyl)piperidine HCl		198.14	20, 18			220			

c228	3-Chloropropyl thiolacetate	$\text{CH}_3\text{C}(=\text{O})\text{SCH}_2\text{CH}_2\text{CH}_2\text{Cl}$	152.64	2 ³ , 493	1.159	1.4946 ²⁰		84 ^{10mm}	77	
c229	3-Chloropropyltri- chlorosilane	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{SiCl}_3$	212.0		1.3590 ²⁰	1.4668 ²⁰		181.5	66	
c229	3-Chloropropyltri- ethoxysilane	$\text{Cl}(\text{CH}_2)_3\text{Si}(\text{OC}_2\text{H}_5)_3$	240.8	1.009 ²⁰	1.420 ²⁰			102 ^{10mm}		
c231	3-Chloropropyltri- methoxysilane	$\text{Cl}(\text{CH}_2)_3\text{Si}(\text{OCH}_3)_3$	198.72		1.077 ²⁵	1.4183 ²⁵		183	66	
c232	3-Chloropropyne	$\text{ClCH}_2\text{C}\equiv\text{CH}$	74.51	1, 248	1.0306 ²⁵	1.4349 ²⁰	−78	58	18	misc bz, alc, eth, EtAc
c233	2-Chloropyridine	$\text{ClC}_5\text{H}_4\text{N}$	113.55	20, 230	1.205 ¹⁵	1.5320 ²⁰		166 ^{714mm}	65	sl s aq; s alc, eth
c234	2-Chloro-3-pyridine- carboxylic acid	$\text{C}_5\text{H}_3\text{N}(\text{Cl})\text{COOH}$	157.56	22 ² , 35			d 175			
c235	6-Chloro-3-pyridine- carboxylic acid	$\text{C}_5\text{H}_3\text{N}(\text{Cl})\text{COOH}$	157.56	22, 43			200 d			
c236	2-Chloroquinoline		163.61	20, 359	1.2464 ²⁵	1.6259 ²⁵	37	267		i aq; s alc, bz, eth
c237	4-Chlorosalicylic acid	$\text{HO}(\text{Cl})\text{C}_6\text{H}_3\text{COOH}$	172.57	10, 101			212			
c238	5-Chlorosalicylic acid	$\text{HO}(\text{Cl})\text{C}_6\text{H}_3\text{COOH}$	172.57	10, 102			172			
c239	<i>N</i> -Chlorosuccinimide		133.53	21, 380	1.65		150–151			1.4 aq; 0.67 alc; 2 bz; sl s chl, eth
c240	Chlorosulfonyl isocyanate	ClSO_2NCO	141.53		1.626	1.4467 ²⁰	−44	107		

β-Chloropropionaldehyde diethyl acetal, c82

3-Chloropropylene-1,2-oxide, c102

1-Chloro-2,5-pyrrolidinedione, c239

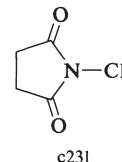
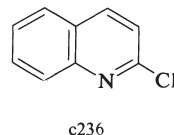
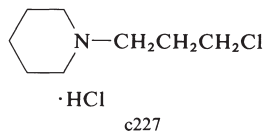


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c241	8-Chlorotheophylline		214.61	26, 473			d 290			s alk
c242	2-Chlorothiophene	$\text{Cl}-\text{C}_4\text{H}_3\text{S}$	118.59	17, 32	1.286	1.5483 ²⁰	−72	129	22	i aq; misc alc, eth
c243	4-Chlorothiophenol	$\text{ClC}_6\text{H}_4\text{SH}$	144.62	6, 326			51	207		
c244	2-Chlorotoluene	$\text{ClC}_6\text{H}_4\text{CH}_3$	126.59	5, 290	1.0826 ²⁰ ₄	1.5250 ²	−34	159.0	47	sl s aq; v s alc, bz, chl, eth
c245	3-Chlorotoluene	$\text{ClC}_6\text{H}_4\text{CH}_3$	126.59	5, 291	1.0760 ¹⁹ ₄	1.5218 ²⁰	−48.9	161.8	50	s alc, bz, chl; misc eth
c246	4-Chlorotoluene	$\text{ClC}_6\text{H}_4\text{CH}_3$	126.59	5, 292	1.0697 ²⁰ ₄	1.5208 ²⁰	7.2	162.0	49	sl s aq; s alc, bz, eth
c247	<i>N</i> -Chloro- <i>p</i> -toluene-sulfonamide, Na salt	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{NCl}^-\text{Na}^+$	227.67				167 d			s aq; i bz, chl, eth
c248	4'-Chloro-1-toluenethiol	$\text{ClC}_6\text{H}_4\text{CH}_2\text{SH}$	158.65	6, 466	1.202	1.5893 ²⁰	20		76	
c249	4-Chloro- <i>o</i> -toloxy-acetic acid, Na salt	$\text{ClC}_6\text{H}_3(\text{CH}_3)\text{O}-\text{CH}_2\text{COO}^-\text{Na}^+$	222.61	6 ³ , 1265			220–225			
c250	4-(4-Chloro- <i>o</i> -tolyl-oxy)butyric acid	$\text{ClC}_6\text{H}_3(\text{CH}_3)\text{O}-(\text{CH}_2)_3\text{COOH}$	228.68				99–100			
c251	Chloro-2,2,2-trifluoroethane	$\text{CF}_3\text{CH}_2\text{Cl}$	118.5		1.389 ⁰	1.3090 ⁰	−105	6.9		
c252	Chlorotrifluoroethylene	$\text{CF}_2=\text{CFCl}$	116.48		1.315		−158.2	−27.9		
c253	Chlorotrifluoromethane	ClCF_3	104.46	1 ³ , 42			−181	−81.5		
c254	Chlorotrimethylgermane	$(\text{CH}_3)_3\text{GeCl}$	153.16		1.2382 ²²	1.4283 ²⁰	−13	102		
c255	Chlorotrimethylsilane	$(\text{CH}_3)_3\text{SiCl}$	108.64		0.8580 ²⁰ ₄	1.3885 ²⁰	−40	57	−40	

c256	Chlorotriphenyl-methane	(C ₆ H ₅) ₃ CCl	278.78	5, 700			110–112	230 ^{20mm}		v s bz, chl, eth
c257	Chlorotripropylsilane	(C ₃ H ₇) ₃ SiCl	192.8		0.882 ₄ ²⁰	1.440 ²⁰		199–201		
c257a	Chlorotris(di-methylamino)silane	[(CH ₃) ₂ N] ₃ SiCl	195.8		0.975 ₄ ²⁰	1.442 ²⁰		62–63 ^{12mm}		
c258	α -Chloro- <i>o</i> -xylene	CH ₃ C ₆ H ₄ CH ₂ Cl	140.61	5, 364	1.063	1.5391 ²⁰		199	73	i aq; misc alc, eth
c259	α -Chloro- <i>m</i> -xylene	CH ₃ C ₆ H ₄ CH ₂ Cl	140.61	5, 373	1.064 ²⁰	1.5350 ²⁰		195–196	75	i aq; misc alc, eth
c260	α -Chloro- <i>p</i> -xylene	CH ₃ C ₆ H ₄ CH ₂ Cl	140.61	5, 384		1.5330 ²⁰	4.5	200	75	misc alc, bz, eth, acet
c261	4-Chloro- <i>o</i> -xylene	ClC ₆ H ₃ (CH ₃) ₂	140.61	5, 363	1.047	1.5283 ²⁰		223	66	misc alc, bz, eth, acet
c262	Cholesterol		386.66		1.067 ₄ ²⁰		148.5	360 sl d		1.29 alc; 35 eth; 22 chl; s bz, PE
c263	Cholic acid		408.58				198			0.028 aq; 0.06 alc; 2.8 acet; 0.036 bz; 0.5 chl

α -Chlorotoluene, b89

Chlorotoluidines, c142, c143, c144, c145, c146

2-Chlorotriethylamine, d272

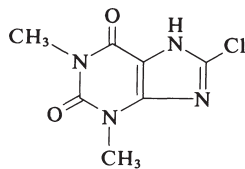
Chloro- α,α,α -trifluorotoluenes, c51, c52, c53

4-Chloro- α,α,α -trifluoro-*o*-toluidine, a144

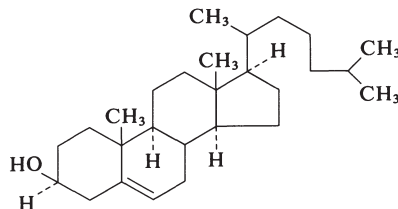
α' -Chloro- α,α,α -trifluoro-*m*-xylene, t299

Chlorotrihexylsilane, t302

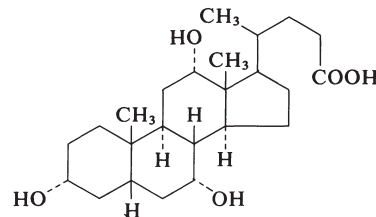
Chloroxylenol, c90



c241



c262



c263

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

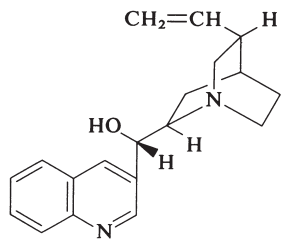
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c264	Cinchonine		294.40	23 ² , 369			~260			1.4 alc; 0.9 chl; 0.2 eth
c265	1,8-Cineole		154.25	17, 23	0.921 ²⁵ ₂₅	1.4572 ²⁰	1.5	174.4		misc alc, chl, eth
c266	<i>trans</i> -Cinnamaldehyde	$C_6H_5CH=CHCHO$	132.16	7, 348	1.050 ²⁵ ₂₅	1.6219 ²⁰	-7.5	246	71	0.014 aq; misc alc, chl, eth
c267	<i>trans</i> -Cinnamic acid	$C_6H_5CH=CHCOOH$	148.16	9, 573	1.2475 ⁴		134	300		0.05 aq; 16 alc; 8 chl
c268	<i>trans</i> -Cinnamoyl chloride	$C_6H_5CH=CHCOCl$	166.61	9 ² , 390	1.1617 ²⁵ ₄	1.614 ⁴³	35-36	258		s hot alc, CCl ₄
c269	Cinnamyl alcohol	$C_6H_5CH=CHCH_2OH$	134.18	6, 570	1.0397 ³⁵ ₃₅	1.5758 ³³	33	250.0		s aq; v s alc, eth
c270	Citraconic acid	$CH_3C(COOH)=CHCOOH$	130.10	2, 768	1.62		92 d			v s aq, alc, eth; sl s chl; i bz, PE
c271	Citraconic anhydride		112.08	17, 440	1.247	1.4712 ²⁰	8	214	101	i aq; s alk
c272	Citrazinic acid		155.11	22, 254			car-bonizes without melting >300			
c273	Citric acid	$HOOCCH_2C(OH)(COOH)-CH_2COOH$	192.12	3, 556	1.665		154			59 aq
c274	Citronellol	$(CH_3)_2C=CHCH_2CH_2CH-(CH_3)CH_2CH_2OH$	156.27	1, 451	0.8570 ²⁰ ₄	1.4556 ²⁰		222	79	
c275	Cocaine		303.35	22 ² , 150		1.5022 ⁹⁸	98	187 ^{0.1mm}		0.17 aq; 15 alc; 140 chl; 28 eth
c276	Coumarin		146.15	17, 328	0.935 ²⁰ ₄		69	298		0.25 aq; v s alc, chl, eth

c277	Creatine	$\text{HOOCCH}_2\text{N}(\text{CH}_3)-\text{C}(=\text{NH})\text{NH}_2$	131.14	4, 363			300			1.3 aq; 0.11 alc; ith
c278	Creatinine		113.12	24, 245			255 d			8 aq; sl s alc; i eth
c279	<i>o</i> -Cresol	$\text{CH}_3\text{C}_6\text{H}_4\text{OH}$	108.14	6, 349	1.0273 ⁴¹	1.5361 ⁴¹	30.9	190.8	81	3.1 aq ⁴⁰ ; misc alc, chl, eth; s alk
c280	<i>m</i> -Cresol	$\text{CH}_3\text{C}_6\text{H}_4\text{OH}$	108.14	6, 373	1.034 ²⁰	1.5438 ²⁰	12.2	202.7	86	2.5 aq ⁴⁰ ; misc alc, chl, eth; s alk
c281	<i>p</i> -Cresol	$\text{CH}_3\text{C}_6\text{H}_4\text{OH}$	108.14	6, 389	1.0179 ⁴¹	1.5312 ⁴¹	34.8	201.9	86	2.3 aq ⁴⁰ ; misc alc, chl, eth; s alk
c282	<i>trans</i> -Crotonaldehyde	$\text{CH}_3\text{CH}=\text{CHCHO}$	70.09	1, 728	0.8516 ²⁰	1.4373 ²⁰	-76.5	104.1	8	18.1 aq
c283	Crotonyl chloride	$\text{CH}_3\text{CH}=\text{CHCOCl}$	104.54	2, 411	1.091	1.4595 ²⁰		123	35	
c284	Cupferron	$\text{C}_6\text{H}_5\text{N}(\text{NO})\text{O}^-\text{NH}_4^+$	155.16	16', 395			163-164			v s aq, alc

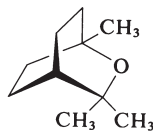
Chromone, b56
 Chromotropic acid, d396
 Chrysoldin, d31
 Cinchophen, p149
 Cinnamyl chloride, c217
 Citral, d562, d563
 Cleland's reagent, d424
 2,4,6-Collidine, t367

p-Coumaric acid, h107
 Cresotic acids, h137, h138
 Cresylic acids, c279, c280, c281
 Crotonic acid, b402
 Crotononitrile, b400
 Crotyl alcohols, b404, b405
 Crotyl bromide, b240
 Crotyl chloride, c68

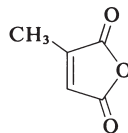
12-Crown-4, t125
 15-Crown-5, p45
 18-Crown-6, h74
 Cumene, i91
 Cumic alcohol, i92
 Cupron, b50



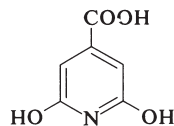
c264



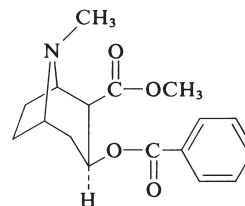
c265



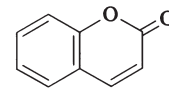
c271



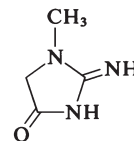
c272



c275



c276



c278

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

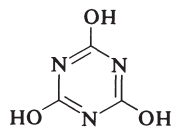
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c285	Cyanamide	H_2NCN	42.04	3 ² , 63	1.282 ₄ ²⁰		46	83 ^{380mm}		78 aq; 29 BuOH; 42 EtAc; s alc, eth
c286	2-Cyanoacetamide	$\text{NCCH}_2\text{CONH}_2$	84.08	2, 589			119.5		215	25 aq; 3.1 alc
c287	Cyanoacetic acid	NCCH_2COOH	85.06	2, 583			65–67	108 ^{15mm}	107	s aq, alc, eth; sl s bz
c288	Cyanoacetohydrazide	$\text{NCCH}_2\text{C}(=\text{O})\text{NHNH}_2$	99.09				110	d		v s aq; s alc; i eth
c289	Cyanoacetylurea	$\text{NCCH}_2\text{C}(=\text{O})\text{NHC}(=\text{O})\text{-NH}_2$	127.10	3, 66			214 d			
c290	2-Cyanoethanol	$\text{NCCH}_2\text{CH}_2\text{OH}$	71.08	3 ² , 213	1.0588 ⁰			106–108 ^{11mm}		misc aq, alc; sl s eth
c291	2-Cyanoethylchloromethylsilane	$\text{NCCH}_2\text{CH}_2\text{Si}(\text{CH}_3)\text{Cl}_2$	168.1		1.202 ₄ ²⁰	1.455 ²⁰		63 ^{4mm}		
c292	1-Cyano-3-methylisothiurea, Na salt	$\text{CH}_3\text{NHC}(=\text{NCN})\text{S}^-\text{Na}^+$	137.14	4, 71			290 d			
c293	1-Cyanonaphthalene	$\text{C}_{10}\text{H}_7\text{CN}$	153.18	9, 649	1.1113 ₂₅ ²⁵	1.6298 ¹⁸	38	299		i aq; v s alc, eth
c293	3-Cyanopropyltrichlorosilane	$\text{NCCH}_2\text{CH}_2\text{CH}_2\text{SiCl}_3$	202.6		1.280 ²⁵	1.465 ²⁵		93–94 ^{8mm}		
c295	2-Cyanopyridine	$\text{NC}(\text{C}_5\text{H}_4\text{N})$	104.11	22, 36		1.5288 ²⁰	28	215	89	s aq; v s alc, bz, eth
c296	3-Cyanopyridine	$\text{NC}(\text{C}_5\text{H}_4\text{N})$	104.11	22, 41			52	240–245		v s aq, alc, bz, eth
c297	4-Cyanopyridine	$\text{NC}(\text{C}_5\text{H}_4\text{N})$	104.11	22, 46			80			s aq, alc, bz, eth
c298	Cyanotrimethylsilane	$(\text{CH}_3)_3\text{SiCN}$	99.21		0.783 ₄ ²⁰	1.3924 ²⁰	11	114–117	1	0.5 aq; s hot alc, pyr; i acet, bz, chl, eth
c299	Cyanuric acid		129.08	26, 239	1.768 ⁰		d to HO-CN			
c300	Cyclobutane	C_4H_8	56.10	5, 17	0.7038 ⁰	1.3752 ⁰	–90.7	12.5		i aq; v s alc, acet
c301	Cyclodecane	$\text{C}_{10}\text{H}_{20}$	140.27			1.4707 ²⁰		201	1	
c302	Cyclododecanol	$\text{C}_{12}\text{H}_{23}\text{OH}$	184.32				77			

c303	Cyclododecanone	$C_{12}H_{22}(=O)$	182.31	7 ² , 48	0.906		61	85 ^{1mm}		
c304	<i>trans,trans,cis</i> -1,5,9-cyclododecatriene		162.28		0.8925 ²⁰ ₄	1.5070 ²⁰	−18	231	87	
c305	<i>trans</i> -Cyclododecene		166.31		0.863	1.4822 ²⁰		232–245	93	
c306	Cycloheptane	C_7H_{14}	98.18	5, 29	0.811 ²⁰ ₄	1.4455 ²⁰	−8.0	118.8	6	v s alc, eth
c307	DL- <i>trans</i> -1,2-Cycloheptanediol	$C_7H_{12}(OH)_2$	130.19	6 ³ , 4086			61–63	138–139 ^{15mm}		
c308	Cycloheptanol	$C_7H_{13}OH$	114.19	6, 10	0.948 ²⁰ ₄	1.4760 ²⁰	2	185	71	sl s aq; v s alc, eth
c309	Cycloheptanone	$C_7H_{12}(=O)$	112.17	7, 13	0.9490 ²⁰ ₄	1.4611 ²⁰		179–181	55	i aq; v s alc; s eth
c310	1,3,5-Cycloheptatriene		92.13	5, 280	0.888	1.5211 ²⁰	−75.3	115.5	26	s alc, eth; v s bz, chl
c311	Cycloheptene	C_7H_{12}	96.17	5, 65	0.824 ²⁰ ₄	1.4585 ²⁰		114.7	−6	s alc, eth
c312	Cyclohexane	C_6H_{12}	84.16	5, 20	0.7786 ²⁰ ₄	1.4262 ²⁰	6.5	80.7	−18	0.01 aq; misc alc, bz, acet, eth, CCl ₄
c313	Cyclohexane-d ₁₂	C_6D_{12}	92.26		0.89	1.4210 ²⁰		78	−18	

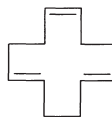
Cyanoacetoneitrile, m5
 Cyanoanilines, a124, a125, a126
 Cyanobenzene, b51
 2-Cyanoethanol, h169
 Cyanoethylene, a64
 Cyanomethane, a29

2-Cyanopropene, m27
 Cyanuric chloride, t250
 Cyclododecane epoxide, e4
 Cyclododecanone isooxime, a318
 Cycloheptanone isooxime, a317
 Cycloheptyl bromide, b260

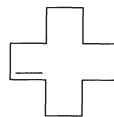
Cyclohexaneacetic acid, c333
 Cyclohexanecarboxylic acid chloride, c316
 2,5-Cyclohexadien-1,4-dione, b59
 2,5-Cyclohexadiene-1,4-dione with 1,4-benzenediol (1:1), q1
 Cyclohexanemethanol, c342



c299



c304



c305



c310

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c314	1,3-Cyclohexanebis-(methylamine)	$C_6H_{10}(NHCH_3)_2$	142.25						106	
c315	Cyclohexanecarbaldehyde	$C_6H_{11}CHO$	112.17	7, 19	0.926	1.4500 ²⁰		163	40	
c316	Cyclohexanecarbonyl chloride	$C_6H_{11}COCl$	146.62	9, 9	1.096	1.4700 ²⁰		184	66	
c317	Cyclohexanecarboxylic acid	$C_6H_{11}COOH$	128.17	7, 19	1.0480 ¹⁵	1.4530 ²⁰	29	232.5		0.21 aq; s alc, bz, eth
c318	<i>cis</i> -1,2-Cyclohexanediamine	$C_6H_{10}(NH_2)_2$	114.19	13, 1	0.931	1.4864 ²⁰		92 ^{18mm}		
c319	<i>trans</i> -1,2-Cyclohexanediamine	$C_6H_{10}(NH_2)_2$	114.19	13, 1	0.931	1.4864 ²⁰		92 ^{18mm}		
c320	<i>cis</i> -1,2-Cyclohexanedicarboxylic anhydride		154.17				34	158 ^{17mm}		
c320	<i>cis</i> -1,4-Cyclohexanedimethanol	$C_6H_{10}(CH_2OH)_2$	144.21		0.978 ¹⁰⁰	1.4893 ²⁰ super-cooled	43	288	74	misc aq, alc; 2.5 eth
c322	1,3-Cyclohexanedione	$C_6H_8(=O)_2$	112.13	7, 554	1.0861 ⁹¹	1.4576 ¹⁰²	103–105			s aq, alc, acet, chl
c323	1,2-Cyclohexanedione dioxime	$C_6H_8(=NOH)_2$	142.16	17 ² , 526			185–188			s aq
c324	Cyclohexanemethylamine	$C_6H_{11}CH_2NH_2$	113.20	12, 12	0.870	1.4630 ²⁰		145–147	43	
c325	Cyclohexanepropionic acid	$C_6H_{11}CH_2CH_2COOH$	156.23	9, 82	0.912	1.4636 ²⁰	14–17	275.8		
c326	Cyclohexanethiol	$C_6H_{11}SH$	116.23	6, 8	0.950	1.4921 ²⁰		158–160	43	
c327	Cyclohexanol	$C_6H_{11}OH$	100.16	6, 5	0.9416 ³⁰	1.4629 ³⁰	25.2	161.1	67	3.8 aq ²⁵ ; misc alc, bz

c328	Cyclohexanone	$C_6H_{10}(=O)$	98.15	7, 8	0.9478^{20}_4	1.4510^{20}	−45 to −47	155.7	46	15 aq ¹⁰ ; s alc, eth
c329	Cyclohexanone oxime	$C_6H_{10}(=NOH)$	113.16	7, 10			89–91	206–210		s aq, eth; sl s alc
c330	Cyclohexene	C_6H_{10}	82.15	5, 63	0.8094^{20}_4	1.4464^{20}	−103.5	83.0	−12	0.02 aq; misc alc, bz, acet, eth v s alc
c331	2-Cyclohexen-1-one	$C_6H_8(=O)$	96.13	7 ² , 55	0.993	1.4885^{20}	−53	168	61	
c332	2,3-Cyclohexeneo- pyridine		133.19	20 ² , 176	1.025	1.5440		218	86	
c332a	[2-(3-Cyclohexenyl)- ethyl]methyldi- chlorosilane	$C_6H_9CH_2CH_2Si(CH_3)Cl_2$	223.2		1.077^{20}_4	1.481^{25}		79–81 ^{2mm}		
c333	Cyclohexylacetic acid	$C_6H_{11}CH_2COOH$	142.20	9 ² , 9	1.007	1.4630^{20}	31–33	242–244	>112	sl s aq; s org solv
c334	Cyclohexylamine	$C_6H_{11}NH_2$	99.18	12, 5	0.8671^{20}	1.4593^{20}	−17.7	134.8	<32	misc aq, alc, eth, chl
c335	2-(Cyclohexylamino)- ethanesulfonic acid	$C_6H_{11}NHCH_2CH_2SO_3H$	207.29				>300			
c336	3-Cyclohexylamino-1- propanesulfonic acid	$C_6H_{11}NHCH_2CH_2-CH_2SO_3H$	221.32				>300			

Cyclohexanone cyanohydrin, h110

cis-4-Cyclohexene-1,2-dicarboximide, t75

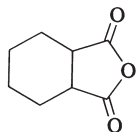
cis-4-Cyclohexene-1,2-dicarboxylic anhydride, t74

Cyclohexene oxide, e5

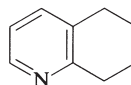
N-(1-Cyclohexen-1-yl)morpholine, m450

N-(1-Cyclohexen-1-yl)pyrrolidine, p274

Cyclohexyl alcohol, c327



c320



c332

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

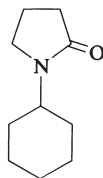
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c337	4-Cyclohexylaniline	$C_6H_{11}C_6H_4NH_2$	175.28	12, 1209			53–56	166 ^{13mm}		i aq; v s alc, eth
c338	Cyclohexylbenzene	$C_6H_{11}C_6H_5$	160.26	5, 503	0.9502 ₄ ²⁰	1.5258 ²⁰	5–6	239–240	98	
c339	<i>N</i> -Cyclohexylformamide	$C_6H_{11}NHCHO$	127.18				38–40	137 ^{10mm}		
c340	Cyclohexyl isocyanate	$C_6H_{11}NCO$	125.17	12 ² , 12	0.980	1.4551 ²⁰		168–170	48	
c341	Cyclohexyl isothiocyanate	$C_6H_{11}NCS$	141.24	12 ² , 12	0.996	1.5350 ²⁰		219		s alc, eth
c342	Cyclohexylmethanol	$C_6H_{11}CH_2OH$	114.19	6, 14	0.9512 ₄ ²⁵	1.4640 ²⁵		181	71	
c343	<i>N</i> -Cyclohexyl-2-pyrrolidinone		167.25		1.026	1.495	12	284		
c344	Cyclohexyltrichlorosilane	$C_6H_{11}SiCl_3$	217.6		1.222 ₄ ²⁰	1.477 ²⁰		90–91 ^{10mm}		
c345	1,5-Cyclooctadiene		108.18	5, 116	0.8818 ₄ ²⁵	1.4905 ²⁵	–69	149–150	45	s CCl ₄
c346	Cyclooctane	C_8H_{16}	112.22	5, 35	0.834	1.4574 ²⁰	14.8	151.1	30	
c347	Cyclooctanol	$C_8H_{15}OH$	128.22	6 ² , 25	0.9740 ₄ ²⁰	1.4850 ²⁰	14–15	106–108 ^{22mm}	86	
c348	Cyclooctanone	$C_8H_{14}(=O)$	126.20	7, 21	0.9584 ₄ ²⁰	1.6494 ²⁰	41–43	195–197		
c349	Cyclooctene	C_8H_{14}	110.20	5 ¹ , 35	0.846	1.4698 ²⁰	–16	145–146	25	i aq; misc alc, eth sl s aq; s MeOH
c350	Cyclooctylamine	$C_8H_{15}NH_2$	127.23		0.928	1.4804 ²⁰	–48	190	62	
c351	Cyclopentamethylene-dichlorosilane		169.1		1.558 ₄ ²⁰	1.4679 ²⁰		169–170		
c352	Cyclopentane	C_5H_{10}	70.13	5, 19	0.7460 ₄ ²⁰	1.4065 ²⁰	–93.9	49.3	–37	
c353	Cyclopentanecarboxylic acid	C_5H_9COOH	114.14	9, 6	1.053 ₄ ²⁰	1.4540 ²⁰	4	216	93	
c354	<i>cis,cis,cis,cis</i> -1,2,3,4-Cyclopentane-tetracarboxylic acid	$C_5H_6(COOH)_4$	246.17	9 ² , 724			192–195 d			

c355	Cyclopentanol	C_5H_9OH	86.13	6, 5	0.9488 ₄ ²⁰	1.4521 ²⁰	−19	140.9	51	sl s aq; s alc
c356	Cyclopentanone	$C_5H_8(=O)$	84.12	7, 5	0.9509 ₄ ¹⁸	1.4366 ²⁰	−58	130.6	30	sl s aq; misc alc, eth
c357	Cyclopentanone oxime	$C_5H_8(=NOH)$	99.13	7, 7			53–55	196		s aq, alc, bz, chl, eth
c358	Cyclopentene	C_5H_8	68.11	5, 61	0.774	1.4228 ²⁰	−135.1	44.2	−28	
c359	2-Cyclopentene-1-acetic acid	$C_5H_7CH_2COOH$	126.16	9, 42	1.047	1.4675 ²⁰	19	93–94 ^{2.5mm}	>112	
c360	2,3-Cyclopenteneo-pyridine		119.17		1.018	1.5445 ²⁰		87–88 ^{11mm}	67	
c361	N-(1-Cyclopentene-1-yl)morpholine		153.23		0.957	1.5105 ²⁰		105–106 ^{12mm}	60	
c362	2-Cyclopentylidene-cyclopentanone		150.22		1.001	1.5231 ²⁰		140 ^{20mm}	103	
c363	3-Cyclopentylpropionic acid	$C_5H_9CH_2CH_2COOH$	142.20		0.996	1.4570 ²⁰		130 ^{12mm}	46	
c364	Cyclopropane	C_3H_6	42.08	5, 15	0.720 ₄ ^{−79}		−127.4	−32.8		37 mL per 100 mL aq ¹⁵ ; v s alc, eth

Cyclohexylbenzene, p104
Cyclohexyl bromide, b261
Cyclohexyl chloride, c77
Cyclohexyl ketone, c328
Cyclohexyl mercaptan, c326

Cyclohexylmethane, m194
Cyclohexylmethyl bromide, b306
Cyclooctene oxide, e7a
Cyclopentanepropanoic acid, c363
Cyclopentene oxide, e37

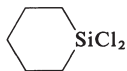
Cyclopentyl bromide, b263
Cyclopentyl chloride, c79
Cyclopropyl bromide, b264
Cyclopropyl cyanide, c365



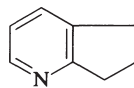
c343



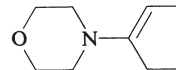
c345



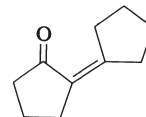
c351



c360



c361



c362

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

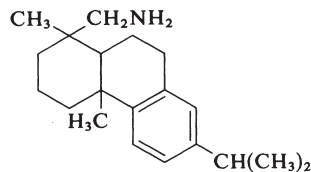
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
c365	Cyclopropanecarbonitrile	C_3H_5CN	67.09	9, 4	0.911 ¹⁶	1.4207 ²⁰		135	32	s eth
c366	Cyclopropane-carbonyl chloride	C_3H_5COCl	104.54	9, 4	1.152	1.4522 ²⁰		119	23	
c367	Cyclopropanecarboxylic acid	C_3H_5COOH	86.09	9, 4	1.008	1.4380 ²⁰	17–19	182–184	71	sl s hot aq; s alc, eth
c368	Cyclopropyl methyl ketone	$C_3H_5COCH_3$	84.12	7, 7	0.8993 ²⁰ ₄	1.4241 ²⁰		114	21	s aq, alc, eth
c369	Cystamine dihydrochloride	$H_2NCH_2CH_2SSCH_2CH_2NH_2 \cdot 2HCl$	225.20	4, 287			217 d			
c370	L-(+)-Cysteine	$HSCH_2CH(NH_2)COOH$	121.16	4, 506			220 d			v s aq, alc; i bz, eth
c371	L-Cystine	$HOOCCH(NH_2)CH_2SSCH_2CH(NH_2)COOH$	240.30	4, 507			d 240			0.01 aq; s acid, alk; i alc
d1	<i>cis</i> -Decahydronaphthalene	$C_{10}H_{18}$	138.26	5, 92	0.8963 ²⁰ ₄	1.4810 ²⁰	–43.0	195.8	58	v s alc, chl, eth; misc most ketones, esters see under <i>cis</i> isomer
d2	<i>trans</i> -Decahydronaphthalene	$C_{10}H_{18}$	138.26	5 ² , 56	0.8700 ²⁰ ₄	1.4697 ²⁰	–30.4	187.3	52	
d3	Dehydro-2-naphthol	$C_{10}H_{17}OH$	154.25	6, 67	0.996	1.4992		109 ^{14mm}	>112	
d4	Decamethylcyclopentasiloxane	$[-Si(CH_3)_2O-]_5$	370.8		0.959 ²⁰ ₄	1.3982 ²⁰	–38	101 ^{20mm}		i aq
d5	Decamethyltetrasiloxane	$(CH_3)_3SiO[Si(CH_3)_2O]_2-Si(CH_3)_3$	310.7		0.8536 ²⁰ ₄	1.3880 ²⁰	–70	194–195	86	sl s alc; s bz, PE
d6	Decanal	$H(CH_2)_9CHO$	156.27	1, 711	0.830 ¹⁵ ₄	1.4280 ²⁰		207–209	85	i aq; s alc, eth
d7	Decane	$CH_3(CH_2)_8CH_3$	142.29	1, 168	0.7301 ²⁰ ₄	1.4119 ²⁰	–29.7	174.1	46	0.07 aq
d8	1,10-Decanediamine	$H_2N(CH_2)_{10}NH_2$	172.32	4, 273			62–63	140 ^{12mm}		
d9	Decanedioic acid	$HOOC(CH_2)_8COOH$	202.25	2, 718	1.207 ²⁰ ₄	1.422 ¹³⁴	134.5	295 ^{100mm}		0.1 aq; v s alc, esters, ketones
d10	1,10-Decanediol	$HO(CH_2)_{10}OH$	174.28	1 ² , 560			72–75	170 ^{8mm}		sl s aq, eth; v s alc

d11	Decanedioyl dichloride	$\text{ClC(O)(CH}_2)_8\text{COC l}$	239.14	2, 719	1.1212 ₄ ²⁰	1.4678 ²⁰		220 ^{75mm}	>112	d aq, alc
d12	Decanenitrile	$\text{CH}_3(\text{CH}_2)_8\text{CN}$	153.27	2, 356	0.8295 ₄ ¹⁵	1.4295 ²⁰	−15	235–237		misc alc, chl, eth
d13	1-Decanesulfonic acid, Na salt	$\text{CH}_3(\text{CH}_2)_9\text{SO}_3^-\text{Na}^+$	244.33	4 ³ , 27			300			
d14	Decanoic acid	$\text{CH}_3(\text{CH}_2)_8\text{COOH}$	172.27	2 ² , 309	0.8782 ₄ ⁵⁰	1.4288 ⁴⁰	31.4	270		0.015 aq; s alc, chl, bz, eth, CS ₂
d15	1-Decanol	$\text{CH}_3(\text{CH}_2)_9\text{OH}$	158.29	1, 425	0.8297 ₄ ²⁰	1.4371 ²⁰	6.9	230.2	82	i aq; s alc, eth
d16	4-Decanone	$\text{CH}_3(\text{CH}_2)_5\text{C(=O)-(CH}_2)_2\text{CH}_3$	156.27	1, 711	0.824 ₀ ²⁰	1.4237 ²⁰		207	71	i aq; misc alc, eth
d17	Decanoyl chloride	$\text{CH}_3(\text{CH}_2)_8\text{C(=O)Cl}$	190.71	2, 356	0.919	1.4410 ²⁰	−34.5	96 ^{5mm}	98	d aq, alc; s eth
d18	1-Decene	$\text{CH}_3(\text{CH}_2)_7\text{CH=CH}_2$	140.27	1 ³ , 858	0.7408 ₄ ²⁰	1.4215 ²⁰	−66.3	170.6	47	i aq; misc alc, eth
d19	Decylamine	$\text{CH}_3(\text{CH}_2)_9\text{NH}_2$	157.30	4, 199	0.787	1.4360 ²⁰	12–14	216–218	85	sl s aq; misc alc, bz, eth, acet
d20	Dehydroabietylamine		285.48			1.5460 ²⁰			>112	
d21	Dehydroacetic acid		168.15	17, 559			111–113	269.9		22 acet; 18 bz; 5 MeOH
d22	Deoxybenzoin	$\text{C}_6\text{H}_5\text{CH}_2\text{C(=O)C}_6\text{H}_5$	196.25	7, 431	1.201 ₄ ⁰		55–56	320		i aq; v s alc, eth

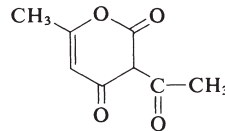
Cymenes, i100, i101, i102
 4-Cymylphenol, m359
 Cysteamine, a162
 Cysteic acid hydrate, a288
 Cytosine, a198

2,4-D, d214
p,p'-DDT, b167
 1,2-Decahydroacenaphthylene, a2
 Decamethylene glycol, d10
 1,10-Decadedicarboxylic acid, d721

Decyl aldehyde, d6
 Decyl chloride, c80
 Decyl iodide, i33
 Dextrose, g6



d20



d21

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d23	Diacetoxymethylsilane	$(\text{CH}_3)_2\text{Si}(\text{OOCCH}_3)_2$	176.3		1.054 ₄ ²⁰	1.4030 ²⁰		164–166		
d24	Diacetoxymethylphenylsilane	$\text{CH}_3(\text{C}_6\text{H}_5)\text{Si}(\text{OCOCH}_3)_2$	238.3			1.487 ²⁰		127 ^{6mm}		
d25	Diallylamine	$(\text{H}_2\text{C}=\text{CHCH}_2)_2\text{NH}$	97.16	4, 208	0.787	1.4405 ²⁰	−88	111–112	15	
d26	Diallyl ether	$(\text{H}_2\text{C}=\text{CHCH}_2)_2\text{O}$	98.15	1 ² , 477	0.805 ₀ ¹⁸	1.4240 ²⁰		94		i aq; misc alc, eth
d27	Diallyl sulfide	$(\text{H}_2\text{C}=\text{CHCH}_2)_2\text{S}$	114.21	1, 440	0.8877 ₄ ²⁷	1.4889 ²⁰	−83	138	46	sl s aq; misc alc, eth
d28	1,2-Diaminoanthraquinone		238.25	14 ¹ , 459			289–291			sl s alc, eth
d29	1,4-Diaminoanthraquinone		238.25	14, 197			265–268			sl s aq, alc; v s bz
d30	2,6-Diaminoanthraquinone		238.25	14, 215			>325			sl s hot aq, pyr
d31	2,5-Diaminoazobenzene HCl	$\text{C}_6\text{H}_5\text{N}=\text{NC}_6\text{H}_5\cdot(\text{NH}_2)_2\cdot\text{HCl}$	248.72	16, 383			235 d			
d32	2,5-Diaminobenzene-sulfonic acid	$(\text{H}_2\text{N})_2\text{C}_6\text{H}_3\text{SO}_3\text{H}$	188.21	14, 713			298 d			sl s aq, alc
d33	3,5-Diaminobenzoic acid	$(\text{H}_2\text{N})_2\text{C}_6\text{H}_3\text{COOH}$	152.15	14, 453			228	−H ₂ O, 110		sl s aq; s alc, eth
d34	4,4'-Diaminodiphenylamine sulfate	$\text{H}_2\text{NC}_6\text{H}_4\text{NHC}_6\text{H}_4\cdot\text{NH}_2\cdot\text{H}_2\text{SO}_4$	297.33	13, 110			300			
d35	4,4'-Diaminodiphenylmethane	$\text{H}_2\text{NC}_6\text{H}_4\text{CH}_2\text{C}_6\text{H}_4\text{NH}_2$	198.27	13, 238			91–92	398	221	sl s aq; v s alc, bz, eth
d36	3,3'-Diaminodiphenyl sulfone	$\text{H}_2\text{NC}_6\text{H}_4\text{SO}_2\text{C}_6\text{H}_4\text{NH}_2$	248.30	13, 426			167–170			i aq; s alc, bz
d37	4,4'-Diaminodiphenyl sulfone	$\text{H}_2\text{NC}_6\text{H}_4\text{SO}_2\text{C}_6\text{H}_4\text{NH}_2$	248.30	13, 536			175–177			i aq; s alc, acet, HCl
d38	2,7-Diaminofluorene		196.25	13, 266			165–166			sl s aq; v s alc

d39	2,4-Diamino-6-hydroxypyrimidine		126.12	24, 469			285 d			s aq
d40	Diaminomaleonitrile	$\text{NCC}(\text{NH}_2)=\text{C}(\text{NH}_2)\text{CN}$	108.10	4 ² , 949			178–179			
d41	1,8-Diamino- <i>p</i> -menthane		170.30	13, 4	0.914	1.4805 ²⁰	–45	107–125 ^{10mm}	93	
d42	3,3'-Diamino- <i>N</i> -methyl-dipropylamine	$\text{CH}_3\text{N}[(\text{CH}_2)_3\text{NH}_2]_2$	145.25	4 ⁴ , 1279				110–112 ^{6mm}	102	

Diacetins, g17, g18

Diacetone acrylamide, d568

Diacetone alcohol, h142

Diacetonitrile, a151

(Diacetoxyiodo)benzene, i28

Diacetyl, b386

Diallyl, h41

2,5-Diaminoanisole, m94

1,4-Diaminobutane, b379

1,2-Diaminocyclohexanes, c318, c319

1,10-Diaminodecane, d8

p-Diaminodiphenyl, b136

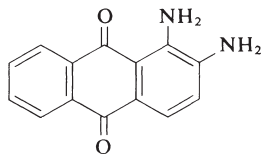
3,3'-Diaminodipropylamine, i9

1,12-Diaminododecane, d720

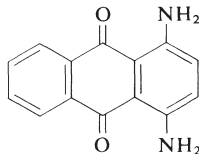
1,2-Diaminoethane, e15

1,7-Diaminoheptane, h7

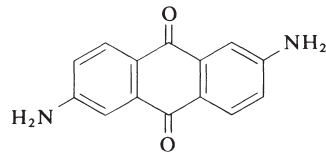
1,6-Diaminohexane, h56



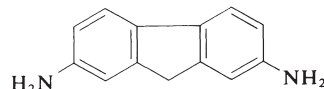
d28



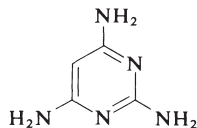
d29



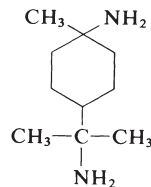
d30



d38



d39



d41

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d43	1,3-Diamino-2-propanol	$\text{H}_2\text{NCH}_2\text{CH}(\text{OH})\text{CH}_2\text{NH}_2$	90.13	4, 290			40–45	235		
d44	2,6-Diaminopyridine	$(\text{H}_2\text{N})_2\text{C}_5\text{H}_3\text{N}$	109.13	22 ¹ , 647			118–120			s aq, alc
d45	1,4-Diazabicyclo-[2.2.2]octane		112.18				158	174		45 aq; 77 EtOH; 51 bz; 13 acet; 26 MeEtKe
d46	1,8-Diazabicyclo-[5.4.0]undec-7-ene		152.24		1.018	1.5219 ²⁰		80 ^{0.6mm}	>112	
d47	Diazomethane	$\text{CH}_2=\text{N}=\text{N}$	42.04	23, 25			–145	–23	very explosive	s eth, diox
d48	1-Diazo-2-naphthol-4-sulfonic acid, Na salt		272.22	16, 595			166			
d49	Dibenz[<i>de,kl</i>]anthracene		252.32	5 ¹ , 363	1.35		273–274	503		s bz; sl s alc, eth
d50	Dibenzofuran		168.20	17, 70	1.0886 ⁹⁹	1.6079 ⁹⁹	81–83	285		i aq; s alc, bz, eth
d51	2,3,11,12-Dibenzo-1,4,7,10,13-hexaoxacyclooctadeca-2,11-diene		360.41				162–164			
d52	Dibenzothiophene		184.26	17, 72			97.100	332–333		s aq; v s alc, bz
d53	Dibenzoylmethane	$\text{C}_6\text{H}_5\text{C}(=\text{O})\text{CH}_2\text{C}(=\text{O})\text{C}_6\text{H}_5$	224.26	7, 769			78–79	220 ^{18mm}		s alc; v s eth
d54	Dibenzoly peroxide	$\text{C}_6\text{H}_5\text{C}(\text{O})\text{OOC}(\text{O})\text{C}_6\text{H}_5$	242.23				103–106	may explode when heated		sl s aq, alc; s bz, chl, eth

d55	(—)-Dibenzoyl-L-tartaric acid hydrate	$[(C_6H_5COOCH-(COOH)-)_2 \cdot H_2O]$	376.34	9, 170						
d56	Dibenzylamine	$C_6H_5CH_2NHCH_2C_6H_5$	197.28	12, 1035	1.026	1.5731^{20}	-26	300	143	i aq; s alc, eth
d57	Dibenzyl disulfide	$C_6H_5CH_2SSCH_2C_6H_5$	246.39	6, 465			69	d > 270		s hot alc, bz, eth
d58	Dibenzyl ether	$C_6H_5CH_2OCH_2C_6H_5$	198.27	6, 434	1.0014^{20}_4	1.5610^{20}	3.5	298 d	135	misc alc, acet, chl, eth

1,3-Diamino-2-hydroxypropane, d43

Diaminonaphthalenes, n4, n5

1,2-Diamino-4-nitrobenzene, n68

1,4-Diamino-2-nitrobenzene, n67

1,9-Diaminononane, n93

1,8-Diaminooctane, o23

1,5-Diaminopentane, p29

2,5-Diaminopentanoic acid, o46

1,2-Diaminopropane, p192

1,3-Diaminopropane, p193

4,6-Diamino-4-pyrimidinol, d39

Diaminotoluenes, t168, t169, t170, t171

1,3-Diaminourea, c11

4,5-Diamino-*o*-xylene, d586

Diamylamine, d650

Diamyl ether, d651

Diamyl ketone, u6

1,2-Dianilinoethane, d669

Diazoacetic ester, e114

1,3-Diazole, i4

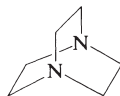
Dibenzo-18-crown-6, d51

Dibenzo[*b,e*]pyridine, a61

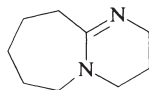
Dibenzopyrrole, d665

Dibenzoyl, b34

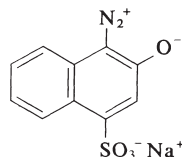
Dibenzyl, d666



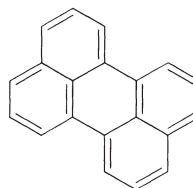
d45



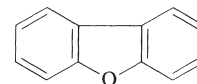
d46



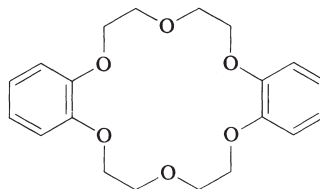
d48



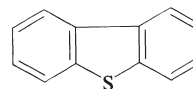
d49



d50



d51



d52

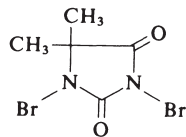
TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d59	<i>N,N'</i> -Dibenzylethyl-enediamine	$(C_6H_5CH_2NHCH_2-)_2$	240.35	12, 1067	1.024 ₄ ²⁰	1.5624 ²⁰	26	195 ^{4mm}	>112	v s alc, bz, chl, eth
d60	Dibenzyl malonate	$CH_2[COOCH_2C_6H_5]_2$	284.31	6, 436	1.137	1.5447 ²⁰		188 ^{0.2mm}	>112	
d61	Dibenzyl phosphonate	$(C_6H_5CH_2O)_2P(O)H$	262.25		1.187	1.5540 ²⁰	-5 to +5	110 ^{0.01mm}	>112	
d62	Dibromoacetic acid	$Br_2CHCOOH$	217.86	2, 218				128–130 ^{16mm}		
d63	Dibromoacetonitrile	Br_2CHCN	198.86	2, 219	2.296	1.5393 ²⁰		67–69 ^{24mm}	none	
d64	2,4'-Dibromoacetophenone	$BrC_6H_4C(=O)CH_2Br$	277.96	7, 285			108–110			s warm alc, eth
d65	1,4-Dibromobenzene	$C_6H_4Br_2$	235.92	5, 211	0.9641 ¹⁰⁰	1.5743 ¹⁰⁰	87.3	219	none	1.4 alc; s bz; 101 eth
d66	4,4'-Dibromobiphenyl	$BrC_6H_4C_6H_4Br$	312.00	5, 580			162–163	355–360		s bz; sl s hot alc
d67	1,3-Dibromobutane	$CH_3CH(Br)CH_2CH_2Br$	215.93	1, 120	1.800 ²⁰	1.5085 ²⁰		175	none	s chl, eth
d68	1,4-Dibromobutane	$BrCH_2CH_2CH_2CH_2Br$	215.93	1, 120	1.8080 ₄ ²⁰	1.5186 ²⁰	-20	198	>112	s chl
d69	1,4-Dibromo-2,3-butanedione	$BrCH_2C(=O)C(=O)CH_2Br$	243.89	1, 774			116–117			
d70	<i>trans</i> -2,3-Dibromo-2-butene-1,4-diol	$HOCH_2C(Br)=C(Br)CH_2OH$	245.91	1 ¹ , 260			112–114			
d71	Dibromo-chloromethane	$HCCLBr_2$	208.29	1, 67	2.451	1.5465 ²⁰	-22	120 ^{748mm}	none	misc alc, bz, eth
d72	1,2-Dibromo-2-chloro-1,1,2-trifluoroethane	$FCCL(Br)C(Br)F_2$	276.5		2.2478 ²⁰	1.4275 ²⁰		93–94		
d73	1,10-Dibromodecane	$Br(CH_2)_{10}Br$	300.09	1 ¹ , 64	1.335 ³⁰	1.4912 ²⁰	27	160 ^{15mm}	>112	sl s alc; s eth
d74	1,2-Dibromo-1,1-difluoroethane	$CH_2BrC(Br)F_2$	223.87	1, 92	2.2238 ²⁰	1.4456 ²⁰	-61.3	93.4		i aq
d75	Dibromodifluoromethane	Br_2CF_2	209.81	1 ¹ , 16	2.288 ₄ ¹⁵	1.3999 ¹²	-141.6	23–24	none	0.1 aq; misc alc, bz, chl, eth

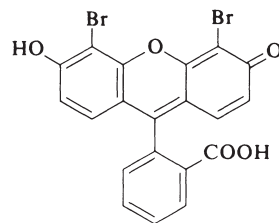
d76	1,3-Dibromo-5,5-dimethylhydantoin		285.93				197 d			
d77	1,1-Dibromoethane	CH_3CHBr_2	187.87	1, 90	2.055^{20}_4	1.5379^{20}		113		i aq; v s alc, eth
d78	1,2-Dibromoethane	$\text{BrCH}_2\text{CH}_2\text{Br}$	187.87	1, 90	2.1802^{20}_4	1.5416^{15}	10.0	131.7	none	0.43 aq; misc alc, eth
d79	(1,2-Dibromoethyl)-benzene	$\text{C}_6\text{H}_5\text{CH}(\text{Br})\text{CH}_2\text{Br}$	263.97	5, 356			70–74	$140^{15\text{mm}}$		
d80	<i>cis</i> -1,2-Dibromoethylene	$\text{BrCH}=\text{CHBr}$	185.86	1, 190	2.21^{17}_4	1.5431^{18}	–53	112.5		s alc, bz, chl, eth
d81	<i>trans</i> -1,2-Dibromoethylene	$\text{BrCH}=\text{CHBr}$	185.86	1, 190	2.246	1.5505^{18}	–6.5	108		
d82	1,2-Dibromoethyltrichlorosilane	$\text{BrCH}_2\text{CH}(\text{Br})\text{SiCl}_3$	321.3		2.046^{20}_4	1.537^{20}		$90^{11\text{mm}}$		
d83	4',5',-Dibromofluorescein		490.12	19, 228			270–273			s hot alc, HOAc
d84	2,4-Dibromo-1-fluorobenzene	$\text{Br}_2\text{C}_6\text{H}_3\text{F}$	253.91		2.047^{20}	1.5840^{20}		$105^{22\text{mm}}$	92	
d85	1,2-Dibromohexafluoropropane	$\text{CF}_3\text{CF}(\text{Br})\text{C}(\text{Br})\text{F}_2$	309.83				72.8			

Dibenzyl ketone, d684

5,7-Dibromo-8-quinolinol, d87



d76



d83

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

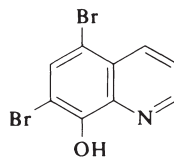
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d86	1,6-Dibromohexane	$\text{Br}(\text{CH}_2)_6\text{Br}$	243.98	1, 145	1.586_4^{18}	1.5066^{20}		243	32	misc eth
d87	5,7-Dibromo-8-hydroxyquinoline		302.96	21, 97			200–201	subl		s alc, bz; v s eth
d88	Dibromomethane	CH_2Br_2	173.85	1, 67	2.4956_4^{20}	1.5419^{20}	–52.7	96.97	none	1.15 aq; misc alc, bz, acet, chl, eth
d89	2,6-Dibromo-4-nitroaniline	$\text{Br}_2\text{C}_6\text{H}_2(\text{NO}_2)\text{NH}_2$	295.93	12, 743			206–208			sl s aq; s HOAc
d90	2,5-Dibromonitrobenzene	$\text{Br}_2\text{C}_6\text{H}_3\text{NO}_2$	280.91	5, 250	1.9581^{111}		82–84			s bz, hot alc
d91	1,5-Dibromopentane	$\text{Br}(\text{CH}_2)_5\text{Br}$	229.95	1, 131	1.6879_4^{15}	1.5092^{15}	–34	$110^{15\text{mm}}$	79	
d92	1,2-Dibromopropane	$\text{CH}_3\text{CH}(\text{Br})\text{CH}_2\text{Br}$	201.90	1, 109	1.933^{20}	1.5203^{20}	–55.5	139.6	none	0.2 aq; misc alc, bz, chl, eth
d93	1,3-Dibromopropane	$\text{BrCH}_2\text{CH}_2\text{CH}_2\text{Br}$	201.90	1, 110	1.9712_4^{25}	1.5233^{20}	–34	166.8	54	0.17 aq; s alc, eth
d94	2,3-Dibromopropanol	$\text{BrCH}_2\text{CH}(\text{Br})\text{CH}_2\text{OH}$	217.90	1, 357	2.120_4^{20}	1.5599^{20}		95–97 ^{10mm}		sl s aq; misc alc, bz, eth, acet
d95	2,3-Dibromopropene	$\text{BrCH}_2\text{C}(\text{Br})=\text{CH}_2$	199.88	1, 201	1.9336_4^{20}	1.5470^{20}		140–143	none	
d96	2,3-Dibromopropionic acid	$\text{BrCH}_2\text{CH}(\text{Br})\text{COOH}$	231.88	2, 258			64–66	$160^{20\text{mm}}$		s aq, alc, bz
d97	2,6-Dibromopyridine	$\text{Br}_2(\text{C}_5\text{H}_3\text{N})$	236.91	20 ² , 153			118–119	255		
d98	DL-2,3-Dibromosuccinic acid	$\text{HOOCCH}(\text{Br})\text{CH}(\text{Br})\text{COOH}$	275.89	2, 625			167			v s aq, alc
d99	1,2-Dibromotetrachloroethane	$\text{BrCCl}_2\text{CCl}_2\text{Br}$	325.65	1, 93	2.713		220–222		none	
d100	1,2-Dibromotetrafluoroethane	$\text{BrCF}_2\text{CF}_2\text{Br}$	259.83		2.163^{25}	1.367^{25}	–110.5	47.3		
d101	2,5-Dibromothiophene	$\text{Br}_2\text{C}_4\text{H}_2\text{S}$	241.94	17, 33	2.147_{23}^{23}	1.6289^{20}	–6	221		i aq; v s alc, eth
d102	α,α -Dibromotoluene	$\text{C}_6\text{H}_5\text{CHBr}_2$	249.94	5, 308	1.510^{15}	1.6147^{20}		$156^{23\text{mm}}$	110	i aq; misc alc, eth
d103	1,2-Dibromo-1,1,2-trifluoroethane	$\text{HC}(\text{Br})\text{FC}(\text{Br})\text{F}_2$	241.8	1, 92	$2, 274^{27}$	1.4191^{24}		76.5		

d104	α,α' -Dibromo- <i>o</i> -xylene	$C_6H_4(CH_2Br)_2$	263.97	5, 366	1.960		92–94			sl s alc, chl, eth
d105	α,α' -Dibromo- <i>p</i> -xylene	$C_6H_4(CH_2Br)_2$	263.97	5, 385	2.012 ⁰		142–143	245		v s alc, chl; s eth
d106	1,2-Dibutoxyethane	$C_4H_9OCH_2CH_2OC_4H_9$	174.28		0.8374 ²⁰ ₂₀	1.4131 ²⁰	–69.1	203.6		0.2 aq; misc alc, acet
d107	Dibutylamine	$(C_4H_9)_2NH$	129.25	4, 157	0.7601 ²⁰ ₄	1.4177 ²⁰	–62	159.6	33	0.47 aq; s alc, acet, eth, EtAc, PE
d108	<i>N,N</i> -Dibutylamino-ethanol	$(C_4H_9)_2NCH_2CH_2OH$	173.29		0.860 ²⁰ ₂₀	1.444 ²⁰	< –70	227–230	93	
d109	<i>N,N</i> -Dibutylaniline	$C_6H_5N(C_4H_9)_2$	205.34	12 ² , 95	0.904 ²⁰	1.5197 ²⁰		267–275	110	i aq, MeOH; s acet, bz, EtOH, EtAc, eth
d110	Dibutyl decanedioate	$C_4H_9OOC(CH_2)_8COO-C_4H_9$	314.45	2, 719	0.9366 ²⁰	1.4415 ²⁰	1.0	344–345	177	0.004 aq
d111	Di- <i>tert</i> -butyldi-carbonate	$(CH_3)_3COC(O)OC-(CH_3)_3$	218.25		0.950	1.4103 ²⁰	23	56 ^{0.5mm}	37	
d112	2,5-Di- <i>tert</i> -butyl-1,4-dihydroxy-benzene	$[(CH_3)_3C]_2C_6H_2(OH)_2$	222.33				217–219			
d113	Dibutyl disulfide	$C_4H_9SSC_4H_9$	178.36	1 ² , 400	0.9383 ²⁰ ₄	1.4920 ²⁰	–71	231.2	93	i aq; misc alc, eth

Dibutyl 1,2-benzenedicarboxylate, d128

Dibutyl butanedioate, d130

Dibutyl Cellosolve, d106



d87

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d114	Di- <i>tert</i> -butyl disulfide	$(\text{CH}_3)_3\text{CSSC}(\text{CH}_3)_3$	178.36		0.935	1.4920		229–33	93	
d115	Dibutyl ether	$\text{C}_4\text{H}_9\text{OC}_4\text{H}_9$	130.22	1, 369	0.7689 ₄ ²⁰	1.3992 ²⁰	−97.9	142.4	25	0.03 aq; misc alc, eth
d116	<i>N,N</i> -Dibutyl-formamide	$\text{HC}(=\text{O})\text{N}(\text{C}_4\text{H}_9)_2$	157.26		0.864	1.4429 ²⁰		120 ^{15mm}	100	
d117	3,5-Di- <i>tert</i> -butyl-4-hydroxybenzoic acid	$[(\text{CH}_3)_3\text{C}]_2\text{C}_6\text{H}_2\text{-(OH)COOH}$	250.34				206–209			
d118	Dibutyl maleate	$\text{C}_4\text{H}_9\text{OOCCH}=\text{CHCOOC}_4\text{H}_9$	228.28		0.9950 ²⁰	1.4454 ²⁰	< −80	d 280	135	0.05 aq
d119	Di- <i>tert</i> -butyl malonate	$\text{CH}_2\text{COOC}(\text{CH}_3)_3$ $\text{COOC}(\text{CH}_3)_3$	216.27			1.4184 ²⁰	−6.0	93 ^{10mm}		
d120	2,6-Di- <i>tert</i> -butyl-4-methylphenol	$[(\text{CH}_3)_3\text{C}]_2\text{C}_6\text{H}_2(\text{CH}_3)\text{OH}$	220.36	6 ³ , 2073	0.894 ₄ ⁷⁵	1.4859 ⁷⁵	70	265		i aq; s alc, bz, acet
d121	Dibutyl oxalate	$\text{C}_4\text{H}_9\text{OOC}-\text{COOC}_4\text{H}_9$	202.25	2, 540	0.986 ₂₀ ²⁰	1.4232 ²⁰	−30.0	239–240	108	misc alc, ketones, PE
d122	Di- <i>tert</i> -butyl peroxide	$(\text{CH}_3)_3\text{CO}-\text{OC}(\text{CH}_3)_3$	146.23		0.794 ²⁰	1.3890 ²⁰	−40	110		misc acet, octane
d123	2,4-Di- <i>tert</i> -butylphenol	$[(\text{CH}_3)_3\text{C}]_2\text{C}_6\text{H}_3\text{OH}$	206.33				56.5	263.5	115	s hot alc; i alk
d124	2,6-Di- <i>sec</i> -butylphenol	$[\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)]_2\text{-C}_6\text{H}_3\text{OH}$	206.33		0.918	1.5100 ²⁰	−42	255–260	127	
d125	2,6-Di- <i>tert</i> -butylphenol	$[(\text{CH}_3)_3\text{C}]_2\text{C}_6\text{H}_3\text{OH}$	206.33	6 ³ , 2061			35–83	253	118	s hot alc; i alk
d126	3,5-Di- <i>tert</i> -butylphenol	$[(\text{CH}_3)_3\text{C}]_2\text{C}_6\text{H}_3\text{OH}$	206.33				87–89			
d127	Dibutyl phosphonate	$(\text{C}_4\text{H}_9\text{O})_2\text{P}(\text{O})\text{H}$	194.21	1, 187	0.995 ₄ ²⁰	1.4231 ²⁰		118 ^{11mm}	121	sl s (hyd) aq; misc alc, acet, eth
d128	Dibutyl <i>o</i> -phthalate	$\text{C}_6\text{H}_4[\text{COOC}_4\text{H}_9]_2$	278.35	9 ² , 586	1.0465 ₄ ²⁰	1.4926 ²⁰	−35	340	171	0.01 aq; v s alc, bz, acet, eth

d129	<i>N,N</i> -Dibutyl-1,3-propanediamine	$C_4H_9NHCH_2CH_2CH_2-NHC_4H_9$	186.34		0.827	1.4463 ²⁰		205	103	
d130	Dibutyl succinate	$[C_4H_9OOCCH_2-]_2$	230.30	2 ² , 551	0.9768 ²⁰	1.4299 ²⁰	-29.0	274.5		i aq; s alc, eth
d131	Dibutyl sulfate	$C_4H_9OSO_2OC_4H_9$	210.29		1.059 ²⁵	1.4213 ²⁰		130-132 ^{11mm}		
d132	Dibutyl sulfide	$C_4H_9SC_4H_9$	146.30	1, 370	0.839 ¹⁶	1.4530 ²⁰	-75.0	188.9	76	i aq; v s alc, eth
d133	Di- <i>tert</i> -butyl sulfide	$(CH_3)_3CSC(CH_3)_3$	146.30		0.815	1.4506 ²⁰		151	48	
d134	Dibutyl sulfite	$(C_4H_9O)_2S(O)$	194.29	1 ² , 397	0.9944 ²²	1.4310 ²⁰		108 ^{15mm}		
d135	Dibutyl sulfone	$(C_4H_9)_2SO_2$	178.29	1, 371			46	295	143	i aq; s alc, eth
d136	<i>N,N'</i> -Dibutylthio-urea	$C_4H_9NHC(=S)NHC_4H_9$	188.34				63.65			i aq; s alc; sl s eth
d136a	Dibutyltin dichloride	$(C_4H_9)_2SnCl_2$	303.83				39-41	135 ^{10mm}	>112	
d137	Dibutyltin oxide	$(C_4H_9)_2SnO$	248.92	4 ¹ , 588			>300			
d138	Dichloroacetic acid	$Cl_2CHCOOH$	128.94	2, 202	1.563 ²⁰	1.4642 ²⁰	9-11	193-194	>112	misc aq, alc, eth
d139	1,1-Dichloroacetone	$CH_3C(O)CHCl_2$	126.97	1, 654	1.305 ¹⁸			150		sl s aq; s alc; misc eth
d140	2',4'-Dichloroacetophenone	$Cl_2C_6H_3COCH_3$	189.04	7 ² , 219		1.5635 ²⁰	33-34	145 ^{15mm}	>112	i aq
d141	Dichloroacetyl chloride	$Cl_2CHCOCI$	147.39	2, 204	1.5315 ¹⁶	1.4603 ²⁰		107-108	66	d aq, alc; misc eth
d142	2,3-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 621		1.5969 ²⁰	23-24	252	>112	s alc; v s eth
d143	2,4-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 621	1.567 ²⁰		59.62	245		sl s aq; s alc, eth
d144	2,5-Dichloroaniline	$Cl_2C_6H_3NH_2$	162.02	12, 625			49-51	251		s alc, bz, eth

Di-*tert*-butylcresol, d120
2,5-Di-*tert*-butylhydroquinone, d112
Dibutyl ketone, n100

Dibutyl phosphite, d127
Dibutyl sebacate, d110
Dichloroacetaldehyde diethyl acetal, d169

Dichloroanisoles, d191, d192

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

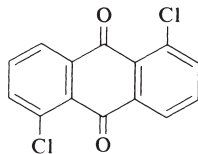
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d145	2,6-Dichloroaniline	$\text{Cl}_2\text{C}_6\text{H}_3\text{NH}_2$	162.02	12, 626			38.41			
d146	3,4-Dichloroaniline	$\text{Cl}_2\text{C}_6\text{H}_3\text{NH}_2$	162.02	12, 626			70–72	272		s alc, eth; sl s bz
d147	3,5-Dichloroaniline	$\text{Cl}_2\text{C}_6\text{H}_3\text{NH}_2$	162.02	12, 626			51–53	259 ^{741mm}		i aq; s alc, eth
d148	1,5-Dichloroanthraquinone		277.11	7, 787			245–247			sl s alc, bz, acet
d149	1,8-Dichloroanthraquinone		277.11	7, 788			202–203			sl s alc
d150	2,4-Dichlorobenzaldehyde	$\text{Cl}_2\text{C}_6\text{H}_3\text{CHO}$	175.01	7, 236			69–73	233		i aq; s alc
d151	2,4-Dichlorobenzamide	$\text{Cl}_2\text{C}_6\text{H}_3\text{CONH}_2$	190.03	9 ³ , 1376			191–194			
d152	1,2-Dichlorobenzene	$\text{C}_6\text{H}_4\text{Cl}_2$	147.01	5, 201	1.3059 ²⁰ ₄	1.5515	–17.0	180.4	65	misc alc, bz, eth
d153	1,3-Dichlorobenzene	$\text{C}_6\text{H}_4\text{Cl}_2$	147.01	5, 202	1.2884 ²⁰ ₄	1.5459	–24.8	173.1	63	0.01 aq; s alc, eth
d154	1,4-Dichlorobenzene	$\text{C}_6\text{H}_4\text{Cl}_2$	147.01	5, 203	1.2417 ⁶⁰	1.5285	53	174.1	65	s alc, bz, chl, eth
d155	2,5-Dichlorobenzene-sulfonyl chloride	$\text{Cl}_2\text{C}_6\text{H}_3\text{SO}_2\text{Cl}$	245.51	11 ¹ , 15			36–37			d hot aq, hot alc
d156	2,4-Dichlorobenzoic acid	$\text{Cl}_2\text{C}_6\text{H}_3\text{COOH}$	191.01	9, 342			157–160			s hot aq, alc, bz, chl
d157	2,5-Dichlorobenzoic acid	$\text{Cl}_2\text{C}_6\text{H}_3\text{COOH}$	191.01	9, 342			151–154	301		sl s aq; s alc, eth
d158	3,4-Dichlorobenzoic acid	$\text{Cl}_2\text{C}_6\text{H}_3\text{COOH}$	191.01	9, 343			207–209			s hot aq, eth; v s alc
d159	4,4'-Dichlorobenzophenone	$(\text{ClC}_6\text{H}_4)_2\text{CO}$	251.11	7, 420			144–146	353		s hot alc; v s chl, eth
d160	2,4-Dichlorobenzoyl chloride	$\text{Cl}_2\text{C}_6\text{H}_3\text{COCl}$	209.46	9, 342	1.494	1.5297 ²⁰	16–18	150 ^{34mm}	137	d aq, alc
d161	3,4-Dichlorobenzoyl chloride	$\text{Cl}_2\text{C}_6\text{H}_3\text{COCl}$	209.46	9, 344			30–33	242	142	d aq, alc
d162	1,2-Dichlorobutane	$\text{CH}_3\text{CH}_2\text{CH}(\text{Cl})\text{CH}_2\text{Cl}$	127.01	1 ¹ , 38	1.118 ²⁰ ₄	1.4474 ¹⁵		124		i aq; s chl, eth

d163	1,4-Dichlorobutane	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$	127.01	1, 119	1.1598 ₄ ²⁰	1.4566 ²⁰	−38	155	40	i aq; s chl
d164	<i>meso</i> -2,3-Dichlorobutane	$\text{CH}_3\text{CH}(\text{Cl})\text{CH}(\text{Cl})\text{CH}_3$	127.01	1, 119	1.1025 ₄ ²⁵	1.4386 ²⁵	−80	115.9	18	i aq; s chl
d165	<i>cis</i> -1,4-Dichloro-2-butene	$\text{ClCH}_2\text{CH}=\text{CHCH}_2\text{Cl}$	125.00	1 ³ , 743	1.188 ₄ ²⁵	1.4887 ²⁵	−48	152	49	i aq; s org solv
d166	<i>trans</i> -1,4-Dichloro-2-butene	$\text{ClCH}_2\text{CH}=\text{CHCH}_2\text{Cl}$	125.00	1 ³ , 743	1.183 ₄ ²⁵	1.4861 ²⁵	1−3	74–76 ^{40mm}	56	i aq; s org solv
d167	3,4-Dichloro-1-butene	$\text{ClCH}_2\text{CH}(\text{Cl})\text{CH}=\text{CH}_2$	125.00		1.150	1.4658 ²⁰	−61	123	28	
d168	1,4-Dichloro-2-butyne	$\text{ClCH}_2\text{C}\equiv\text{CCH}_2\text{Cl}$	122.98	1 ³ , 927	1.258 ₄ ²⁰	1.5048 ²⁰		165–168	160	
d169	1,1-Dichloro-2,2-diethoxyethane	$\text{Cl}_2\text{CHCH}(\text{OC}_2\text{H}_5)_2$	187.07	1, 614	1.138	1.4360 ²⁰		183–184	60	
d170	Dichlorodifluoromethane	Cl_2CF_2	120.92	1, 61	1.486 ^{−30}		−158	−29.8		0.02 aq; 9 bz; 5.5 chl; 6 diox; s alc, eth
d171	4,6-Dichloro-1,3-dihydroxybenzene	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})_2$	179.00	6 ¹ , 403			104–106	254		sl s aq, bz; s eth
d172	2,5-Dichloro-3,6-dihydroxy- <i>p</i> -benzoquinone		208.98	8, 379			283–284			

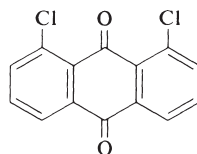
2,6-Dichlorobenzyl chloride, t249
2,2'-Dichlorodiethyl ether, b158

5,5'-Dichloro-2,2'-dihydroxydiphenylmethane, m233

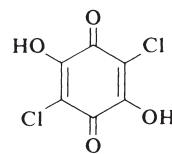
1,1-Dichlorodimethyl ether, d197
Dichlorohydrin, d220



d148



d149



d172

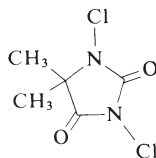
TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d173	1,3-Dichloro-3,5-dimethylhydantoin		197.02	24 ² , 158			134–136			
d174	Dichlorodimethylsilane	(CH ₃) ₂ SiCl ₂	129.06		1.064 ₄ ²⁰	1.4038 ²⁰	–16	70	–16	
d175	Dichlorodiphenylsilane	(C ₆ H ₅) ₂ SiCl ₂	253.20	16, 910	1.222 ₄ ²⁰	1.582 ²⁰		308–309	157	d aq, alc
d176	1,1-Dichloroethane	CH ₃ CHCl ₂	98.96	1, 83	1.1757 ₄ ²⁰	1.4164 ²⁰	–97.0	57.3	–5	0.51 aq; misc alc
d177	1,2-Dichloroethane	ClCH ₂ CH ₂ Cl	98.96	1, 84	1.2531 ₄ ²⁰	1.4448 ²⁰	–35.7	83.5	15	0.8 aq; misc alc, chl, eth
d178	1,1-Dichloroethylene	H ₂ C=CCl ₂	96.94	1, 186	1.2129 ₄ ²⁰	1.4247 ²⁰	–122.6	31.6	–15	0.02 aq; s alc, bz, chl, eth
d179	<i>cis</i> -1,2-Dichloroethylene	ClCH=CHCl	96.94	1, 188	1.2818 ₄ ²⁰	1.4490 ²⁰	–80.1	60.7	6	0.7 aq; s alc, eth
d180	<i>trans</i> -1,2-Dichloroethylene	ClCH=CHCl	96.94	1, 188	1.2546 ₄ ²⁰	1.4462 ²⁰	–49.8	47.7	6	0.6 aq; s alc, eth
d181	2,2'-Dichloroethyl ether	ClCH ₂ CH ₂ OCH ₂ CH ₂ Cl	143.01	1 ² , 335	1.2220 ₂₀ ²⁰	1.457 ²⁰		178.5	55	1.1 aq; s alc, bz, eth
d182	1,2-Dichloroethyltrichlorosilane	ClCH ₂ CH(Cl)SiCl ₃	232.4		1.516 ₄ ²⁵	1.449 ²⁵		82–84 ^{26mm}		
d183	Dichlorofluoromethane	FCHCl ₂	102.92	1, 61	1.345 ³⁰		–135	8.9		69 HOAc; 108 diox; s alc, eth; i aq
d184	Dichloroheptylmethylsilane	C ₇ H ₁₅ Si(CH ₃)Cl ₂	225.2		0.9780 ₄ ²⁰	1.4396 ²⁵		207–208		
d185	1,2-Dichlorohexafluorocyclobutane	F ₆ C ₄ Cl ₂	233.0			1.3342 ²⁵		59–60		
d186	1,5-Dichlorohexamethyltrisiloxane	[ClC(CH ₃) ₂ O] ₂ –Si ₃ (CH ₃) ₂	277.4		1.018 ₄ ²⁰	1.4071		184		
d187	1,6-Dichlorohexane	Cl(CH ₂) ₆ Cl	155.07	1, 144	1.068	1.4568 ²⁰		87 ^{15mm}	73	s chl

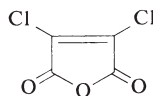
d188	1,2-Dichloro-2-iodo-1,1,2-trifluoroethane	F(I)C(Cl)C(Cl)F_2	278.9		2.200 ²⁰	1.4490 ²⁰		100–101		
d189	Dichloromaleic anhydride		166.95	17, 434						
d190	Dichloromethane	CH_2Cl_2	84.93	1, 60	1.3255 ²⁰ ₄	1.4246 ²⁰	−96.7	40.5	none	1.3 aq; misc alc, eth
d191	2,3-Dichloro-1-methoxybenzene	$\text{Cl}_2\text{C}_6\text{H}_3\text{OCH}_3$	177.03	6 ¹ , 102			31–33			
d192	3,5-Dichloro-1-methoxybenzene	$\text{Cl}_2\text{C}_6\text{H}_3\text{OCH}_3$	177.03	6, 190			40–42			
d193	2,4-Dichloro-6-methoxy-1,3,5-triazine		179.99				86–88	132 ^{49mm}		
d194	(Dichloromethyl)dimethylchlorosilane	$\text{Cl}_2\text{CHSi(Cl)(CH}_3)_2$	177.5		1.237 ²⁰ ₄	1.461 ²⁰	−49	149		
d195	2,2-Dichloro-1-methylcyclopropane-carboxylic acid	$\text{Cl}_2(\text{C}_3\text{H}_2)(\text{CH}_3)\text{COOH}$	169.01				60–65	85 ^{8mm}		
d196	<i>N</i> -(Dichloromethylene)aniline	$\text{C}_6\text{H}_5\text{N}=\text{CCl}_2$	174.03	12, 447	1.265	1.5710 ²⁰		106 ^{30mm}	79	
d197	Dichloromethyl ether	$\text{Cl}_2\text{CHOCH}_3$	114.96		1.271	1.4300 ²⁰		85	42	

Dichloroisopropyl alcohol, d220

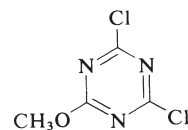
4,4'-Dichloro- α -methylbenzhydrol, b164



d173



d189



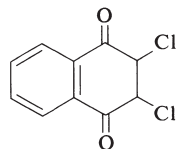
d193

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d198	Dichloro(methyl)-phenylsilane	$C_6H_5Si(CH_3)Cl_2$	191.13		1.176	1.5190 ²⁰		205	82	
d199	Dichloro(methyl)-silane	$HSi(CH_3)Cl_2$	115.04	4 ¹ , 581	1.105		−93	41	−32	
d200	Dichloro(methyl)-vinylsilane	$H_2C=CHSi(CH_3)Cl_2$	141.07		1.087 ₄ ²⁰	1.4300 ²⁰		92–93	4	
d201	2,3-Dichloro-1,4-naphthoquinone		227.05	7, 729			190–192			sl s alc, bz, eth
d202	2,6-Dichloro-4-nitroaniline	$Cl_2C_6H_2(NO_2)NH_2$	207.02	12, 735			190–192			
d203	2,3-Dichloronitrobenzene	$Cl_2C_6H_3NO_2$	192.00	5, 245	1.721 ¹⁴		61–62	257–258		s PE
d204	2,4-Dichloronitrobenzene	$Cl_2C_6H_3NO_2$	192.00	5, 245	1.439 ⁸⁰		29–32	258		s hot alc; misc eth
d205	3,4-Dichloronitrobenzene	$Cl_2C_6H_3NO_2$	192.00	5, 246	1.456 ₄ ⁷⁵		41–42	255–256	123	
d206	2,3-Dichlorooctafluorobutane	$CF_3CF(Cl)CF(Cl)CF_3$	271.0		1.6801 ²⁰	1.3100 ²⁰	−68	63		
d207	1,7-Dichlorooctamethyltetrasiloxane	$[Cl(CH_3)_2SiOSi(CH_3)_2]_2O$	351.6		1.011 ₄ ²⁰	1.403 ²⁰		222		
d208	2,3-Dichloro-4-oxo-2-butenic acid	$ClC(CHO)=C(Cl)COOH$	168.96	3, 727			125–128		100	sl s aq; s alc, hot bz
d209	1,5-Dichloropentane	$Cl(CH_2)_3Cl$	141.04	1, 131	1.1058 ₄ ¹⁵	1.4553 ²⁰	−72	63 ^{10mm}	26	i aq; s alc, eth
d210	2,3-Dichlorophenol	$Cl_2C_6H_3OH$	163.00	6 ¹ , 102			58.60	206		s alc, eth
d211	2,4-Dichlorophenol	$Cl_2C_6H_3OH$	163.00	6, 189			42–43	210	113	v s alc, bz, chl, eth
d212	2,5-Dichlorophenol	$Cl_2C_6H_3OH$	163.00	6, 189			56–58	211		v s alc, bz, eth
d213	2,6-Dichlorophenol	$Cl_2C_6H_3OH$	163.00	6, 190			65–68	218–220		v s alc, eth
d214	2,4-Dichlorophenoxyacetic acid	$Cl_2C_6H_3OCH_2COOH$	221.04				138	160 ^{0.4mm}		s alc, bz, chl, eth

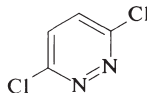
d215	2,5-Dichloro- <i>p</i> -phenylenediamine	$\text{Cl}_2\text{C}_6\text{H}_2(\text{NH}_2)_2$	177.03	13, 118			165 d			
d216	Dichlorophenylphosphine	$\text{C}_6\text{H}_5\text{PCl}_2$	178.99	16, 763	1.319	1.5980 ²⁰	−51	222	>112	
d217	4,5-Dichloro- <i>o</i> -phthalic acid	$\text{Cl}_2\text{C}_6\text{H}_2(\text{COOH})_2$	235.02	9 ¹ , 366			193–195			s aq; v s eth
d218	1,2-Dichloropropane	$\text{CH}_3\text{CH}(\text{Cl})\text{CH}_2\text{Cl}$	112.99	1, 105	1.1558 ²⁰	1.4390 ²⁰	−100.4	96.4	4	0.26 aq; misc alc, bz, chl, eth
d219	1,3-Dichlopropane	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{Cl}$	112.99	1, 105	1.878 ₄ ²⁰	1.4487 ²⁰	−99.5	120.5	32	v s alc, eth
d220	1,3-Dichloro-2-propanol	$\text{ClCH}_2\text{CH}(\text{OH})\text{CH}_2\text{Cl}$	128.99	1, 364	1.3506 ₄ ¹⁷	1.4835 ²⁰	−4	174.3	74	9.1 aq; misc alc, eth
d221	1,3-Dichloropropene	$\text{ClCH}_2\text{CH}=\text{CHCl}$	110.97	1, 199	1.217 ₄ ²⁰	1.470 ²⁰		112		i aq; s chl, eth
d222	2,3-Dichloro-1-propene	$\text{ClCH}_2\text{C}(\text{Cl})=\text{CH}_2$	110.97	1, 199	1.204 ₂₅ ²⁵	1.4611 ²⁰		94	10	misc alc; s eth
d223	3,6-Dichloropyridazine		148.98				66–69			
d224	2,6-Dichloropyridine	$\text{Cl}_2(\text{C}_5\text{H}_3\text{N})$	147.99	20, 231			86–88			
d225	4,7-Dichloroquinoline		198.05				84–86	148 ^{10mm}		
d226	Dichlorosilane	H_2SiCl_2	101.0				−122	8.3		
d227	1,2-Dichloro-1,1,2,2-tetrafluoroethane	$\text{ClCF}_2\text{CF}_2\text{Cl}$	170.93		1.470 ₄ ²⁰	1.290 ²⁰	−94	3.6		s alc, eth

1,1-Dichloro-2-propanone, d139



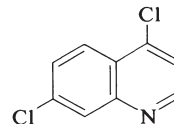
d201

4,6-Dichlororesorcinol, d171



d223

α,α -Dichlorotoluene, c59



d225

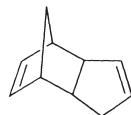
TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d228	2,5-Dichlorothio- phenene	$\text{Cl}_2(\text{C}_4\text{H}_2\text{S})$	153.03	17, 33	1.442	1.5621 ²⁰	−40.5	162		i aq; misc alc, eth
d229	2,4-Dichlorotoluene	$\text{Cl}_2\text{C}_6\text{H}_3\text{CH}_3$	161.03	5, 295	1.2460 ²⁰ ₂₀	1.5454 ²⁰	−13	200.5	79	i aq
d230	2,6-Dichlorotoluene	$\text{Cl}_2\text{C}_6\text{H}_3\text{CH}_3$	161.03	5, 296	1.254	1.5507 ²⁰		196–203	82	i aq; s chl
d231	3,4-Dichlorotoluene	$\text{Cl}_2\text{C}_6\text{H}_3\text{CH}_3$	161.03	5, 296	1.251 ²⁵ ₂₅	1.5472 ²⁰	−14	201 ^{740mm}	85	i aq
d232	2,2-Dichloro-1,1,1-trifluoroethane	CF_3CHCl_2	152.9					28		
d233	α, α' -Dichloro- <i>p</i> -xylene	$\text{C}_6\text{H}_4(\text{CH}_2\text{Cl})_2$	175.06	5, 384			100	254		22.5 acet; 20 bz; 4.5 CCl_4 ; 11 eth; 18 EtAc
d234	2,5-Dichloro- <i>p</i> -xylene	$\text{Cl}_2\text{C}_6\text{H}_2(\text{CH}_3)_2$	175.06	5, 384			71	222		27 acet; 44 bz; 39 eth 32 EtAc; 5 MeOH
d235	Dicyanodiamide	$\text{H}_2\text{NC}(=\text{NH})\text{NHCN}$	84.08	3 ² , 75	1.400 ²⁵ ₄		208–211			2.3 aq; 1.3 alc; i bz
d236	1,2-Dicyanobenzene	$\text{C}_6\text{H}_4(\text{CN})_2$	128.13	9, 815			139–141			v s bz, alc; s hot eth
d237	1,3-Dicyanobenzene	$\text{C}_6\text{H}_4(\text{CN})_2$	128.13	9, 836			158–160			s alc, bz, chl, eth
d238	1,4-Dicyanobutane	$\text{NC}(\text{CH}_2)_4\text{CN}$	108.14	2, 653	0.951	1.4380 ²⁰	1–3	295	>112	
d239	1,6-Dicyanohexane	$\text{NC}(\text{CH}_2)_6\text{CN}$	136.20	2, 694	0.954	1.4436 ²⁰	−3.5	185 ^{15mm}	>112	
d240	2,4-Dicyano-3-methylglutaramide	$\text{CH}_3\text{CH}[\text{CH}(\text{CN})-\text{CONH}_2]_2$	194.19	2 ² , 704			159–160			
d241	Dicyclohexyl	$\text{C}_6\text{H}_{11}\text{C}_6\text{H}_{11}$	166.31	5, 108	0.864	1.4782 ²⁰	3–4	227	101	7 MeOH; misc bz, acet, eth
d242	Dicyclohexylamine	$(\text{C}_6\text{H}_{11})_2\text{NH}$	181.32	12, 6	0.910	1.4842 ²⁰	−0.1	255.8	96	misc alc, bz, chl, eth
d243	<i>N, N'</i> -Dicyclohexyl-carbodiimide	$\text{C}_6\text{H}_{11}\text{N}=\text{C}=\text{NC}_6\text{H}_{11}$	206.33				34–35	122–124 ^{6mm}		
d244	Dicyclopentadiene		132.21	5, 495	0.930 ²⁵ ₄	1.5050 ²⁵	−1	170	26	s alc, eth

d245	Diethanolamine	$\text{HOCH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{OH}$	105.14	4, 283	1.088_4^{30}	1.4747^{30}	28.0	268.0	137	96 aq; 4 bz; 0.8 eth; misc MeOH, acet
d246	2,2-Diethoxyacetophenone	$\text{C}_6\text{H}_5\text{C}(=\text{O})\text{CH}(\text{OC}_2\text{H}_5)_2$	208.26	7 ¹ , 361	1.034	1.4995^{20}		131–134 ^{10mm}	110	
d247	4,4-Diethoxybutylamine	$\text{H}_2\text{N}(\text{CH}_2)_3\text{CH}(\text{OC}_2\text{H}_5)_2$	161.25	4, 319	0.933	1.4275^{20}		196	62	
d248	2,2-Diethoxy- <i>N,N</i> -dimethylethylamine	$(\text{C}_2\text{H}_5\text{O})_2\text{CHCH}_2\text{N}(\text{CH}_3)_2$	161.25	4, 308	0.883	1.4129^{20}		170	45	
d249	Diethoxydimethylsilane	$(\text{C}_2\text{H}_5\text{O})_2\text{Si}(\text{CH}_3)_2$	148.28		0.840_4^{20}	1.3811^{20}	–87	114	11	5 aq; misc alc, eth 21 aq s alc, eth
d250	Diethoxydiphenylsilane	$(\text{C}_2\text{H}_5\text{O})_2\text{Si}(\text{C}_6\text{H}_5)_2$	272.42		1.0329_4^{20}	1.5269^{20}		130 ^{2mm}		
d251	1,1-Diethoxyethane	$\text{CH}_3\text{CH}(\text{OC}_2\text{H}_5)_2$	118.18	1, 603	0.8254_4^{20}	1.3825^{20}	2.8	102.7	–21	
d252	1,2-Diethoxyethane	$\text{C}_2\text{H}_5\text{OCH}_2\text{CH}_2\text{OC}_2\text{H}_5$	118.18	1, 468	0.842	1.3922^{20}	–74	121.4	27	
d253	2,2-Diethoxyethanol	$(\text{C}_2\text{H}_5\text{O})_2\text{CHCH}_2\text{OH}$	134.18	1, 818	0.888_4^{24}	1.4160^{20}		167	67	
d254	2,2-Diethoxyethylamine	$(\text{C}_2\text{H}_5\text{O})_2\text{CHCH}_2\text{NH}_2$	133.19	4, 308	0.916	1.4170		162–163	45	
d255	Diethoxymethylsilane	$(\text{C}_2\text{H}_5\text{O})_2\text{SiH}(\text{CH}_3)$	134.3		0.829_4^{25}	1.372^{25}		94–95		
d256	Diethoxymethylvinylsilane	$(\text{C}_2\text{H}_5\text{O})_2\text{Si}(\text{CH}_3)\text{CH}=\text{CH}_2$	160.3		0.858_4^{20}	1.400^{20}		133–134		
d257	1,1-Diethoxypropane	$\text{CH}_3\text{CH}_2\text{CH}(\text{OC}_2\text{H}_5)_2$	132.20	1, 630	0.8232_4^{20}	1.3884^{20}		122.8	12	v s alc, eth
d258	3,3-Diethoxy-1-propene	$(\text{C}_2\text{H}_5\text{O})_2\text{CHCH}=\text{CH}_2$	130.19	1, 727	0.854	1.4000^{20}		89–90	4	

α ,*p*-Dichlorotoluene, c60

1,2-Dicyanoethane, b380



d244

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

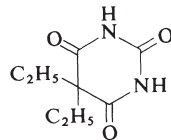
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d259	2,2-Diethoxytriethylamine	$(C_2H_5O)_2CHCH_2N-(C_2H_5)_2$	189.30	4, 309	0.850	1.4189 ²⁰		194–195	65	
d260	<i>N,N</i> -Diethylacetamide	$CH_3C(=O)N(C_2H_5)_2$	115.18	4, 110	0.925	1.4401 ²⁰		182–186	70	
d261	Diethyl acetamidomalonate	$C_2H_5OOCCH(NHCOCH_3)COOC_2H_5$	217.22	4 ² , 891			97–98	185 ^{20mm}		
d262	Diethyl 1,3-acetonedicarboxylate	$C_2H_5OOCCH_2COCH_2COOC_2H_5$	202.21	3, 791	1.113	1.4385 ²⁰		250	86	
d263	Diethyl acetylenedicarboxylate	$C_2H_5OOC \equiv CCOOC_2H_5$	170.16	2, 803	1.063	1.4426 ²⁰		107 ^{11mm}	94	
d264	Diethyl 2-acetylglutarate	$C_2H_5OOCCH_2CH_2CH(COCH_3)COOC_2H_5$	230.26		1.071	1.4386 ²⁰		154 ^{11mm}	>112	
d265	Diethyl acetylsuccinate	$C_2H_5OOCCH_2CH(COCH_3)COOC_2H_5$	216.23	3, 801	1.081	1.4346 ²⁰		180–183 ^{50mm}	>112	
d266	Diethyl allylmalonate	$C_2H_5OOCCH(CH_2CH=CH_2)COOC_2H_5$	200.23	2, 776	1.015	1.4304 ²⁰		222–223	92	
d267	Diethylamine	$(C_2H_5)_2NH$	73.14	4, 95	0.7074 ²⁰	1.3864 ²⁰	–50.0	55.5	–28	misc aq, alc
d268	Diethylamine HCl	$(C_2H_5)_2NH \cdot HCl$	109.60	4, 95	1.048 ²¹			320–330		s aq, alc, chl; i eth
d269	4-(Diethylamino)benzaldehyde	$(C_2H_5)_2NC_6H_4CHO$	177.25	14 ² , 25			39–41	174 ^{7mm}		
d270	2-Diethylaminoethanol	$(C_2H_5)_2NCH_2CH_2OH$	117.19	4, 282	0.8800 ²⁵	1.4389 ²⁵	–70	163	48	s aq, alc, bz, eth
d271	2-(Diethylamino)ethyl-4-amino benzoate	$H_2NC_6H_4COOCH_2CH_2N(C_2H_5)_2$	236.30	14, 424			61			0.5 aq; s alc, bz, eth
d272	2-Diethylaminoethyl chloride HCl	$ClCH_2CH_2N(C_2H_5)_2 \cdot HCl$	172.10	4 ² , 618			208–210			
d273	3-(Diethylamino)phenol	$(C_2H_5)_2NC_6H_4OH$	165.24	13, 408			65–69	170 ^{15mm}		s aq, alc, eth

d274	3-Diethylamino-1,2-propanediol	$(C_2H_5)_2NCH_2CH(OH)-CH_2OH$	147.22	4, 302	0.973 ₂₀ ²⁰	1.4602 ²⁰	233–235		107	s aq, alc, chl, eth
d275	1-Diethylamino-2-propanol	$(C_2H_5)_2NCH_2CH(OH)-CH_3$	131.22	4 ² , 737	0.889	1.4255 ²⁰	13.5	55–59 ^{13mm}	33	s alc
d276	4-(Diethylamino)-salicylaldehyde	$(C_2H_5)_2NC_6H_3(OH)CHO$	193.25	14, 234			62–64			
d277	<i>N,N</i> -Diethylaniline	$C_6H_5N(C_2H_5)_2$	149.24	12, 164	0.9302 ₄ ²⁵	1.5394 ²⁵	–34.4	216.3	97	1 aq; sl s alc, eth
d278	2,6-Diethylaniline	$(C_2H_5)_2C_6H_3NH_2$	149.24		0.906	1.5452 ²⁰	3	243	123	
d279	Diethyl azodicarboxylate	$C_2H_5OOCN=NCOOC_2H_5$	174.16	3, 123	1.106	1.4280 ²⁰		106 ^{13mm}	26	
d280	5,5-Diethylbarbituric acid		184.19	24 ² , 279	1.220		188–192			0.7 aq; 7 alc; 1.3 chl; 3.2 eth; s acet, HOAc
d281	Diethyl benzal-malonate	$C_6H_5CH=C(COOC_2H_5)_2$	248.28	9, 892	1.107	1.5365 ²⁰		215 ^{30mm}	>112	
d282	1,2-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.8800 ²⁰	1.5022 ²⁰	–31.3	183.4	49	s alc, eth
d283	1,3-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.8640 ₄ ²⁰	1.4950 ²⁰	–83.9	181.1	50	s alc, eth
d284	1,4-Diethylbenzene	$C_6H_4(C_2H_5)_2$	134.22	5, 426	0.8620 ₄ ²⁰	1.4940 ²⁰	–42.85	183.8	56	s alc, eth
d285	Diethyl benzyl-malonate	$C_6H_5CH_2CH(COOC_2H_5)_2$	250.29	9, 869	1.064	1.4868 ²⁰		162 ^{10mm}	>112	
d286	Diethyl bromomalonate	$BrCH(COOC_2H_5)_2$	239.07	2, 594	1.4022 ₄ ²⁵	1.4550 ²⁰	–54	233–235 d		i aq; misc alc, eth

Diethyl acetal, d251
Diethylacetic acid, e89

Diethyl 2-acetylpentanedioate, d264
Diethylaminoacetaldehyde diethyl acetal, d259

3-Diethylaminopropylamine, d330
Diethyl (Z)-2-butenedioate, d316



d280

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d287	Diethyl butylmalonate	$C_4H_9CH(COOC_2H_5)_2$	216.28	2 ¹ , 282	0.983	1.4220		235–240	93	v s alc, eth
d288	Diethylcarbamoyl chloride	$(C_2H_5)_2NCOCI$	135.59	4, 120		1.4515 ²⁰		187–190	75	d hot aq, hot alc
d289	Diethyl carbonate	$(C_2H_5O)_2C=O$	118.13	3, 5	0.9764 ²⁰ ₄	1.3843 ²⁰	–43.0	126.8	25	69 aq; misc alc, bz, eth, esters
d290	Diethyl chloromalonate	$ClCH(COOC_2H_5)_2$	194.61	2 ² , 537	1.2040 ²⁰ ₄	1.4310 ²⁰		222–223		misc alc, chl, eth
d291	Diethyl chlorophosphate	$(C_2H_5O)_2P(O)Cl$	172.55	1, 332	1.194	1.4165 ²⁰		60 ^{2mm}		
d292	Diethyl chlorothiophosphate	$(C_2H_5O)_2P(S)Cl$	188.61		1.200	1.4715 ²⁰		45 ^{3mm}		
d293	Diethylcyanamide	$(C_2H_5)_2NCN$	98.15	4, 121	0.846	1.4229 ²⁰		186–188	69	
d293a	Diethyl cyanomethylphosphonate	$(C_2H_5O)_2P(O)CH_2CN$	177.14		1.095	1.4312 ²⁰		101 ^{0.4mm}	>112	
d294	<i>N,N</i> -Diethylcyclohexylamine	$C_6H_{11}N(C_2H_5)_2$	155.29	12, 6	0.850	1.4562 ²⁰		194–195	57	
d294a	Diethyl disulfide	$C_2H_5SSC_2H_5$	122.25	1, 347	0.998 ²⁰ ₄	1.5063 ²⁰	–101.5	154.0		sl s aq; misc alc, eth
d295	Diethyldithiocarbamic acid, Na salt	$(C_2H_5)_2NC(=S)S^-Na^+ \cdot 3H_2O$	225.31	4 ² , 613			95–99			
d296	Diethyl dithiophosphate	$(C_2H_5O)_2P(S)SH$	186.23	1, 333	1.111	1.5120 ²⁰		60 ^{1mm}		
d297	<i>N,N</i> -Diethyldodecanamide	$CH_3(CH_2)_{10}C(O)N(C_2H_5)_2$	255.45		0.847	1.4545 ²⁰		166 ^{2mm}	>112	
d298	Diethylenetriamine	$(H_2NCH_2CH_2)_2NH$	103.17	4, 255	0.9542 ²⁰ ₂₀	1.4826 ²⁰	–35	207.1	101	misc aq, alc, bz, eth

d299	Diethylenetriamine-pentaacetic acid	$[(\text{HOOCCH}_2)_2\text{NCH}_2\text{-CH}_2]_2\text{NCH}_2\text{COOH}$	393.35				220 d			
d300	Diethyl ether	$\text{C}_2\text{H}_5\text{OC}_2\text{H}_5$	74.12	1, 314	0.7134 ²⁰	1.3527 ²⁰	−116.3	34.6	−40	6 aq; misc alc, bz, chl
d301	Diethyl ethoxymethyl-enemalonate	$(\text{C}_2\text{H}_5\text{OOC})_2\text{C}=\text{CH-OC}_2\text{H}_5$	216.23	3, 469	1.070	1.4620 ²⁰		279–281	155	
d302	<i>N,N</i> -Diethylethyl-enediamine	$(\text{C}_2\text{H}_5)_2\text{NCH}_2\text{CH}_2\text{NH}_2$	116.21	4,251	0.827	1.4360 ²⁰		145–147	30	
d303	Diethyl ethyl-malonate	$\text{C}_2\text{H}_5\text{CH}(\text{COOC}_2\text{H}_5)_2$	188.2	2,644	1.004 ²⁰ ₂₀	1.4158 ²⁰		75–77 ^{5mm}	88	sl s aq; v s alc, eth
d304	<i>N,N</i> -Diethyl-formamide	$(\text{C}_2\text{H}_5)_2\text{NCHO}$	101.15	4, 109	0.908	1.4340 ²⁰		176–177	60	misc aq; v s alc, eth
d305	Diethyl fumarate	$\text{C}_2\text{H}_5\text{OOCCH}=\text{CH-COOC}_2\text{H}_5$	172.18	2,742	1.052 ²⁰ ₄	1.4406 ²⁰	1–2	218–219	91	
d306	Diethyl 3,4-furandi-carboxylate	$(\text{C}_2\text{H}_5\text{OOC})_2\text{C}_4\text{H}_2\text{O}$	212.20		1.140	1.4717 ²⁰		155 ^{13mm}	82	
d307	Diethyl glutarate	$\text{C}_2\text{H}_5\text{OOCCH}_2\text{CH}_2\text{CH}_2\text{-COOC}_2\text{H}_5$	188.22	2, 633	1.022	1.4240 ²⁰	−23.8	237	96	0.9 aq; v s alc; s eth
d308	2,4-Diethyl-2,6-heptadienal	$\text{H}_2\text{C}=\text{CHCH}_2\text{CH}(\text{C}_2\text{H}_5)\text{-CH}=\text{C}(\text{C}_2\text{H}_5)\text{CHO}$	166.27					91 ^{12mm}		
d309	Diethyl heptane-dioate	$\text{C}_2\text{H}_5\text{OOC}(\text{CH}_2)_5\text{-COOC}_2\text{H}_5$	216.28	2, 671	0.9945 ²⁰	1.4280 ²⁰	−24	192 ^{100mm}	>112	i aq; s alc, eth
d310	2,4-Diethyl-1-heptanol	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{C}_2\text{H}_5)\text{-CH}_2\text{CH}(\text{C}_2\text{H}_5)\text{CH}_2\text{OH}$	172.31					109 ^{12mm}		

Diethyl carbitol, b176
Diethylene dioxide, d646
Diethylene glycol, b181
Diethylene glycol dibutyl ether, b151
Diethylene glycol diethyl ether, b176
Diethylene glycol dimethyl ether, b191

Diethylene glycol monobutyl ether, b411
Diethylene glycol monoethyl ether, e35
Diethylene glycol monoethyl ether acetate, e36
Diethylene glycol monomethyl ether, m66
Diethyleneimine oxide, m448

Diethyl ethoxycarbonylmethylphosphonate, t283
N,N-Diethylethanamine, t264
N,N-Diethylethanolamine, d270
Di-2-ethylhexyl adipate, d312
Di-2-ethylhexyl sebacate, d311

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d311	Di-(2-ethylhexyl) decanedioate	$C_4H_9CH(C_2H_5)CH_2OOC-(CH_2)_8COOCH_2CH-(C_2H_5)C_4H_9$	426.68		0.912 ₄ ²⁵	1.451 ²⁵		256 ^{5mm}	227	i aq; s alc, bz, acet
d312	Di-(2-ethylhexyl) hexanedioate	$C_4H_9CH(C_2H_5)CH_2OOC-(CH_2)_4COOCH_2CH-(C_2H_5)C_4H_9$	370.57		0.925 ₂₅ ²⁵	1.4474 ²⁰		214 ^{5mm}	193	s alc, eth, acet; i aq
d313	Di-(2-ethylhexyl) <i>o</i> -phthalate	$C_6H_4[COOCH_2CH-(C_2H_5)C_4H_9]$	390.56		0.981 ₂₅ ²⁵	1.4853 ²⁰	−50	384	207	
d314	Diethyl hydrogen phosphonate	$(C_2H_5O)_2P(O)H$	138.10	1, 330	1.079 ₄ ²⁰	1.4076 ²⁰		50–51 ^{2mm}	90	s aq (hyd), alc, eth
d315	<i>N,N</i> -Diethylhydroxylamine	$(C_2H_5)_2NOH$	89.14	4, 536	1.867	1.4195 ²⁰	−25	125–130	45	
d316	Diethyl maleate	$C_2H_5OOCCH=CH-COOC_2H_5$	172.18	2, 751	1.0687 ²⁰	1.4400 ²⁰	−8.8	225.3	93	1.4 aq; s alc, eth
d317	Diethyl malonate	$C_2H_5OOCCH_2COOC_2H_5$	160.17	2, 573	1.0550	1.4136 ²⁰	−48.9	199.3	100	2.7 aq; misc alc, eth
d318	Diethylmalonic acid	$HOOC(C_2H_5)_2COOH$	160.17	2, 686			127	d 170–180		v s aq, alc, eth
d319	<i>N,N</i> -Diethyl-3-methylbenzamide	$CH_3C_6H_4C(=O)N-(C_2H_5)_2$	191.27	9 ² , 325	0.996 ₄ ²⁰	1.5212 ²⁰		111 ^{1mm}		s aq; v s alc, bz, eth
d320	Diethyl methylmalonate	$C_2H_5OOCCH(CH_3)-COOC_2H_5$	174.20	2, 629	1.018 ₄ ²⁰	1.4130 ²⁰		198	76	sl s aq; v s alc, eth
d321	Diethyl 2-methyl-2'-oxosuccinate	$C_2H_5OOCCH(CH_3)-C(=O)C(=O)OC_2H_5$	202.21	3, 794	1.073	1.4313 ²⁰		138 ^{23mm}	>112	
d322	Diethyl methylsuccinate	$C_2H_5OOCCH_2CH(CH_3)-COOC_2H_5$	188.22	2, 639	1.012	1.4199 ²⁰		217–218		
d323	<i>N,N</i> -Diethyl-4-nitrosoaniline	$C_6H_4(NO)N(C_2H_5)_2$	178.24	12, 684			82–84			
d324	Diethyl octanedioate	$C_2H_5OOC(CH_2)_6-COOC_2H_5$	230.30	2, 693	0.9822 ₄ ²⁰	1.4323 ²⁰	5.9	282	>112	i aq; s alc, eth

d325	Diethyl oxalate	$C_2H_5OOC COOC_2H_5$	146.14	2, 535	1.0785 ₄ ²⁰	1.4102	−40.6	185.4	75	3.6aq (gradual d); misc alc, eth
d326	Diethyl oxydiformate	$[C_2H_5OC(=O)]_2O$	162.14		1.12 ₄ ²⁰	1.3980 ²⁰		93 ^{18mm}	69	s alc, esters, ketones
d327	<i>N</i> ¹ , <i>N</i> ¹ -Diethyl-1,4-pentanediamine	$CH_3CH(NH_2)(CH_2)_3-N(C_2H_5)_2$	158.29		0.817	1.4429 ²⁰		200 ^{753mm}	68	s aq, alc, eth
d328	Diethyl phenyl-malonate	$C_6H_5CH(COOC_2H_5)_2$	236.27	9, 854	1.0950 ₄ ²⁰	1.4913 ²⁰	16	170 ^{14mm}	>112	i aq; s alc
d329	Diethyl o-phthalate	$C_6H_4(COOC_2H_5)_2$	222.24	9, 798	1.232 ₄ ¹⁴	1.5049 ¹⁴	−3	295	140	i aq; misc alc, eth
d330	<i>N,N</i> -Diethyl-1,3-propanediamine	$(C_2H_5)_2NCH_2CH_2-CH_2NH_2$	130.24		0.826	1.4416 ²⁰		159	58	
d331	2,2-Diethyl-1,3-propanediol	$(C_2H_5)_2C(CH_2OH)_2$	132.20		1.052 ²⁰	1.4574 ²⁵	61.3	125 ^{10mm}		25 aq; v s alc, eth
d332	Diethyl propyl-malonate	$C_2H_5OOCCH(C_2H_7)-COOC_2H_5$	202.25	2, 657	0.987	1.4185 ²⁰		221–222	91	
d333	1,1-Diethyl-2-propynylamine	$HC\equiv CC(C_2H_5)_2NH_2$	111.19		0.828	1.4409 ²⁰		71 ^{90mm}	21	
d334	<i>N,N</i> -Diethyl-3-pyridine-carboxamide	$C_5H_4N-C(=O)N-(C_2H_5)_2$	178.24	22 ² , 34	1.060 ₄ ²⁵	1.5240 ²⁰	24–26	296–300	>112	
d335	Diethyl succinate	$C_2H_5OOCCH_2CH_2-COOC_2H_5$	174.20	2, 609	1.040 ₄ ²⁰	1.4200 ²⁰	−21	217.7	110	i aq; misc alc, eth
d336	Diethyl sulfate	$(C_2H_5O)_2SO_2$	154.18	1, 327	1.172 ₄ ²⁵	1.4004 ²⁰	−25	209 d	78	misc alc, eth
d337	Diethyl sulfide	$(C_2H_5)_2S$	90.19	1, 344	0.8367 ₄ ²⁰	1.4430 ²⁰	−103.9	92.1	−9	i aq; misc alc, eth
d338	Diethyl sulfite	$(C_2H_5O)_2S(O)$	138.19	1, 325	1.077 ₄ ²⁵			157.7		s aq(d), alc

Diethyl ketone, p42
N,N-Diethylnicotinamide, d334
O,O-Diethyl *O-p*-nitrophenyl
phosphorothioate, p3
Diethyl 3-oxoglutarate, d262

Diethyl 2-pentenedioate, d307
Diethyl phosphite, d314
Diethyl phosphorochloridate, d291
Diethyl phosphorochloridothionate, d292
Diethyl pimelate, d309

Diethyl propanedioate, d317
1,1-Diethylpropargylamine, d333
Diethyl pyrocarbonate, d326
Diethyl suberate, d324

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d339	(+)-Diethyl-L-tartrate	[—CH(OH)COOC ₂ H ₅] ₂	206.19	3, 512	1.204 ₄ ²⁰	1.4459 ²⁰	17	280	93	sl s aq; misc alc, eth
d340	(-)-Diethyl-D-tartrate	[—CH(OH)COOC ₂ H ₅] ₂	206.19	3 ¹ , 181	1.205	1.4467 ²⁰		162 ^{19mm}	93	
d341	Diethyl 3,3'-thio-propionate	S(CH ₂ CH ₂ COOC ₂ H ₅) ₂	234.32		1.095	1.4655 ²⁰		121 ^{2mm}		
d342	<i>N,N</i> -Diethyl- <i>m</i> -toluamide	CH ₃ C ₆ H ₄ C(=O)N-(C ₂ H ₅) ₂	191.27	9 ² , 325	0.996	1.5212 ²⁰		111 ^{1mm}		
d343	<i>N,N</i> -Diethyl-1,1,1-trimethylsilyl-amine	(C ₂ H ₅) ₂ NSi(CH ₃) ₃	145.32		0.767	1.4081 ²⁰		125–126	10	
d344	Diethylzinc	(C ₂ H ₅) ₂ Zn	123.49		1.2065 ²⁰		–28	118		
d345	1,4-Difluorobenzene	C ₆ H ₄ F ₂	114.09	5, 199	1.1701 ²⁰	1.4415 ²⁰	–23.7	88.9	2	
d346	1,1-Difluoroethane	CH ₃ CHF ₂	66.05		0.909 ²¹		–117	–24.7		0.32 aq
d347	1,1-Difluorotetra-chloroethane	Cl ₃ CCClF ₂	203.83	1, 86	1.649	1.413	41	91	none	sl s alc; v s eth
d348	1,2-Difluorotetra-chloroethane	FCI ₂ CCCl ₂ F	203.83	1 ³ , 365	1.6447 ₄ ²⁵	1.413 ²⁵	23.8	203.8		i aq; s alc, eth
d349	Dihexylamine	(C ₆ H ₁₃) ₂ NH	185.36	4 ¹ , 384	0.795	1.4320 ²⁰		192–195	95	s alc, eth
d350	Dihexyl ether	(C ₆ H ₁₃) ₂ O	186.34	1 ³ , 1656	0.7936 ₄ ²⁰	1.4204 ²⁰		226.2	77	i aq; s eth
d351	9,10-Dihydro-anthracene		180.25	5, 641	0.880		108–110	312		i aq; s alc, bz, eth
d352	(+)-Dihydrocarvone		152.24	7 ³ , 337	0.929 ¹⁹	1.4718 ²⁰		221–222	81	
d353	Dihydrocoumarin		148.16	17, 315	1.169 ¹⁸	1.5563 ²⁰	25	272		sl s alc, eth; s chl
d354	10,11-Dihydro-5 <i>H</i> -dibenzo- <i>[a,d]</i> cyclo-hepten-5-one		208.26		1.156	1.6332 ²⁰	32–34	148 ^{0.3mm}	>112	
d355	3,4-Dihydro-2-ethoxy-2 <i>H</i> -pyran		128.17		0.957	1.4394 ²⁰		42 ^{16mm}	24	

d356	2,3-Dihydrofuran		70.09	17 ³ , 141	0.927	1.4239 ²⁰		54–55	<1
d357	Dihydrolinalool	(CH ₃) ₂ C=CHCH ₂ CH ₂ - C(OH)(CH ₃)CH ₂ CH ₃	156.27		0.925 ²⁵	1.433 ²⁰			178
d358	3,4-Dihydro-1(2 <i>H</i>)- 6-methoxynaphtha- lenone		176.22	9 ² , 889			80	171 ^{11mm}	
d359	3,4-Dihydro-2- methoxy-2 <i>H</i> -pyran		114.14			1.4425 ²⁰			16
d360	2,3-Dihydro-2- methylbenzofuran		134.18	17 ¹ , 23	1.061	1.5308 ²⁰		197–198	62
d361	5,6-Dihydro-4- methyl-2 <i>H</i> -pyran		98.15	17 ³ , 160	0.912	1.4495 ²⁰		117–118	21

Diglycine, i10

Diglycol, b181

Diglycolic acid, o61

Diglyme, b191

Dihydroanisoles, m61, m62

6,7-Dihydro-5*H*-cyclopenta[*b*]pyridine, c360

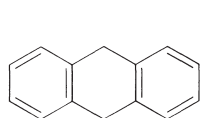
10,11-Dihydro-5*H*-dibenz[*b,f*]acepine, i12

2,5-Dihydro-2,5-dimethoxyfuran, d436

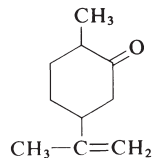
3,7-Dihydro-3,7-dimethyl-1*H*-pyridine-2,6-
dione, t138

2,3-Dihydroindene, i13

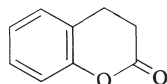
Dihydromyrcenol, m303



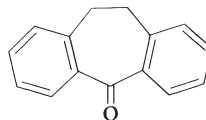
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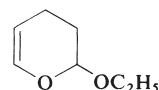
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d353



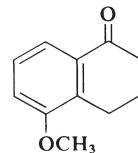
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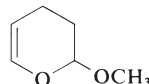
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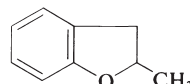
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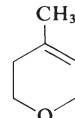
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d359



d360

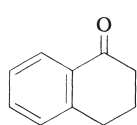


d361

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d362	3,4-Dihydro-1(2 <i>H</i>)-naphthalenone	$(\text{HO})_2\text{C}_6\text{H}_3\text{C}(=\text{O})\text{CH}_3$	146.19	7, 370	1.099	1.5685 ²⁰	5–6	116 ^{6mm}	>112	s aq, alc
d363	Dihdropyran		84.12		0.922 ¹⁹ ₁₅	1.4410 ²⁰	–70	86	–15	
d364	5,6-Dihydro-2 <i>H</i> -pyran-3-carbaldehyde		112.13		1.100	1.4980 ²⁰		78 ^{12mm}	77	
d365	3,4-Dihydro-2 <i>H</i> -pyran-2-carboxylic acid, Na salt		150.11				242–244			
d366	Dihydroterpineol		256.27		0.907 ²⁵	1.4670 ²⁰			88	s aq, alc, bz, chl, eth
d367	5,6-Dihydro-2,4,4,6-tetramethyl-4 <i>H</i> -1,3-oxazine		141.21		0.886	1.4410 ²⁰		48 ^{17mm}		
d368	2,5-Dihydrothiophene-1,1-dioxide		118.15				64–66		>112	
d369	1,2-Dihydro-2,2,4-trimethylquinoline		173.26		0.934	1.5895 ²⁰		90 ^{0.02mm}	101	
d370	2',4',-Dihydroxyacetophenone		152.15	8, 266	1.180		145–147			s warm alc, pyr, HOAc; i bz, chl, eth
d371	1,2-Dihydroxyanthraquinone		240.21	8, 439			287–289	430		s alc, bz, chl, HOAc
d372	1,4-Dihydroxyanthraquinone		240.21	8, 450			196			s alc, alk, eth
d373	1,8-Dihydroxyanthraquinone		240.21	8, 458			193–197	subl		0.005 alc; 0.2 eth; s chl
d374	2,6-Dihydroxyanthraquinone		240.21	8, 463			360 d			sl s aq, alc
d375	2,4-Dihydroxybenzaldehyde		138.12	8, 241			135–136	226 ^{22mm}		v s aq, alc, chl, eth

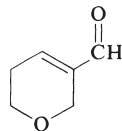
d376	3,4-Dihydroxybenzaldehyde	$(\text{HO})_2\text{C}_6\text{H}_3\text{CHO}$	138.12	8, 246		153			5 aq; 79 hot alc; v s eth
d377	1,2-Dihydroxybenzene	$\text{C}_6\text{H}_4(\text{OH})_2$	110.11	6, 759	1.344 ⁴	104–106	245.5	137	43 aq; s alc, bz, chl, eth; v s pyr, alk
d378	1,3-Dihydroxybenzene	$\text{C}_6\text{H}_4(\text{OH})_2$	110.11	6 ² , 802	1.272 ¹⁵	109–110	276	171	110 aq; 110 alc; v s eth, glyc; sl s chl
d379	1,4-Dihydroxybenzene	$\text{C}_6\text{H}_4(\text{OH})_2$	110.11	6, 836	1.332 ¹⁵	170–171	285–287		7 aq; v s alc, eth
4,5-Dihydro-2-(phenylmethyl)-1H-imidazole, b102			3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione, c1			2,2'-Dihydroxy-2,2'-biindan-1,2',3,3'-tetrone, h85			
Dihydroresorcinol, c322			1,3-Dihydroxyacetone, d397						



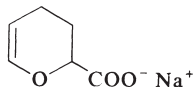
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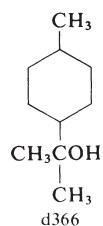
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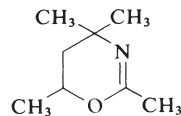
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d365



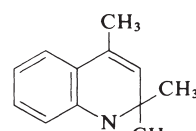
d366



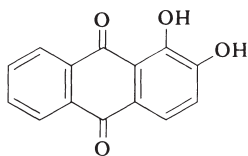
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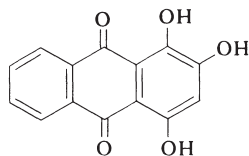
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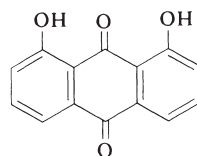
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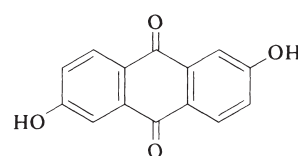
d371



d372



d373



d374

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d380	1,3-Dihydroxybenzene monoacetate	$\text{HOC}_6\text{H}_4\text{OOCCH}_3$	152.15	6, 816		1.5350 ²⁰		283	>112	
d381	2,5-Dihydroxy-p-benzenedisulfonic acid, K salt	$(\text{HO})_2\text{C}_6\text{H}_2(\text{SO}_3^-\text{K}^+)_2$	346.43	11, 300			>300			v s aq
d382	2,5-Dihydroxy-benzenesulfonic acid, K salt	$(\text{HO})_2\text{C}_6\text{H}_3\text{SO}_3^-\text{K}^+$	228.27	11, 300			251 d			v s aq
d383	2,4-Dihydroxybenzoic acid	$(\text{HO})_2\text{C}_6\text{H}_3\text{COOH}$	154.12	10, 377			213			s hot aq, alc, eth
d384	2,5-Dihydroxybenzoic acid	$(\text{HO})_2\text{C}_6\text{H}_3\text{COOH}$	154.12	10, 384			199–200			0.5 aq; s alc, eth
d385	3,5-Dihydroxybenzoic acid	$(\text{HO})_2\text{C}_6\text{H}_3\text{COOH}$	154.12	10, 404			236 d			sl s aq; s alc, eth
d386	2,4-Dihydroxybenzophenone	$(\text{HO})_2\text{C}_6\text{H}_3\text{C}(=\text{O})\text{C}_6\text{H}_5$	214.22	8, 312			144–145			v s alc, eth, HOAc
d387	2,2'-Dihydroxybiphenyl	$\text{HOC}_6\text{H}_4\text{C}_6\text{H}_4\text{OH}$	186.21	6, 989			110	315		s alc, bz, eth; sl s aq
d388	4,6-Dihydroxy-2-mercaptopyrimidine		144.15	24, 476			236			
d389	1,2-Dihydroxy-4-methylbenzene	$(\text{HO})_2\text{C}_6\text{H}_3\text{CH}_3$	124.14	6, 878	1.129 ⁷⁴ ₄	1.5425 ⁷⁴	67–69	251		v s aq, alc, eth
d390	1,3-Dihydroxy-2-methylbenzene	$(\text{HO})_2\text{C}_6\text{H}_3\text{CH}_3$	124.14	6, 878			115–118	264		s aq, alc, bz, eth
d391	2,4-Dihydroxy-6-methylpyrimidine		126.12	24, 342			318 d			
d392	1,5-Dihydroxynaphthalene	$\text{C}_{10}\text{H}_6(\text{OH})_2$	160.17	6, 980			259 d			sl s aq; s alc; v s eth

d393	1,7-Dihydroxynaphthalene	$C_{10}H_6(OH)_2$	160.17	6, 981			177–180		v s alc, eth
d394	2,3-Dihydroxynaphthalene	$C_{10}H_6(OH)_2$	160.17	6, 982			162–164		v s alc, eth
d395	2,7-Dihydroxynaphthalene	$C_{10}H_6(OH)_2$	160.17	6, 985			187 d		sl s aq; v s alc, eth
d396	4,5-Dihydroxynaphthalene-2,7-disulfonic acid	$(HO)_2C_{10}H_4(SO_3H)_2$	296.26	11, 307					v s aq; i alc, eth
d397	1,3-Dihydroxy-2-propanone	$HOCH_2C(=O)CH_2OH$	90.08	1, 846			65–71		v s aq, alc, acet, eth
d398	2,3-Dihydroxypropionaldehyde	$HOCH_2CHOCHO$	90.08	1, 845	1.455^{18}_{18}		145	$140^{0.8mm}$	3 aq; i bz, PE
d399	7-(2,3-Dihydroxypropyl)theophylline		254.25				158		33 aq; 2 alc; 1 chl
d400	3,6-Dihydroxypyridazine		112.09	24, 312			d 260		sl s hot alc; s hot aq
d401	2,3-Dihydroxypyridine	$(HO)_2C_5H_3N$	111.10	21 ² , 107			245 d		

2,2'-Dihydroxydiethylamine, d245

N,N-Di(hydroxyethyl)aminoacetic acid, b182

2,2-Dihydroxy-1,3-indandione, i16

2,2-Dihydroxymethyl-1-butanol, e156

1,8-Dihydroxynaphthalene-3,6-disulfonic acid, d396

Dihydroxypropanes, p194, p195

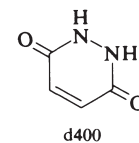
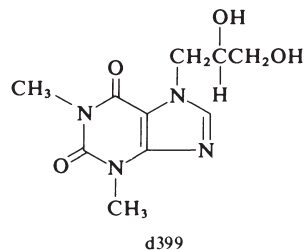
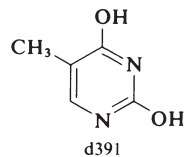
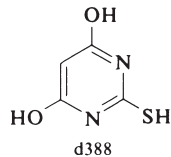


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

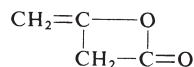
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d402	1,4-Diiodobenzene	$C_6H_4I_2$	329.91	5, 227			131–133	285		sl s alc; v s eth
d403	1,2-Diiodoethane	ICH_2CH_2I	281.86	1, 99	2.132 ¹⁰		81	200		sl s aq; s alc, eth
d404	Diiodomethane	CH_2I_2	267.84	1, 71	3.325 ²⁰ ₄	1.7411 ²⁰	5.6	181		0.12 aq; misc alc, bz, eth, PE
d405	1,3-Diiodopropane	$ICH_2CH_2CH_2I$	295.88	1, 115	2.5755 ²⁰ ₄	1.6423 ²⁰	–13	222		i aq; s chl, eth
d406	Diisobutylamine	$[(CH_3)_2CHCH_2]_2NH$	129.25	4, 166	0.740	1.4081 ²⁰	–77	137–139	29	s alc, acet, eth, EtAc
d407	Diisobutyl ether	$[(CH_3)_2CHCH_2]_2O$	130.22		0.761 ¹⁵			122–124		i aq; misc alc, eth
d408	Diisobutyl hexanedioate	$[(CH_3)_2CHCH_2OOC-CH_2CH_2-]_2$	258.36		0.950 ²⁵ ₂₅				160	
d409	Diisobutyl- <i>o</i> -phthalate	$C_6H_4[COOCH_2CH(CH_3)_2]_2$	278.35		1.038 ²⁵ ₂₅				174	
d410	1,6-Diisocyanato-hexane	$OCN(CH_2)_6NCO$	168.20	4 ² , 711	1.040	1.4525 ²⁰		255	140	
d411	Diisopropylamine	$[(CH_3)_2CH]_2NH$	101.19	4, 154	0.7169 ²⁰	1.3924 ²⁰	–96.3	83.5	–6	11 aq
d412	2-(Diisopropylamino)-ethanol	$[(CH_3)_2CH]_2NCH_2CH_2OH$	145.25	4 ¹ , 430	0.826	1.4417 ²⁰		187–192	57	
d413	2,6-Diisopropylaniline	$[(CH_3)_2CH]_2C_6H_3NH_2$	177.29	12, 168	0.940	1.5332 ²⁰	–45	257	123	
d414	1,3-Diisopropylbenzene	$C_6H_4[CH(CH_3)_2]_2$	162.28	5, 447	0.856 ²⁰ ₄	1.4980 ²⁰	–63	203	76	misc alc, bz, eth, acet
d415	1,4-Diisopropylbenzene	$C_6H_4[CH(CH_3)_2]_2$	162.28	5 ² , 339	0.857 ²⁰ ₄	1.4889 ²⁰		203	76	misc alc, bz, eth, acet
d416	Diisopropylcyanamide	$[(CH_3)_2CH]_2NCN$	126.20	4 ³ , 279	0.839	1.4270 ²⁰		93 ^{25mm}	78	
d417	Diisopropyl ether	$[(CH_3)_2CH]_2O$	102.17	1, 362	0.7258 ²⁰ ₄	1.3689 ²⁰	–86.9	68.4	–12	1.2 aq; misc alc, bz, chl, eth
d418	<i>N,N</i> -Diisopropylethylamine	$[(CH_3)_2CH]_2NC_2H_5$	129.25		0.742	1.4133 ²⁰		127	10	

d419	2,6-Diisopropyl-phenol	$[(\text{CH}_3)_2\text{CH}]_2\text{C}_6\text{H}_3\text{OH}$	178.28	6 ¹ , 272	0.962	1.5140 ²⁰	18	256	>112	
d420	Diisopropyl phosphite	$[(\text{CH}_3)_2\text{CHO}]_2\text{P}(\text{O})\text{H}$	166.16	1, 363	0.997	1.4070 ²⁰		72–75 ^{10mm}	>112	
d421	(+)-Diisopropyl L-tartrate	$[\text{—CH}(\text{OH})\text{COOCH}(\text{CH}_3)_2]$	234.25	3, 517	1.114	1.4387 ²⁰		152 ^{12mm}	109	
d422	Diketene		84.07		1.073	1.4330 ²⁰		127	33	
d423	Dilauryl phosphite	$[\text{CH}_3(\text{CH}_2)_{11}\text{O}]_2\text{P}(\text{O})\text{H}$	418.64		0.946	1.4520 ²⁰			>112	
d424	<i>threo</i> -1,4-Dimercapto-2,3-butanediol	$\text{HSCH}_2\text{CH}(\text{OH})\text{CH}(\text{OH})\text{—CH}_2\text{SH}$	154.25				42–43			v s aq, alc, chl, eth
d425	2,3-Dimercapto-1-propanol	$\text{HSCH}_2\text{CH}(\text{SH})\text{CH}_2\text{OH}$	124.22		1.2385 ²⁵ ₄	1.5720 ²⁵		120 ^{15mm}	>112	8 aq(d); s alc, eth
d426	3',4'-Dimethoxyacetophenone	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{COCH}_3$	180.20	8 ² , 298			49–51	286–288		sl s aq, alc, eth
d427	2,4-Dimethoxyaniline	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{NH}_2$	153.18	13, 784			34–37			s alc, bz, eth
d428	2,5-Dimethoxyaniline	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{NH}_2$	153.18	13, 788			80–82	270 sl d		s aq, alc
d429	3,4-Dimethoxyaniline	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{NH}_2$	153.18	13, 780			88	176 ^{22mm}		s hot eth
d430	3,4-Dimethoxybenzaldehyde	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{CHO}$	166.18	8, 255			42–43	281		v s alc, eth
d431	1,2-Dimethoxybenzene	$\text{C}_6\text{H}_4(\text{OCH}_3)_2$	138.17	6, 771	1.0819 ²⁵	1.5232 ²⁵	22.5	206.3	87	sl s aq; s alc, eth
d432	1,3-Dimethoxybenzene	$\text{C}_6\text{H}_4(\text{OCH}_3)_2$	138.17	6, 813	1.055	1.5240	–55	85–87 ^{7mm}	87	s alc, bz, eth; sl s aq
d433	1,4-Dimethoxybenzene	$\text{C}_6\text{H}_4(\text{OCH}_3)_2$	138.17	6, 843	1.036 ⁶⁸ ₄		55–60	213		s alc; v s bz, eth

Dihydroxytoluene, d390
3, 5-Diiodosalicylic acid, h111
2Diisobutyl adipate, d408

Diisobutylene, t357
Diisobutyl ketone, d531
Diisopropyl ketone, d578

Diisopropylmethane, d572
Dimedone, d508
1, 1-Dimethoxytrimethylamine, d523



d422

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d434	3,4-Dimethoxybenzoic acid	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{COOH}$	182.18	10 ¹ , 188			180–181			0.047 aq; v s alc, eth
d435	1,1-Dimethoxy-3-butanone	$(\text{CH}_3\text{O})_2\text{CHCH}_2\text{COCH}_3$	132.16		0.993	1.4150 ²⁰			49	
d436	2,5-Dimethoxy-2,5-dihydrofuran		130.14		1.073	1.4339 ²⁰		160–162	47	
d437	Dimethoxydiphenylsilane	$(\text{C}_6\text{H}_5)_2\text{Si}(\text{OCH}_3)_2$	244.4		1.0771 ²⁰ ₄	1.5447 ²⁰		161 ^{15mm}		
d438	1,1-Dimethoxyethane	$\text{CH}_3\text{CH}(\text{OCH}_3)_2$	90.12	1, 603	0.8502 ²⁰		–113	64.5		s aq, alc, chl, eth
d439	1,2-Dimethoxyethane	$\text{CH}_3\text{OCH}_2\text{CH}_2\text{OCH}_3$	90.12	1, 467	0.8629 ²⁰ ₄	1.3796 ²⁰	–68	85.2	1	misc aq, alc; s PE
d440	(2,2-Dimethoxy)-ethylamine	$\text{H}_2\text{NCH}_2\text{CH}(\text{OCH}_3)_2$	105.14	4 ² , 758	0.965	1.4170 ²⁰		135 ^{95mm}	53	
d441	Dimethoxymethane	$\text{CH}_2(\text{OCH}_3)_2$	76.10	1, 574	0.8601 ²⁰ ₂₀	1.3534 ²⁰	–104.8	42.3	–17	32 aq
d442	1,1-Dimethoxy-2-methylaminoethane	$\text{CH}_3\text{NHCH}_2\text{CH}(\text{OCH}_3)_2$	119.16	4 ² , 759	0.928	1.4115 ²⁰		140	29	
d443	Dimethoxymethylphenylsilane	$(\text{CH}_3\text{O})_2\text{Si}(\text{CH}_3)\text{C}_6\text{H}_5$	182.3		0.993 ²⁰ ₄	1.469 ²⁰		199–200		
d444	1,2-Dimethoxy-4-nitrobenzene	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{NO}_2$	183.16	6, 789	1.1888 ¹³³ ₄		95–98	230 ^{17mm}		v s alc, eth; s chl
d445	2,5-Dimethoxy-4'-nitrostilbene	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{CH}=\text{CH}-\text{C}_6\text{H}_4\text{NO}_2$	285.30	6 ² , 987			117–119			
d446	2,6-Dimethoxyphenol	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{OH}$	154.17	6, 1081			53–56	261		s alc, alk; v s eth
d447	(3,4-Dimethoxy)-phenylacetic acid	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{CH}_2\text{COOH}$	196.20	10, 409			96–98			s aq; v s alc, eth
d448	(3,4-Dimethoxy)-phenylacetonitrile	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{CH}_2\text{CN}$	177.20	10 ¹ , 198			62–63	171–178 ^{10mm}		
d449	2,2-Dimethoxy-2-phenylacetophenone	$\text{C}_6\text{H}_5\text{C}(\text{O})\text{C}(\text{OCH}_3)_2-\text{C}_6\text{H}_5$	256.30				67–70			

d450	1,1-Dimethoxy-2-phenylethane	$C_6H_5CH_2CH(OCH_3)_2$	166.22	7, 293	1.004	1.4950 ²⁰		221	83	
d451	β -(3,4-Dimethoxy)-phenylethylamine	$(CH_3O)_2C_6H_3CH_2CH_2NH_2$	181.24	13, 800	1.074	1.5464 ²⁰		188 ^{15mm}		
d452	2,2-Dimethoxy-propane	$(CH_3)_2C(OCH_3)_2$	104.15	1, 648	0.847	1.3780		83	4	
d453	1,1-Dimethoxy-2-propanone	$CH_3C(O)CH(OCH_3)_2$	118.13	1 ¹ , 395	0.976	1.3978 ²⁰		143–147	37	
d454	3,3-Dimethoxy-1-propene	$(CH_3O)_2CHCH=CH_2$	102.13	1 ¹ , 378	0.862	1.3954 ²⁰		89–90		
d455	1,2-Dimethoxy-4-propenylbenzene	$CH_3CH=CHC_6H_3(OCH_3)_2$	178.23	6, 956	1.055	1.5680 ²⁰		262–264	>112	
d456	2,6-Dimethoxy-pyridine	$(CH_3O)_2C_5H_3N$	139.15		1.053	1.5029 ²⁰		178–180	61	
d457	2,5-Dimethoxytetrahydrofuran	$(CH_3O)_2C_4H_6O$	132.16		1.020	1.4180 ²⁰		145–147	35	
d458	<i>N,N</i> -Dimethylacetamide	$CH_3C(O)N(CH_3)_2$	87.12	4, 59	0.9366 ²⁵	1.4356 ²⁵	–20	165.5	70	misc aq, alc, bz, eth
d459	Dimethyl 1,3-acetone-dicarboxylate	$[CH_3OOCCH_2]_2C=O$	174.15	3, 790	1.185	1.4434 ²⁰		150 ^{25mm}	>112	
d460	Dimethyl acetylene-dicarboxylate	$CH_3OOC\equiv CCOOCH_3$	142.11	2, 803	1.156	1.4470 ²⁰		95–98 ^{19mm}	86	
d461	Dimethylamine	$(CH_3)_2NH$	45.09	4, 39	0.680 ⁰		–92.2	6.9		v s aq; s alc, eth

Dimethyl acetal, d438
Dimethylacetic acid, m390

2,3-Dimethylacrylic acids, m161, m162
3,3-Dimethylacrylic acid, m163

3,3-Dimethylallene, m148
Dimethylaminoacetaldehyde diethyl acetal, d249

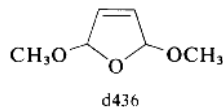


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d462	4-Dimethylamino-benzaldehyde	$(\text{CH}_3)_2\text{NC}_6\text{H}_4\text{CHO}$	149.19	14, 31			74	176 ^{17mm}		s alc, chl, eth, HOAc
d463	<i>p</i> -(Dimethylamino)-benzenesulfonic acid, Na salt	$(\text{CH}_3)_2\text{NC}_6\text{H}_4\text{SO}_3^-\text{Na}^+$	223.23	14 ³ , 2023			>300			
d464	4-Dimethylamino-benzoic acid	$(\text{CH}_3)_2\text{NC}_6\text{H}_4\text{COOH}$	165.19	14, 426			241 d			s alc; sl s eth
d465	2-(Dimethylamino)-ethanol	$(\text{CH}_3)_2\text{NCH}_2\text{CH}_2\text{OH}$	89.14	4, 276	0.8876 ₄ ²⁰	1.4294 ²⁰		135	40	misc aq, alc, eth
d466	2-(Dimethylamino)-ethyl benzoate	$\text{C}_6\text{H}_5\text{COOCH}_2\text{CH}_2\text{-N}(\text{CH}_3)_2$	193.26		1.014	1.5077 ²⁰		155 ^{20mm}		
d467	2-Dimethylamino-ethyl chloride HCl	$(\text{CH}_3)_2\text{NCH}_2\text{CH}_2\text{Cl} \cdot \text{HCl}$	144.05	4, 133			205–208			
d468	2-(Dimethylamino)-ethyl methacrylate	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COOCH}_2\text{-CH}_2\text{N}(\text{CH}_3)_2$	157.22	4 ³ , 649	0.933	1.4391 ²⁰		182–192	70	
d469	4-Dimethylamino-3-methyl-2-butanone	$(\text{CH}_3)_2\text{NCH}_2\text{CH}(\text{CH}_3)\text{-COCH}_3$	129.20	4 ¹ , 452	0.841	1.4250 ²⁰		73 ^{35mm}	38	
d470	3-Dimethylamino-phenol	$(\text{CH}_3)_2\text{NC}_6\text{H}_4\text{OH}$	137.18	13, 405	1.5895 ²⁶		82–84	265–268		v s alc, bz, eth, acet
d471	3-(Dimethylamino)-1,2-propanediol	$(\text{CH}_3)_2\text{NCH}_2\text{CH}(\text{OH})\text{-CH}_2\text{OH}$	119.16	4, 302	1.004	1.4609 ²⁰		216–217	105	s aq, alc, chl, eth
d472	1-Dimethylamino-2-propanol	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{N}(\text{CH}_3)_2$	103.17		0.837	1.4193 ²⁰		121–127	35	
d473	3-Dimethylamino-1-propanol	$(\text{CH}_3)_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$	103.17	4 ¹ , 433	0.872	1.4360 ²⁰		163–164	36	
d474	3-(Dimethylamino)-propionitrile	$(\text{CH}_3)_2\text{NCH}_2\text{CH}_2\text{CN}$	98.15	4 ³ , 1265	0.870	1.4258 ²⁰	–43	171 ^{750mm}	62	
d475	3-Dimethylaminopropyl chloride HCl	$(\text{CH}_3)_2\text{NCH}_2\text{CH}_2\text{-CH}_2\text{Cl} \cdot \text{HCl}$	158.07	4, 148			141–144		35	

d476	4-(Dimethylamino)-pyridine	$(\text{CH}_3)_2\text{N}(\text{C}_5\text{H}_4\text{N})$	122.17	22 ² , 341			108–110			v s aq, alc, bz, chl
d477	<i>N,N</i> -Dimethyl-aniline	$\text{C}_6\text{H}_5\text{N}(\text{CH}_3)_2$	121.18	12, 141	0.9559 ²⁰ ₄	1.5584 ²⁰	2.5	194.2	62	v s alc, chl, eth
d478	2,3-Dimethyl-aniline	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{NH}_2$	121.18	12, 1101	0.9931 ²⁰	1.5685 ²⁰	2.5	221–222	96	sl s aq; s alc, eth
d479	2,4-Dimethyl-aniline	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{NH}_2$	121.18	12, 1111	0.980 ²⁰ ₄	1.5586 ²⁰		218	90	s alc, bz, eth
d480	2,5-Dimethyl-aniline	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{NH}_2$	121.18	12, 1135	0.9790 ²¹ ₄	1.5592 ²⁰	11.5	218	93	sl s aq; s alc, eth
d481	2,6-Dimethyl-aniline	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{NH}_2$	121.18	12, 1107	0.984 ²⁰	1.5601 ²⁰	10–12	216	91	sl s aq; s alc, eth
d482	3,4-Dimethylaniline	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{NH}_2$	121.18	12, 1103	1.076 ¹⁸		49–51	226		sl s aq; s alc
d483	3,5-Dimethylaniline	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{NH}_2$	121.18	12, 1131	0.972 ²⁰ ₄	1.5578 ²⁰		104 ^{14mm}	93	sl s aq; s alc
d484	Dimethylarsinic acid	$(\text{CH}_3)_2\text{As}(\text{O})\text{OH}$	137.99				195–196			v s alc; 200 aq; i eth
d485	3,4-Dimethylbenzoic acid	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{COOH}$	150.18	9 ² , 353			165–167	subl		s alc, bz
d486	2,5-Dimethylbenzonitrile	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{CN}$	131.18	9, 535	0.957	1.5284 ²⁰	13–14	223 ^{730mm}	92	
d487	<i>N,N</i> -Dimethylbenzylamine	$\text{C}_6\text{H}_5\text{CH}_2\text{N}(\text{CH}_3)_2$	135.21	12, 1019	0.900	1.5011 ²⁰	–75	183	54	
d488	2,3-Dimethyl-1,3-butadiene	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$	82.15	1 ³ , 991	0.7222 ²⁵ ₄	1.4362 ²⁵	–76.0	69.2	<1	
d489	2,2-Dimethylbutane	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_3$	86.18	1, 150	0.6492 ²⁰	1.3688 ²⁰	–99.9	49.7	–28	
d490	2,3-Dimethylbutane	$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$	86.18	1, 151	0.6616 ²⁰	1.3750 ²⁰	–128.5	58.0	–28	
d491	2,3-Dimethyl-2,3-butanediol	$(\text{CH}_3)_2\text{C}(\text{OH})\text{C}(\text{OH})(\text{CH}_3)_2$	118.18	1, 487			41.1	174.4		v s hot aq, alc, eth

3-Dimethylaminopropylamine, d593
Dimethylanisoles, d547, d548
2,4-Dimethyl-3-azapentane, d411

Dimethylbenzenes, x4, x5, x6
6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-ethanol,
n105

Dimethyl (Z)-butenedioate, d544

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

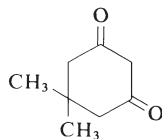
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d492	2,2-Dimethyl-1-butanol	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{OH}$	102.18	1 ³ , 1675	0.8286 ₄ ²⁰	1.4208 ²⁰	< -15	136.8		sl s aq; s alc, eth
d493	2,3-Dimethyl-1-butanol	$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}_2\text{OH}$	102.18	1 ³ , 1677	0.8300 ₄ ²⁰	1.4205 ²⁰		149		s alc, eth
d494	2,3-Dimethyl-2-butanol	$(\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2\text{OH}$	102.18	1, 413	0.8236 ₄ ²⁰	1.4176 ²⁰	-10.6	118.7	29	s aq; misc alc, eth
d495	3,3-Dimethyl-1-butanol	$(\text{CH}_3)_3\text{CCH}_2\text{CH}_2\text{OH}$	102.18	1 ³ , 1677	0.8147 ²⁰	1.4120 ²⁰	-60	143	47	s alc, eth
d496	3,3-Dimethyl-2-butanol	$(\text{CH}_3)_3\text{CCH}(\text{OH})\text{CH}_3$	102.18	1, 412	0.8185 ₄ ²⁰	1.4151 ²⁰	5.3	120.4	28	s alc; misc eth
d497	3,3-Dimethyl-2-butanone	$(\text{CH}_3)_3\text{CCOCH}_3$	100.16	1, 694	0.7250 ₂₅ ²⁵	1.3939 ²⁵	-52.5	106.2	23	2.5 aq; s alc, eth
d498	2,3-Dimethyl-2-butene	$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	84.16	1, 218	0.7081 ₄ ²⁰	1.4124 ²⁰	-74.3	73.2	-16	s alc, eth
d499	3,3-Dimethyl-1-butene	$(\text{CH}_3)_3\text{CCH}=\text{CH}_2$	84.16	1, 217	0.6531 ₄ ²⁰	1.3762 ²⁰	-115.2	41.3	-28	
d500	3,3-Dimethylbutyric acid	$(\text{CH}_3)_3\text{CCH}_2\text{COOH}$	116.16	2, 337	0.9124 ₄ ²⁰	1.4100 ²⁰	6-7	190	88	s alc, eth
d501	Dimethylcadmium	$(\text{CH}_3)_2\text{Cd}$	142.48		1.9846 ₄ ¹⁷	1.5488	-4.5	105.5	≥150 ex- plo- des	d aq; s PE
d502	Dimethylcarbamyl chloride	$(\text{CH}_3)_2\text{NCOCI}$	107.54	4, 73	1.168	1.4540 ²⁰	-33	168	68	
d503	Dimethyl carbonate	$(\text{CH}_3\text{O})_2\text{C}=\text{O}$	90.08	3, 4	1.065 ₄ ¹⁷	1.3682 ²⁰	0.5	90-91	18	i aq; misc alc, eth
d504	Dimethyl chlorothio-phosphate	$(\text{CH}_3\text{O})_2\text{P}(\text{S})\text{Cl}$	160.56	1 ¹ , 143	1.322	1.4819 ²⁰		67 ^{16mm}		
d505	Dimethylcyanamide	$(\text{CH}_3)_2\text{NCN}$	70.09	4, 74	0.867	1.4100 ²⁰		161-163	58	

d506	<i>cis</i> -1,2-Dimethyl- cyclohexane	$(\text{CH}_3)_2\text{C}_6\text{H}_{10}$	112.22	5, 36	0.7692 ²⁰	1.4335 ²⁰	−49.9	129.7	15	i aq; s alc, bz
d507	<i>trans</i> -1,2-Dimethyl- cyclohexane	$(\text{CH}_3)_2\text{C}_6\text{H}_{10}$	112.22	5, 36	0.7772 ²⁰	1.4273 ²⁰	−88.2	123.4	15	i aq; s alc, eth
d508	5,5-Dimethyl-1,3- cyclohexanedione		140.18	7, 559			d 149			0.4 aq; s alc, bz
d509	2,3-Dimethylcyclo- hexanol	$(\text{CH}_3)_2\text{C}_6\text{H}_9\text{OH}$	128.22		0.934	1.4653 ²⁰			65	
d510	2,6-Dimethylcyclo- hexanone		126.20	7, 23	0.925	1.4460 ²⁰		175	51	i aq; s alc, eth
d511	2,3-Dimethylcyclo- hexylamine	$(\text{CH}_3)_2\text{C}_6\text{H}_9\text{NH}_2$	127.23		0.835	1.4595 ²⁰		160	51	
d512	Dimethyl decanedioate	$\text{CH}_3\text{OOC}(\text{CH}_2)_8\text{COOCH}_3$	230.30	2, 719	0.983 ³⁰ ₂₀	1.4335 ²⁸	23	144 ^{5mm}		i aq; s alc, eth
d513	5,7-Dimethyl-3,5,9- decatrien-2-one	$\text{H}_2\text{C}=\text{CHCH}_2\text{CH}(\text{CH}_3)-$ $\text{CH}=\text{C}(\text{CH}_3)\text{CH}=\text{CH}-$ COCH_3	178.28					79 ^{0.05mm}		
d514	Dimethyl 2,5-dioxo- 1,4-cyclohexanedi- carboxylate		228.20	10, 894			155–157			

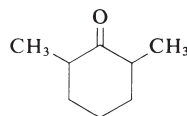
Dimethyl 2-butyndioate, d460
 Dimethyl Cellosolve, d439
 Dimethylchlorosilane, c92

(*Z*)-2-Dimethylcrotonic acid, m162
 Dimethyl 1,4-cyclohexanedione-2,5-
 dicarboxylic acid, d514

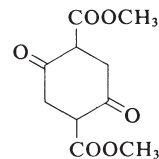
Dimethyl diphenyl sulfone 4,4'-dicarboxylate, s26



d508



d510



d514

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

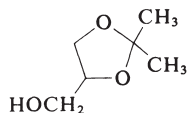
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d515	2,3-Dimethyl-1,3-dioxolane-4-methanol		132.16		1.064 ₄ ²⁰	1.4383 ²⁰		188–189	80	misc aq, alc, eth
d516	Dimethyl disulfide	CH ₃ SSCH ₃	94.20	1, 291	1.046	1.5253 ²⁰	−84.7	109.8	24	i aq; misc alc, eth
d517	Dimethyldithiocarbamic acid dihydrate, Na salt	(CH ₃) ₂ NCSS [−] Na ⁺ · 2H ₂ O	179.24	4, 75						
d518	Dimethyl ether	(CH ₃) ₂ O	46.07	1, 281	0.661 ²⁰		−141.5	−24.9	−41	35% aq (5 atm); 15% bz; 11.8% acet
d519	Dimethylethoxyphenylsilane	C ₂ H ₅ O(C ₆ H ₅)Si(CH ₃) ₂	180.3		0.9263 ₄ ²⁰	1.4799 ²⁰		93 ^{35mm}		
d520	<i>N,N</i> -Dimethylethylamine	C ₂ H ₅ N(CH ₃) ₂	73.14	4, 94	0.675	1.3720 ²⁰	−140	36–38	−36	
d521	<i>N,N</i> -Dimethylethylenediamine	(CH ₃) ₂ NCH ₂ CH ₂ NH ₂	88.15	4 ² , 690	0.803	1.4260 ²⁰			23	
d522	<i>N,N</i> -Dimethylformamide	(CH ₃) ₂ NCHO	73.10	4, 58	0.9445 ₄ ²⁵	1.4282 ²⁵	−60.4	153.0	57	misc aq, alc, bz, eth
d523	<i>N,N</i> -Dimethylformamide dimethyl acetal	(CH ₃) ₂ NCH(OCH ₃) ₂	119.16		0.897	1.3972 ²⁰		103 ^{720mm}	7	
d524	Dimethyl fumarate	CH ₃ OOCC [−] CHCOOCH ₃	144.13	2, 741	1.045 ¹⁰⁶		105	193		sl s alc, eth
d525	2,5-Dimethylfuran	(CH ₃) ₂ (C ₄ H ₃ O)	96.13	17, 41	0.9000 ₄ ²⁰	1.4414 ²⁰	−62	93	<1	i aq; misc alc, eth
d526	Dimethylglyoxime	CH ₃ C(=NOH)C(=NOH)CH ₃	116.12	1, 772			238–240			s alc, acet, eth, pyr
d527	2,4-Dimethyl-2,6-heptadienal	H ₂ C=CHCH ₂ CH(CH ₃)-CH=C(CH ₃)CHO	138.21					47 ^{2mm}		
d528	2,4-Dimethyl-2,6-heptadien-1-ol	H ₂ C=CHCH ₂ CH(CH ₃)-CH=C(CH ₃)CH ₂ OH	140.23					88 ^{10mm}		

d529	2,6-Dimethyl-2,5-heptadien-4-one	$(\text{CH}_3)_2\text{C}=\text{CHC}(=\text{O})-\text{CH}=\text{C}(\text{CH}_3)_2$	138.21	1, 751	0.885^{20}_4	1.4968^{21}	28	198–199	79	sl s aq; s alc, eth
d530	Dimethyl heptanedioate	$\text{CH}_3\text{OOC}(\text{CH}_2)_5\text{COOCH}_3$	188.22	2 ¹ , 281	1.0625^{20}_4	1.4314^{20}	–21	$122^{11\text{mm}}$	> 112	s alc
d531	2,6-Dimethyl-4-heptanone	$[(\text{CH}_3)_2\text{CHCH}_2]_2\text{C}=\text{O}$	142.24	1, 710	0.806^{20}_{20}	1.4114^{20}	–41.5	168.1	48	0.06 aq; misc alc, bz, chl, eth
d532	2,5-Dimethyl-2,4-hexadiene	$(\text{CH}_3)_2\text{C}=\text{CHCH}=\text{C}-(\text{CH}_3)_2$	110.20	1, 259	0.7636^{20}_4	1.4741^{20}	12–14	132–134	29	i aq; s alc, eth
d533	2,5-Dimethylhexane	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2-\text{CH}(\text{CH}_3)_2$	114.24	1 ³ , 283	0.6936^{20}_4	1.3925^{20}	–91.2	109.1	26	i aq; sl s alc; s eth
d534	2,5-Dimethyl-2,5-hexanediamine	$[(\text{CH}_3)_2\text{C}(\text{NH}_2)\text{CH}_2-]_2$	144.26		0.832	1.4459^{20}		$64^{8\text{mm}}$	62	
d534a	Dimethyl hexanedioate	$\text{CH}_3\text{OOC}(\text{CH}_2)_4\text{COOCH}_3$	174.20	1, 652	1.0600^{20}_4	1.4285^{20}	8	$112^{10\text{mm}}$	107	i aq; s alc, eth
d535	2,5-Dimethyl-2,5-hexanediol	$[(\text{CH}_3)_2\text{C}(\text{OH})\text{CH}_2-]_2$	146.23	1, 492			86–90	214–215	126	
d536	1,5-Dimethylhexylamine	$(\text{CH}_3)_2\text{CH}(\text{CH}_2)_3-\text{CH}(\text{NH}_2)\text{CH}_3$	129.25		0.767	1.4209^{20}		154–156	48	
d537	2,5-Dimethyl-3-hexyne-2,5-diol	$(\text{CH}_3)_2\text{CC}\equiv\text{CC}(\text{CH}_3)_2$ OH OH	142.20	1, 501			94–95	205–206		

Dimethyleneimine, e131
Dimethylene oxide, e129

N,N-Dimethylethanolamine, d465
Dimethyl glutarate, d574

Dimethylglutaric acids, d575, d576



d515

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d538	5,5-Dimethyl-hydantoin		128.13	24, 289			176–178			v s aq, alc, bz, chl, eth, acet
d539	1,1-Dimethyl-hydrazine	$(\text{CH}_3)_2\text{NNH}_2$	60.10	4, 547	0.791 ₄ ²²	1.4075 ²⁰	–58	63.9	1	misc aq, alc, eth, PE
d540	1,2-Dimethyl-hydrazine	$\text{CH}_3\text{NHNHCH}_3$	60.10	4, 547	0.8274 ₄ ²⁰	1.4209 ²⁰		81	flammable	misc aq, alc, eth, PE
d541	Dimethyl hydrogen phosphonate	$(\text{CH}_3\text{O})_2\text{P}(=\text{O})\text{H}$	110.05	1, 285	1.200 ₄ ²⁰	1.4009 ²⁰		170–171	96	s aq(hyd); misc alc, acet, eth
d542	1,2-Dimethyl-imidazole		96.13	23, 66	1.084		29–30	204	92	
d543	1,3-Dimethyl-2-imidazolidinone		114.15		1.044	1.4720 ²⁰		108 ^{17mm}	80	
d543a	Dimethylketene	$(\text{CH}_3)_2\text{C}=\text{C}=\text{O}$	70.09	1, 731			–97.5	34		d aq, alc; s eth
d544	Dimethyl maleate	$\text{CH}_3\text{OOCCH}=\text{CHCOOCH}_3$	144.13	2, 751	1.1513 ₄ ²⁰	1.4422 ²⁰	–17.5	200.4		8.7 aq
d545	Dimethyl malonate	$\text{CH}_3\text{OOCCH}_2\text{COOCH}_3$	132.12	2, 572	1.154 ₄ ²⁰	1.4135 ²⁰	–62	180–181	90	sl s aq; misc alc, eth
d546	Dimethylmercury	$(\text{CH}_3)_2\text{Hg}$	230.66	4, 678	3.1874 ₄ ²⁰	1.5452 ²⁰		92 ^{740mm}		i aq; s alc, eth
d547	3,4-Dimethyl-1-methoxybenzene	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OCH}_3$	136.19	6, 481	0.9744 ₄ ¹⁴	1.5198 ¹⁴		200		i aq; s alc, bz, eth
d548	3,5-Dimethyl-1-methoxybenzene	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OCH}_3$	136.19	6, 493	0.9627 ₄ ¹⁵	1.5107 ¹⁵		193	65	i aq; s alc, bz, eth
d549	<i>N,N</i> -Dimethylmethyl-eneammonium iodide	$\text{H}_2\text{C}=\text{N}(\text{CH}_3)_2^+\text{I}^-$	185.01	4 ⁴ , 153			219 d			
d550	Dimethyl methylene-succinate	$\text{CH}_3\text{OOCCH}_2\text{C}(=\text{CH}_2)\text{COOCH}_3$	158.15	2, 762	1.1241 ₄ ¹⁸	1.4442 ²⁰	38	208		s alc, eth
d551	Dimethyl methyl-phosphonate	$(\text{CH}_3\text{O})_2\text{P}(\text{O})\text{CH}_3$	124.08	4 ¹ , 572	1.145	1.4130 ²⁰		181	43	
d552	Dimethyl methyl-succinate	$\text{CH}_3\text{OOCCH}_2\text{CH}(\text{CH}_3)\text{COOCH}_3$	160.17	2 ³ , 1696	1.076	1.4200 ²⁰		196	83	

d553	2,6-Dimethyl-morpholine		115.18		0.9346 ²⁰	1.4470 ²⁰	−85	147	48	misc aq, alc, bz
d554	2,3-Dimethylnaphthalene	(CH ₃) ₂ C ₁₀ H ₆	156.23	5, 571	1.008 ₄ ²⁰		102–104	269		sl s alc; s bz, eth
d555	2,6-Dimethylnaphthalene	(CH ₃) ₂ C ₁₀ H ₆	156.23	5, 570	1.142 ₄ ⁰		110.2	262		i aq; sl s alc
d556	1,2-Dimethyl-3-nitrobenzene	(CH ₃) ₂ C ₆ H ₃ NO ₂	151.17	5, 367	1.129	1.5434 ²⁰	7–9	245	107	i aq; s alc
d557	1,2-Dimethyl-4-nitrobenzene	(CH ₃) ₂ C ₆ H ₃ NO ₂	151.17	5, 368	1.139		29–31	143 ^{20mm}		i aq; s alc
d558	1,3-Dimethyl-2-nitrobenzene	(CH ₃) ₂ C ₆ H ₃ NO ₂	151.17	5, 378	1.112	1.5220 ²⁰	14–16	225 ^{744mm}	87	i aq; s alc
d559	1,3-Dimethyl-4-nitrobenzene	(CH ₃) ₂ C ₆ H ₃ NO ₂	151.17	5, 378	1.117	1.5497 ²⁰	2	237–239	107	s alc, bz, chl, eth
d560	<i>N,N</i> -Dimethyl-4-nitrosoaniline	(CH ₃) ₂ NC ₆ H ₄ NO	150.18	12, 677			86	flammable solid		i aq; s alc, eth
d561	Dimethyl 2-nitro-1,4-phthalate	O ₂ NC ₆ H ₃ (COOCH ₃) ₂	239.18	9, 826			72–75			

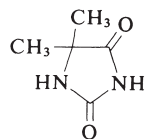
Dimethyl isophthalate, d589

1,4-*a*-Dimethyl-7-isopropyl-1,2,3,4,4*a*,9,10,10*a*-octahydro-1-phenanthrenemethylamine, d20

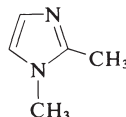
Dimethyl itaconate, d550

2,2-Dimethyl-3-methylenenorbornane, c2

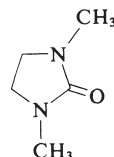
6,6-Dimethyl-2-methylenenorpinene, p176



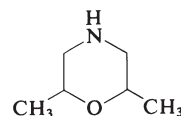
d538



d542



d543



d553

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d562	<i>cis</i> -3,7-Dimethyl-2,6-octadienal		152.24		0.8888 ₄ ²⁰	1.4898 ²⁰		229	101	misc alc, eth, glyc
d563	<i>trans</i> -3,7-Dimethyl-2,6-octadienal		152.24		0.8869 ₄ ²⁰	1.4869 ²⁰		229	101	misc alc, eth, glyc
d564	3,7-Dimethyl-2,6-octadienenitrile		149.24		0.853	1.4753 ²⁰			>112	
d565	Dimethyl octanedioate	CH ₃ OOC(CH ₂) ₆ COOCH ₃	202.25	2, 693	1.0210 ₄ ²⁰	1.4325 ²⁰	−4.8	268		i aq; s alc
d566	Dimethyl oxalate	CH ₃ OOC ₂ COOCH ₃	118.08	2, 534	1.148 ⁵⁴	1.379 ⁸⁰	50–54	163.5	75	6 aq; s alc, eth
d567	<i>N</i> ¹ -(4,5-Dimethyl-oxazol-2-yl)-sulfanilamide		267.31				193–194			s aq, acids, alk
d568	<i>N</i> -(1,1-Dimethyl-3-oxobutyl)acrylamide	CH ₂ =CHC(=O)NHC-(CH ₃) ₂ CH ₂ COCH ₃	169.23				57–58	120 ^{8mm}		
d569	2,3-Dimethylpentanal	CH ₃ CH ₂ CH(CH ₃)CH(CH ₃)CHO	114.19		0.832	1.4132 ²⁰			58	
d570	2,2-Dimethylpentane	CH ₃ CH ₂ CH ₂ C(CH ₃) ₃	100.21	1, 157	0.674 ₄ ²⁰	1.3824 ²⁰	−123.8	79.2	15	i aq; s alc, eth
d571	2,3-Dimethylpentane	CH ₃ CH ₂ CH(CH ₃)-CH(CH ₃) ₂	100.21	1 ² , 120	0.6951 ₄ ²⁰	1.3920 ²⁰	glass	89.8	−6	i aq; s alc, eth
d572	2,4-Dimethylpentane	(CH ₃) ₂ CHCH ₂ CH(CH ₃) ₂	100.21		0.6727 ₄ ²⁰	1.3815 ²⁰	−119.2	80.5		s alc, eth
d573	3,3-Dimethylpentane	CH ₃ CH ₂ C(CH ₃) ₂ CH ₂ CH ₃	100.21	1, 158	0.6933 ₄ ²⁰	1.3905 ²⁰	−134.4	86.1	−6	i aq; s alc, eth
d574	Dimethyl pentanedioate	CH ₃ OOC(CH ₂) ₃ -COOCH ₃	160.17	2, 633	1.0934 ₄ ¹⁵	1.4234 ²⁰		94–95 ^{13mm}	102	v s alc, eth
d575	2,2-Dimethyl-pentanedioic acid	HOOC(CH ₃) ₂ CH ₂ -CH ₂ COOH	160.17	2, 676			83–85			v s aq, alc, chl
d576	3,3-Dimethyl-pentanedioic acid	(CH ₃) ₂ C(CH ₂ COOH) ₂	160.17	2, 684			100–103			v s aq, alc, eth

d577	2,4-Dimethyl-3-pentanol	$(\text{CH}_3)_2\text{CHCH}(\text{OH})\text{-CH}(\text{CH}_3)_2$	116.20	1, 417	0.829^{20}_4	1.4254^{20}	<70	140	37	sl s aq; s alc, eth
d578	2,4-Dimethyl-3-pentanone	$(\text{CH}_3)_2\text{CHC}(=\text{O})\text{-CH}(\text{CH}_3)_2$	114.19	1, 703	0.8062^{20}_4	1.3986^{20}	-80	124	15	misc alc, eth; s bz
d579	2,3-Dimethylphenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	6, 480		1.5420^{20}	75	218		v s alc, bz, chl, eth
d580	2,4-Dimethylphenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	6, 486	1.0276^{14}_4	1.5390^{20}	27	210-212	>112	v s alc, bz, chl, eth
d581	2,5-Dimethylphenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	6, 494	0.965^{80}		74.5	211.5		v s alc, bz, chl, eth
d582	2,6-Dimethylphenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	6, 485			49.0	203	73	v s alc, bz, chl, eth
d583	3,4-Dimethylphenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	6, 480	1.064^{28}_{21}		62.5	225		v s alc, bz, chl, eth
d584	3,5-Dimethylphenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	6, 492	1.008^{28}_{24}		64-68	219.5		v s alc, bz, chl, eth
d585	Dimethylphenyl-chlorosilane	$(\text{CH}_3)_2\text{Si}(\text{Cl})\text{C}_6\text{H}_5$	170.7		1.032^{20}_4	1.508^{20}		192-193		
d586	4,5-Dimethyl- <i>o</i> -phenylenediamine	$(\text{CH}_3)_2\text{C}_6\text{H}_2(\text{NH}_2)_2$	136.20	13, 179			127-129			
d587	Dimethylphenyl-silane	$(\text{CH}_3)_2\text{Si}(\text{H})\text{C}_6\text{H}_5$	136.3		0.8891^{20}_4	1.4995^{20}		156-157		

3,7-Dimethyl-6-octen-1-ol, c274
Dimethylolpropionic acid,

Dimethyl 3-oxoglutarate, d459

2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one, a309

1,5-Dimethyl-2-phenyl-4-aminopyrazolone, a113

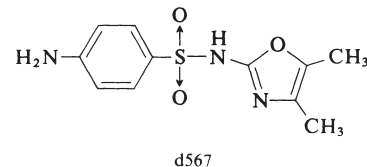
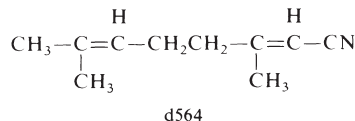
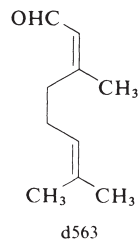
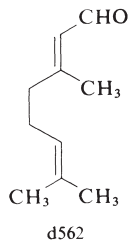


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

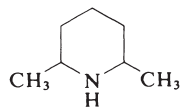
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d588	Dimethyl- <i>o</i> -phthalate	$C_6H_4(COOCH_3)_2$	194.19	9, 797	1.1940 ²⁰ ₂₀	1.515 ²¹	5.5	283.7	146	0.4 aq; misc alc, chl, eth; i PE
d589	Dimethyl- <i>m</i> -phthalate	$C_6H_4(COOCH_3)_2$	194.19	9, 834	1.194 ²⁰ ₄	1.5168 ²⁰	67–68	282		i aq
d590	Dimethyl- <i>p</i> -phthalate	$C_6H_4(COOCH_3)_2$	194.19	4.3303	1.2		140–142	288		i aq, hot alc, eth
d591	2,6-Dimethyl-piperidine		113.20	20, 108	0.840	1.4394 ²⁰		127	11	
d592	2,2-Dimethylpropane	$(CH_3)_4C$	72.15		0.613 ⁰	1.3476 ⁶	–16.6	9.5		
d593	<i>N,N</i> -Dimethyl-1,3-propanediamine	$(CH_3)_2N(CH_2)_3NH_2$	102.18		0.812	1.4350 ²⁰		123	35	
d594	2,2-Dimethyl-1,3-propanediol	$(CH_3)_2C(CH_2OH)_2$	104.15	1, 483	1.11 ²⁵		127–128	208–210		180 aq; 12 bz; 60 acet; v s alc, eth
d595	2,2-Dimethyl-1-propanol	$(CH_3)_3CCH_2OH$	88.15	1, 406	0.812 ²⁰ ₄		52–54	113.1	36	3.6 aq; misc alc, eth
d596	2,2-Dimethylpropionaldehyde	$(CH_3)_3CCHO$	186.25		0.793	1.3794 ²⁰	6	74 ^{730mm}	<1	
d597	2,2-Dimethylpropionamide	$(CH_3)_3CC(O)NH_2$	101.15	2, 320			154–157	212		
d598	2,2-Dimethylpropionic acid	$(CH_3)_3CCOOH$	102.13	2, 319	0.905 ⁵⁰	1.3931 ³⁷	35.5	163.8	63	2.5 aq; v s alc, eth
d599	2,2-Dimethylpropionic anhydride	$[(CH_3)_3CC(O)]_2O$	186.25	2, 320	0.918	1.4092 ²⁰		193	57	
d600	2,2-Dimethylpropionyl chloride	$(CH_3)_3CCOCl$	120.58	2, 320	0.979	1.4120 ²⁰		105–106	<1	d aq, alc; v s eth
d601	1,1-Dimethylpropylamine	$CH_3CH_2C(CH_3)_2NH_2$	87.17	4, 179	0.731 ²⁵ ₄	1.3996 ²⁰	–105	77	65	misc aq, alc, eth
d602	1,1-Dimethyl-2-propynylamine	$HC\equiv CC(CH_3)_2NH_2$	83.13		0.790	1.4235 ²⁰		79–80	<1	

d603	3,5-Dimethylpyrazole		96.13	23, 74			108	218		s aq; v s bz, eth
d604	2,4-Dimethylpyridine	(CH ₃) ₂ (C ₅ H ₃ N)	107.16	20, 244	0.927 ₄ ²⁵	1.4991 ²⁰	<−60	158.3	37	17 aq; v s alc, bz, eth
d605	2,6-Dimethylpyridine	(CH ₃) ₂ (C ₅ H ₃ N)	107.16	20, 244	0.9200 ₄ ²⁵	1.4956 ²⁵	−6.0	143–144	33	43 aq ⁴⁵ ; s alc, eth
d606	3,4-Dimethylpyridine	(CH ₃) ₂ (C ₅ H ₃ N)	107.16	20, 246	0.939 ₄ ²⁵	1.5100 ²⁵	−12	164	53	sl s aq; s alc, eth
d607	3,5-Dimethylpyridine	(CH ₃) ₂ (C ₅ H ₃ N)	107.16	20, 246	0.939 ₄ ²⁵	1.5033 ²⁵	−9	170	53	s aq, alc, eth
d608	Dimethyl succinate	CH ₃ OOCCH ₂ CH ₂ COOCH ₃	146.14	2, 609	1.202 ₄ ¹⁸	1.4190 ²⁰	19.5	195–200	85	0.83 aq; 2.9 alc
d609	Dimethylsulfamoyl chloride	(CH ₃) ₂ NSO ₂ Cl	143.59	4, 84	1.337	1.4518 ²⁰		114 ^{75mm}		
d610	Dimethyl sulfate	(CH ₃ O) ₂ SO ₂	126.13	1, 283	1.3322 ₄ ²⁰	1.3874 ²⁰	−31.8	188 d	83	2.8 aq(hyd); s acet, bz, diox, eth
d611	Dimethyl sulfide	(CH ₃) ₂ S	62.13	1, 288	0.846 ₄ ²¹	1.4354 ²⁰	−98.3	37.3	−36	2 aq; s alc, eth
d612	Dimethyl sulfite	(CH ₃ O) ₂ SO	110.13	1, 282	1.294	1.4083 ²⁰		126–127	30	
d613	Dimethyl sulfone	(CH ₃) ₂ SO ₂	94.13	1, 289			109	238	143	v s aq, alc, acet
d614	Dimethyl sulfoxide	(CH ₃) ₂ SO	78.13	1, 289	1.100 ₄ ²⁰	1.4783 ²⁰	18.5	189.0	95	s alc, acet, bz, chl
d615	Dimethyl- <i>d</i> ₆ sulfoxide	(CD ₃) ₂ SO	84.18		1.18	1.4758 ²⁰		55 ^{5mm}	95	

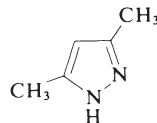
Dimethyl phosphite, d541
 Dimethyl pimelate, d530
 Dimethyl propanedioate, d545

1,1-Dimethylpropargylamine, d602
N'-(4,6-Dimethyl-2-pyrimidinyl)sulfanilamide,
 s21

Dimethyl sebacate, d512
 Dimethyl suberate, d565



d591



d603

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d616	(+)-Dimethyl-L-tartrate	$\text{CH}_3\text{OOCCH}(\text{OH})\text{CH}(\text{OH})\text{COOCH}_3$	178.14	3, 510	1.328_4^{20}		48–50	$163^{23\text{mm}}$		s aq; 200 alc ¹⁵ ; v s bz
d617	Dimethyltelluride	$(\text{CH}_3)_2\text{Te}$	157.68	1, 291			–10	91–92		d aq; v s alc; i eth
d618	2,5-Dimethyltetrahydrofuran	$(\text{CH}_3)_2(\text{C}_4\text{H}_6\text{O})$	100.16	17, 14	0.833	1.4041		90–92	26	
d619	Dimethyl-3,3'-thiodipropionate	$(\text{CH}_3\text{OOCCH}_2\text{CH}_2)_2\text{S}$	206.26		1.198	1.4740^{20}		$148^{18\text{mm}}$	>112	
d620	<i>N,N</i> -Dimethylthioformamide	$(\text{CH}_3)_2\text{NC}(\text{S})\text{H}$	89.16	4, 70	1.047	1.5757^{20}		$58^{1\text{mm}}$	99	
d621	<i>N,N'</i> -Dimethylthiourea	$(\text{CH}_3\text{NH})_2\text{C}=\text{S}$	104.18	4, 70			60–62			v s aq, alc, acet
d622	<i>N,N</i> -Dimethyl- <i>p</i> -toluidine	$\text{CH}_3\text{C}_6\text{H}_4\text{N}(\text{CH}_3)_2$	135.21	12, 902	0.937	1.5458^{20}		211	83	
d623	1,3-Dimethylurea	$(\text{CH}_3\text{NH})_2\text{C}=\text{O}$	88.11	4, 65			101–104	268–270		v s aq, alc, i eth
d624	Dimethylzinc	$(\text{CH}_3)_2\text{Zn}$	95.45		1.386_4^{11}		–40	46	ignites in air	misc bz, PE; s eth
d625	2,4-Dinitroaniline	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_3\text{NH}_2$	183.12	12, 747	1.615^{14}		188			i aq; 0.75 alc
d626	1,3-Dinitrobenzene	$\text{C}_6\text{H}_4(\text{NO}_2)_2$	168.11	5, 258	1.575_4^{18}		89–90	300–303		0.05 aq; 2.7 alc; v s bz, chl, EtAc
d627	2,4-Dinitrobenzenesulfonyl chloride	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_3\text{SOCl}$	234.62	6 ² , 316			96			s bz, HOAc; d alc
d628	3,4-Dinitrobenzoic acid	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_3\text{COOH}$	212.12	9, 413			166	subl		0.7 aq; v s alc, eth
d629	3,5-Dinitrobenzoic acid	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_3\text{COOH}$	212.12	9, 413			207			1.9 hot aq; v s alc; sl s bz, eth
d630	3,5-Dinitrobenzoyl chloride	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_3\text{COCl}$	230.56	9, 414			69.5	$196^{11\text{mm}}$		d aq, alc; s eth
d631	2,6-Dinitro- <i>p</i> -cresol	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_2(\text{OH})\text{CH}_3$	198.13	6, 414			77–79 (an-hyd)			

d631a	4,6-Dinitro-o-cresol	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_2(\text{OH})\text{CH}_3$	198.13	6, 368			87.5			v s alc, acet, eth, alk
d632	1,1-Dinitroethane	$\text{CH}_3\text{CH}(\text{NO}_2)_2$	120.07	1, 102	1.3503 ²⁴ ₂₄			185–186		s alc, eth
d633	2,4-Dinitro-1-fluorobenzene	$\text{FC}_6\text{H}_3(\text{NO}_2)_2$	186.10	5, 262		1.5690 ²⁰	26	178 ^{25mm}	>112	s bz, eth, glyc
d634	1,5-Dinitro-naphthalene	$\text{C}_{10}\text{H}_6(\text{NO}_2)_2$	218.17	5, 558			216–217	subl		s bz; v s eth; sl s alc
d635	2,4-Dinitrophenol	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_3\text{OH}$	184.11	6, 251	1.683		112–114			s alc, bz; 16 EtAc; 36 acet; 5 chl; 20 pyr
d636	2,4-Dinitrophenyl-acetic acid	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_3\text{CH}_2\text{COOH}$	226.15	9, 459			169–175			s alc, eth
d637	2,4-Dinitrophenyl-hydrazine	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_3\text{NHNH}_2$	198.14	15, 489			~200	flammable solid		sl s aq, alc; s acid
d638	3,5-Dinitrosalicyclic acid	$(\text{O}_2\text{N})_2\text{C}_6\text{H}_2(\text{OH})\text{COOH}$	228.12	10, 122			169–172			s aq; v s alc, eth
d639	2,4-Dinitrotoluene	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)_2$	182.14	5, 339	1.321 ⁷¹	1.442	64.66	300 sl d		1.2 alc; 9 eth
d640	2,6-Dinitrotoluene	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)_2$	182.14	5, 341	1.2833 ¹¹¹	1.479	64–66			s alc
d641	3,4-Dinitrotoluene	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)_2$	182.14	5, 341	1.2594 ¹¹¹		54–57			i aq; s alc
d641a	Dinonyl hexanedioate	$\text{C}_9\text{H}_{19}\text{OOC}(\text{CH}_2)_4\text{COOC}_9\text{H}_{19}$	398.63		0.917 ²⁵ ₂₅				218	
d642	Diocetyl phosphite	$(\text{C}_{18}\text{H}_{37}\text{O})\text{P}(\text{O})\text{H}$	586.97				57–59			
d643	Diocetylamine	$(\text{C}_8\text{H}_{17})_2\text{NH}$	241.46	4, 196			14–16	298	>112	i aq; v s alc, eth
d644	Diocetyl sulfide	$(\text{C}_8\text{H}_{17})_2\text{S}$	258.51	1, 419	0.842	1.4610 ²⁰		180 ^{10mm}	>112	
d645	4,9-Dioxa-1,12-dodecanediamine	$\text{H}_2\text{N}(\text{CH}_2)_3\text{O}(\text{CH}_2)_4\text{O}(\text{CH}_2)_3\text{NH}_2$	204.32		0.962	1.4609 ²⁰		134–136 ^{4mm}	>112	

Dimethyl terephthalate, d590
 2,3-Dimethylvaleraldehyde, d569
 2,4-Dinitrochlorobenzene, c94

3,4-Dinitrochlorobenzene, c95
 3,5-Dinitro-1-toluic acid, m228
 Diocetyl phthalates, b179, d313

6,8-Dioxabicyclo[3.2.1]octan-7-one, h183

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d646	1,4-Dioxane		88.10	19, 3	1.0329 ₄ ²⁰	1.4224 ²⁰	11.7	101.2	12	misc aq, alc, bz, chl, eth, PE
d647	1,3-Dioxolane		74.08	19 ² , 3	1.060 ₄ ²⁰	1.4000 ²⁰	−95	74–75	<1	misc aq; s alc, eth
d648	Dipentaerythritol	(HOCH ₂) ₃ CCH ₂ OCH ₂ -C(CH ₂ OH) ₃	254.28				215–218			
d649	Dipentene		136.24	5, 137	0.8402 ₄ ²¹	1.4739 ²⁰		176	42	i aq; misc alc
d650	Dipentylamine	(C ₅ H ₁₁) ₂ NH	157.29	4 ¹ , 378	0.777	1.4272		195–202	39	v s alc, eth
d651	Dipentyl ether	(C ₅ H ₁₁) ₂ O	158.29	1 ¹ , 193	0.7833 ₄ ²⁰	1.4120 ²⁰	−69.4	186.8	63	misc alc, eth; s acet
d652	Diphenylacetic acid	(C ₆ H ₅) ₂ CHCOOH	212.25	9, 673	1.258 ₁₅ ¹⁵		148	195 ^{5mm}		s hot aq, alc, chl, eth
d653	Diphenylacetonitrile	(C ₆ H ₅) ₂ CHCN	193.25	9, 674			76	181 ^{12mm}		s alc, eth
d654	Diphenylacetylene	C ₆ H ₅ C≡CC ₆ H ₅	178.23	5, 656	0.990		60–61	300		v s hot alc, eth
d655	Diphenylamine	(C ₆ H ₅) ₂ NH	169.23	12, 174	1.160		53–54	302	152	45 alc; v s bz, eth
d656	<i>cis,cis</i> -1,4-Diphenyl-1,3-butadiene	C ₆ H ₅ CH=CH-CH=CHC ₆ H ₅	206.29	5, 676	0.9697 ₄ ¹⁰¹	1.6347 ¹⁰¹ (He line)	70.5			s bz, chl, eth, PE
d657	<i>cis,trans</i> -1,4-Diphenyl-1,3-butadiene	C ₆ H ₅ CH=CH-CH=CHC ₆ H ₅	206.29	5, 676	0.9974 ₄ ²²	1.6053 ²²	88	133 ^{0.1mm}		s alc, bz, eth, chl
d658	1,3-Diphenyl-2-buten-1-one	C ₆ H ₅ C(O)CH=C(C ₆ H ₅)CH ₃	222.27	7 ² , 433	1.1080 ₄ ¹⁵	1.6343 ²⁰	−30 glass	246 ^{50mm}		i aq; s alc, eth
d659	Diphenylcarbamoyl chloride	(C ₆ H ₅) ₂ NCOCI	231.68				82–84			
d660	1,5-Diphenylcarbohydrazide	(C ₆ H ₅ NHNH) ₂ C=O	242.28	15, 292			168–171			s hot alc, acet, HOAc
d661	Diphenyl carbonate	(C ₆ H ₅ O) ₂ C=O	214.22	6, 158			80–81	302–306		s hot alc, bz, eth
d662	Diphenyl chlorophosphate	(C ₆ H ₅ O) ₂ P(O)Cl	268.64	6, 179	1.296	1.5500 ²⁰		314 ^{272mm}	>112	

d663	Diphenyl diselenide	$C_6H_5SeSeC_6H_5$	312.13	6, 346	1.557^{80}_4		61–64			s hot alc
d664	Diphenyl disulfide	$C_6H_5SSC_6H_5$	218.34	6, 323	1.353^{20}_4		58–60	310		s alc, bz, eth; i aq
d665	Diphenylenimine		167.21	20, 433	1.10^{18}_4		246	355		0.8 bz; 3 eth; 16 pyr; 11 acet; i aq
d666	1,2-Diphenylethane	$C_6H_5CH_2CH_2C_6H_5$	182.27	5, 598	0.995^{20}_4	1.5338	52.5	284		s alc; v s chl, eth
d667	Diphenyl ether	$C_6H_5OC_6H_5$	170.21	6, 146	1.0661^{20}_4	1.5763^{30}	26.9	258.3	115	s alc, bz, eth, HOAc
d668	1,2-Diphenylethyl-amine	$C_6H_5CH_2CH(C_6H_5)NH_2$	197.28	12, 1326	1.020	1.5802^{20}		311	>112	
d669	<i>N,N'</i> -Diphenylethyl-enediamine	$C_6H_5NHCH_2CH_2NHC_6H_5$	212.30	12, 543			67.5	228–330		v s alc, eth
d670	<i>N,N'</i> -Diphenyl-formamidine	$C_6H_5N=CHNHC_6H_5$	196.25	12, 236			138–141			s eth; v s chl
d671	1,3-Diphenyl-guanidine	$C_6H_5NHC(=NH)NHC_6H_5$	211.27	12, 369	1.13		150	d 170		s alc, hot bz, chl

3,6-Dioxa-1,8-octanediol, t270
 4,8-Dioxa-1,11-undecanediol, t408
 (2,5-Dioxo-4-imidazolidinyl)urea, a77
 1,3-Dioxolane-2-one, e124
 3,4-Dioxypentane, d439
 Dipentyl ketone, u6

Diphenic acid, b137
 Diphenylacetone, d684
 Diphenylcarbamyl chloride, d659
sym-Diphenylcarbazine, d660
 Diphenyldiazone, a322
 Diphenylethanedione, b34

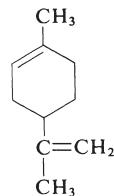
Diphenylethanedione dioxime, b35
 1,2-Diphenylethene, s9
 Diphenylethyne, d654
 Diphenylglycolic acid, b36
 Diphenylglyoxime, b35



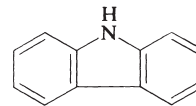
d646



d647



d649



d665

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

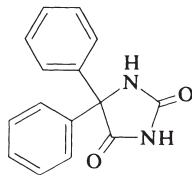
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d672	5,5-Diphenyl-hydantoin		252.27	24, 410			295–298			i aq; 1.7 alc; 3.3 acet
d673	1,2-Diphenyl-hydrazine	$C_6H_5NHNHC_6H_5$	184.24	15, 123	1.158 ₄ ¹⁶		123–126			v s alc; sl s bz
d674	Diphenyl isooctyl-phosphite	$(CH_3)_2CH(CH_2)_5PH-(OC_6H_5)_2$	346.40		1.044	1.522				
d675	Diphenylmercury	$(C_6H_5)_2Hg$	354.81	16, 946	2.318 ₄ ⁴		124–125	d > 306		s chl; sl s hot alc
d676	Diphenylmethane	$C_6H_5CH_2C_6H_5$	168.24	5 ² , 498	1.3421 ₄ ¹⁰	1.5768	25.9	264.5	> 112	v s alc, bz, chl, eth
d677	Diphenylmethanol	$(C_6H_5)_2CHOH$	184.24	6, 678			66.7	298		0.05 aq; v s alc, chl, eth
d678	1,1-Diphenylmethyl-amine	$C_6H_5CH(NH_2)C_6H_5$	183.25	12, 1323	1.0635 ₄ ²² super-cooled	1.5956 ⁹⁹	34	295	> 112	sl s aq
d679	2,5-Diphenyloxazole		221.26	27, 78			72–73	360		
d680	2,6-Diphenylphenol	$(C_6H_5)_2C_6H_3OH$	246.31	6 ³ , 3631			100–102			
d681	Diphenyl phosphite	$(C_6H_5O)_2P(=O)H$	234.19	6 ¹ , 94	1.223	1.5575 ²⁰	12	219 ^{26mm}	176	
d682	Diphenylphosphoryl azide	$(C_6H_5O)_2P(=O)N_3$	275.20		1.277	1.5518 ²⁰		157 ^{0.17mm}	> 112	
d683	2,2-Diphenyl-1-picrylhydrazyl		394.32	16 ² , 363			127 d			
d684	1,3-Diphenyl-2-propanone	$C_6H_5CH_2C(=O)-CH_2C_6H_5$	210.28	7, 445	1.2		32–34	330		i aq; v s alc, eth
d685	1,3-Diphenyl-2-propen-1-one	$C_6H_5CH=CHC(=O)-C_6H_5$	208.26	7, 478	1.0712 ₄ ⁶²	1.6458 ⁶²	57–58	208 ^{25mm}		v s bz, chl, eth
d686	2,2-Diphenyl-propionic acid	$CH_3C(C_6H_5)_2COOH$	226.28	9 ² , 474			175–177	300		s alc; v s bz, eth
d687	Diphenylsilanediol	$(C_6H_5)_2Si(OH)_2$	216.31	16, 909			140 d		53	
d688	Diphenyl sulfide	$(C_6H_5)_2S$	186.28	6, 299	1.118 ₁₅ ¹⁵	1.6327 ²⁰	–40	296	> 112	misc bz, eth, CS ₂
d689	Diphenyl sulfone	$(C_6H_5)_2SO_2$	218.27	6, 300			128–129	379		i aq; s hot alc, bz

d690	Diphenyl sulfoxide	$(C_6H_5)_2S=O$	202.28	6, 300			69–71	207 ^{13mm}	
d691	Diphenylthio- carbazone	$C_6H_5N=NC(S)NH-$ NHC_6H_5	256.33	16, 26			168 d		i aq; v s chl, CCl_4
d692	1,3-Diphenylthio- urea	$C_6H_5NHC(S)NHC_6H_5$	228.32	12, 394	1.32		154		i aq; v s alc, eth
d693	1,3-Diphenylurea	$C_6H_5NHC(O)NHC_6H_5$	212.25	12, 352	1.239		238	260 d	0.015 aq; s eth, HOAc
d694	1,2-Dipiperidino- ethane		196.34	20 ¹ , 19	0.916	1.4876 ²⁰	−0.5	265	110
d695	Dipiperidinomethane		182.31		0.915	1.4820 ²⁰		123 ^{15mm}	
d696	Dipropylamine	$(C_3H_7)_2NH$	101.19	4, 138	0.7375 ²⁰ ₄	1.4043 ²⁰	−39.6	109.2	17
d697	Dipropylene glycol butyl ether	$CH_3CH(OH)CH_2OCH_2-$ $CH(OC_4H_9)CH_3$	190.3		0.917 ²⁵ ₂₅	1.425 ²⁵		229	113
									4 aq; v s alc, eth, PE

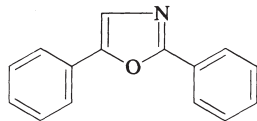
5,5-Diphenyl-2,4-imidazolidinedione, d672
Diphenyl ketone, b53
Diphenyl oxide, d667
Diphenylphosphorochloridate, d662

1,3-Diphenyl-1,3-propanedione, d53
sym-Diphenylthiourea, t146
Dipicolinic acid, p261
Di-2-propenylamine, d25

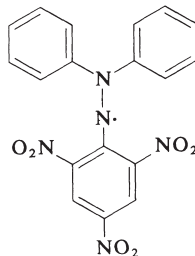
Dipropyl adipate, d702
Dipropylene glycol, h172



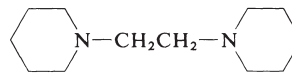
d672



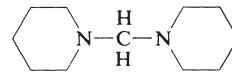
d679



d683



d694



d695

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d698	Dipropylene glycol ethyl ether	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{OCH}_2\text{-CH}(\text{OC}_2\text{H}_5)\text{CH}_3$	162.2		0.930 ₂₅ ²⁵	1.419 ²⁵		388	90	
d699	Dipropylene glycol isopropyl ether	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{OCH}_2\text{-CH}[\text{OCH}(\text{CH}_3)_2]\text{CH}_3$	176.2		0.878 ₂₅ ²⁵	1.421 ²⁵		80.1	90	
d700	Dipropylene glycol methyl ether	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{OCH}_2\text{-CH}(\text{OCH}_3)\text{CH}_3$	148.2		0.951 ₂₀ ²⁰	1.419 ²⁰	−117	188.3	85	
d701	Dipropyl ether	$(\text{C}_3\text{H}_7)_2\text{O}$	102.18	1, 354	0.7466 ₂₀ ²⁰	1.3803 ²⁰	−123.2	89.6	4	0.4 aq
d702	Dipropyl hexanedioate	$\text{C}_3\text{H}_7\text{OOC}(\text{CH}_2)_4\text{-COOC}_3\text{H}_7$	230.30	2 ² , 574	0.9790 ₄ ²⁰	1.4314 ²⁰	−20	144 ^{10mm}		i aq; s alc, eth
d703	Dipropyl sulfate	$(\text{C}_3\text{H}_7\text{O})_2\text{SO}_2$	182.24	1, 354	1.106 ₄ ²⁰		d 140	120 ^{20mm}		v s PE
d704	Dipropyl sulfone	$(\text{C}_3\text{H}_7)_2\text{SO}_2$	150.24	1, 359	1.028 ₄ ⁵⁰		28–30	270	126	
d705	2,2'-Dipyridyl		156.19	23, 199			69.7	273		0.5 aq; v s alc, bz, chl, eth, PE
d706	2,2'-Dipyridylamine		171.20	22 ¹ , 630			89–90	222 ^{50mm}		
d707	1,3-Dithiane		120.24				53–55		90	
d708	4,4'-Dithiobutyric acid	$\text{HOOC}(\text{CH}_2)_3\text{SS}(\text{CH}_2)_3\text{-COOH}$	238.32	3, 312			110			
d709	3,3'-Dithiopropionic acid	$\text{HOOCCH}_2\text{CH}_2\text{SSCH}_2\text{-CH}_2\text{COOH}$	210.27				157–159			
d710	Dithiooxamide	$\text{H}_2\text{NC}(=\text{S})\text{C}(=\text{S})\text{NH}_2$	120.20	2, 565			170 d	subl		sl s aq; s alc; i eth
d711	1,3-Di- <i>o</i> -tolylguanidine	$(\text{CH}_3\text{C}_6\text{H}_4\text{NH})_2\text{C}=\text{NH}$	239.32	12, 803	1.10 ₄ ²⁰		176–178			s hot alc, eth
d712	1,5-Di(vinyloxy)-3-oxapentane	$(\text{CH}_2=\text{CHOCH}_2\text{CH}_2)_2\text{O}$	158.20		0.975 ²⁹	1.445		81 ^{10mm}		
d713	1,3-Divinyltetramethyldisiloxane	$[\text{CH}_2=\text{CHSi}(\text{CH}_3)_2\text{O}]_2$	186.39		0.811 ₄ ²⁰	1.412 ²⁰	−99.7	139		
d714	3,9-Divinyl-2,4,8,10-tetraoxaspiro[5.5]undecane		212.25		1.251		40–54	120 ^{2mm}	110	

d715	Docosane	$\text{CH}_3(\text{CH}_2)_{20}\text{CH}_3$	310.61	1, 174	0.7782 ⁴⁵	1.4358 ⁴⁵	44.4	369		i aq; sl s alc; v s eth
d716	Docosanoic acid	$\text{CH}_3(\text{CH}_2)_{20}\text{COOH}$	340.60	2, 391	0.8221 ¹⁰⁰	1.4270 ¹⁰⁰	80–82	206 ^{60mm}		0.2 alc; 0.19 eth
d717	1-Docosanol	$\text{CH}_3(\text{CH}_2)_{21}\text{OH}$	326.61	1, 431			65–72	180 ^{0,22mm}		sl s eth; s alc, chl
d718	1 <i>H</i> , 7 <i>H</i> -Dodecafluoro-1-heptanol	$\text{HCF}_2(\text{CF}_2)_5\text{CH}_2\text{OH}$	332.0		1.7616 ²⁰	1.3180 ²⁰		169–170		
d719	Dodecane	$\text{CH}_3(\text{CH}_2)_{10}\text{CH}_3$	170.41	1, 171	0.7490 ²⁰	1.4216 ²⁰	–9.6	216.28	71	
d720	1,12-Dodecanediamine	$\text{H}_2\text{N}(\text{CH}_2)_{12}\text{NH}_2$	200.37	4, 273			62–65		155	
d721	Dodecanedioic acid	$\text{HOOC}(\text{CH}_2)_{10}\text{COOH}$	230.30	2, 729			128–130	245 ^{10mm}		
d722	1,2-Dodecanediol	$\text{CH}_3(\text{CH}_2)_9\text{CH}(\text{OH})\text{CH}_2\text{OH}$	202.34	1 ³ , 2237			58–60			
d723	1,12-Dodecanediol	$\text{HOCH}_2(\text{CH}_2)_{10}\text{CH}_2\text{OH}$	202.34	1 ² , 562			81–84	189 ^{12mm}		
d724	Dodecanenitrile	$\text{CH}_3(\text{CH}_2)_{10}\text{CN}$	181.32	2, 363	0.827	1.4360 ²⁰		198 ^{100mm}	>112	misc alc, bz, chl, eth
d725	1-Dodecanethiol	$\text{CH}_3(\text{CH}_2)_{11}\text{SH}$	202.40		0.845 ²⁰	1.4587 ²⁰		266–283	87	i aq; s alc, eth
d726	Dodecanoic acid	$\text{CH}_3(\text{CH}_2)_{10}\text{COOH}$	200.32	2, 359	0.869 ⁵	1.4183 ⁸²	44	225 ^{100mm}		i aq; 100 alc; v s bz, eth
d727	1-Dodecanol	$\text{CH}_3(\text{CH}_2)_{11}\text{OH}$	186.34	1, 428	0.8308 ²⁵	1.4413 ²⁵	23.8	259	>112	i aq; s alc, eth
d728	Dodecanoyl chloride	$\text{CH}_3(\text{CH}_2)_{10}\text{COCl}$	218.77	2, 363	0.946	1.4459 ²⁰		134 ^{11mm}	>112	
d729	1-Dodecene	$\text{CH}_3(\text{CH}_2)_9\text{CH}=\text{CH}_2$	168.32	1, 225	0.7584 ²⁰	1.4294 ²⁰	–35.2	213.4	77	s alc, eth, PE

Dipropyl ketone, h17

Distearyl pentaerythritoldiphosphite, b196

Disulfiram, t61

2,3-Dithiabutane, d516

5,6-Dithiadecane, d113

3,4-Dithiahexane, d294

2,2'-Dithiodiethanol, h118

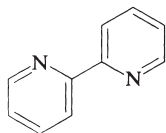
1,4-Dithiothreitol, d424

Dithizone, d691

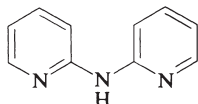
Divinylene oxide, f40

DMSO, d614

Dodecyl alcohol, d727



d705



d706



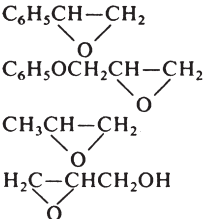
d707



d714

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

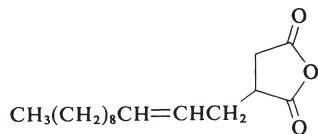
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
d730	2-Dodecen-1-yl-succinic anhydride		266.38					180 ^{5mm}	177	
d731	Dodecanal	$\text{CH}_3(\text{CH}_2)_{10}\text{CHO}$	184.32	1, 714	0.835	1.4344 ²⁰		185 ^{100mm}	101	
d732	Dodecylamine	$\text{CH}_3(\text{CH}_2)_{11}\text{NH}_2$	185.36	4, 200			28–30	247–249	>112	misc alc, bz, chl, eth
d733	4-Dodecylaniline	$\text{CH}_3(\text{CH}_2)_{11}\text{C}_6\text{H}_4\text{NH}_2$	261.46	12 ³ , 2776			40–41	220–221 ^{15mm}		
d734	Dodecylcyclohexane	$\text{CH}_3(\text{CH}_2)_{11}\text{C}_6\text{H}_{11}$	252.50		0.8250	1.4580 ²⁰	12	131 ^{0.8mm}		
d735	Dodecyl sulfate, Na salt	$\text{CH}_3(\text{CH}_2)_{11}\text{OSO}_3^-\text{Na}^+$	288.38				204–207			10 aq
d736	Dodecyltrichlorosilane	$\text{CH}_3(\text{CH}_2)_{11}\text{SiCl}_3$	303.8			1.458 ²⁰		155 ^{10mm}		
d737	Dotriacontane	$\text{CH}_3(\text{CH}_2)_{30}\text{CH}_3$	450.88	1, 177	0.8124 ²⁰	1.4364 ⁷⁰	68–70	467		sl s alc, bz, eth
d738	Dulcitol		182.17	1, 544	1.47 ²⁰		188–189	275 ^{1mm}		3.3 aq; sl s alc
e1	D-Ephedrine	$\text{CH}_3\text{NHCH}(\text{CH}_3)\text{CH}(\text{OH})-\text{C}_6\text{H}_5$	165.24	13, 637			119	225		v s alc, eth
e2	L-Ephedrine	$\text{CH}_3\text{NHCH}(\text{CH}_3)\text{CH}(\text{OH})-\text{C}_6\text{H}_5$	165.24	13, 636			34	255		5 aq; v s alc; s chl
e3	1,2-Epoxybutane	$\text{CH}_3\text{CH}_2\text{CH}-\text{CH}_2$ O	72.11	17 ² , 17	0.8297 ²⁰	1.3840 ²⁰	–150	63.2	–17	6 aq; misc alc, bz, chl, eth
e4	1,2-Epoxy-cyclo-dodecane		182.31		0.939	1.4773 ²⁰				
e5	1,2-Epoxy-cyclo-hexane		98.15	17, 21	0.970	1.4520 ²		129–130	27	v s alc, bz, eth
e6	1,4-Epoxy-cyclohexane		98.15		0.969	1.4480 ²⁰		119 ^{713mm}	12	
e7	2-(3,4-Epoxy-cyclo-hexyl)ethyltri-methoxysilane		246.37		1.070 ²⁵	1.449 ²⁵		310	146	

e7a	1,2-Epoxyoctane		126.20				53–56	55 ^{5mm}	56	
e8	1,2-Epoxyoctane		84.12	17, 21	0.964	1.4336 ²⁰		102	10	
e9	1,2-Epoxyethylbenzene		120.15	17, 49	1.0523 ¹⁶ ₄	1.5338 ²⁰	–37	194	79	i aq; s alc, eth
e9a	1,2-Epoxy-3-phenoxypropane		150.18				2			
e10	1,2-Epoxypropane		58.08	17, 6	0.859 ⁰ ₄	1.3660 ²⁰	–112.1	34.2	–37	41 aq; misc alc, eth
e11	2,3-Epoxy-1-propanol		74.08	17, 104	1.1143 ²⁵ ₄	1.4315 ²⁰		66 ^{2.5mm}	81	misc aq

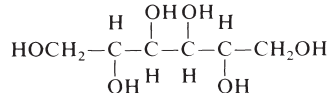
Dodecyl aldehyde
DPPH, d683
Durene, t99
Durenol, t116
EDTA, e125

Eicosane, i2
1-Eicosene, i3
Elaidic acid, o11
Embonic acid, m235
Enanthic acid, h10

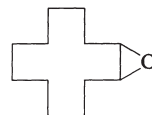
Epibromohydrin, b276
Epichlorohydrin, c101
1,4-Epoxybutane, t66
Epoxyethane, e129
1,3-Epoxypropane, t345



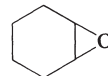
d730



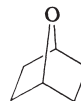
d738



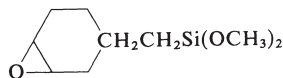
e4



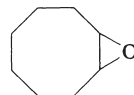
e5



e6



e7


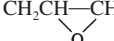


e7a



e8

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e12	2,3-Epoxypropyl methacrylate	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COO}-$ $\text{CH}_2\text{CH}-\text{CH}_2$ 	142.15		1.042	1.4494 ²⁰		189	83	
e13	1,2-Epoxy-3,3,3-tri-chloropropane	$\text{CH}_2\text{CH}-\text{CH}_2$ 	161.42	17 ² , 14	1.495	1.4778 ²⁰		151 ^{745mm}	66	
e14	Ethane	CH_3CH_3	30.07	1, 80	0.5462, ⁻⁸⁸ 1.0493 ⁰ ₄ , g · L		−183.3	−88.6		4.7 mL aq; 46 mL alc ⁴
e15	1,2-Ethanediamine	$\text{H}_2\text{NCH}_2\text{CH}_2\text{NH}_2$	60.10	4, 230	0.8977 ²⁰ ₄	1.4568 ²⁰	8.5	117.3	33	misc aq, alc; i bz
e16	1,2-Ethandiol	$\text{HOCH}_2\text{CH}_2\text{OH}$	62.07	1, 465	1.1135 ²⁰ ₄	1.4318 ²⁰	−12.6	197.3	110	misc aq, alc, glyc, pyr
e17	1,2-Ethandiol diacetate	$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{OOCCH}_3$	146.14	2, 142	1.1043 ²⁰	1.4150 ²⁰	−31	190.2	82	misc alc, eth
e18	1,2-Ethanedithiol	$\text{HSCH}_2\text{CH}_2\text{SH}$	94.20	1, 471	1.123 ²⁴	1.5580 ²⁰		146	50	v s alc, alk
e19	Ethanesulfonyl chloride	$\text{CH}_3\text{CH}_2\text{SO}_2\text{Cl}$	128.57	4 ² , 526	1.357 ²²	1.4339 ²⁰		171		d aq, alc; v s eth
e20	Ethanethiol	$\text{CH}_3\text{CH}_2\text{SH}$	62.13	1, 340	0.8315 ²⁵	1.420 ²⁵	−147.9	35.0	−17	0.7 aq; s alc, eth
e21	Ethanol	$\text{CH}_3\text{CH}_2\text{OH}$	46.07	1, 292	0.7894 ²⁰ ₄	1.3614 ²⁰	−114.5	78.3	8	misc aq, alc, eth, chl
e22	Ethanol- <i>d</i>	$\text{CH}_3\text{CH}_2\text{OD}$	47.08	1 ³ , 1287	0.801	1.3595 ²⁰		78.8	12	misc aq, alc, eth
e23	Ethoxyacetic acid	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{COOH}$	104.11	3, 233	1.1021 ²⁰ ₄	1.4190 ²⁰		97 ^{11mm}	97	s aq, alc, eth
e24	4-Ethoxyaniline	$\text{CH}_3\text{CH}_2\text{OC}_6\text{H}_4\text{NH}_2$	137.18	13, 436	1.0652 ¹⁶ ₄	1.5609 ²⁰	4	250	115	i aq; s alc
e25	2-Ethoxybenzaldehyde	$\text{CH}_3\text{CH}_2\text{OC}_6\text{H}_4\text{CHO}$	150.18	8, 43	1.074	1.5422 ²⁰	20	136 ^{24mm}	107	misc alc, eth
e26	4-Ethoxybenzaldehyde	$\text{CH}_3\text{CH}_2\text{OC}_6\text{H}_4\text{CHO}$	150.18	8, 73	1.080 ²⁵ ₂₅	1.5584 ²⁰	13–14	255	>112	v s alc, bz, eth
e27	2-Ethoxybenzamide	$\text{CH}_3\text{CH}_2\text{OC}_6\text{H}_4\text{CONH}_2$	165.19	10, 93			132–133			sl s aq; s alc, eth
e28	Ethoxybenzene	$\text{CH}_3\text{CH}_2\text{OC}_6\text{H}_5$	122.17	6, 140	0.967 ²⁰ ₄	1.5074 ²⁰	−29.5	170.0		0.12 aq; misc alc, eth
e29	2-Ethoxybenzoic acid	$\text{CH}_3\text{CH}_2\text{OC}_6\text{H}_4\text{COOH}$	166.18	10, 64	1.105	1.5400 ²⁰	19.4	174 ^{15mm}	>112	sl s aq

e30	4-Ethoxybenzoic acid	$\text{CH}_3\text{CH}_2\text{OC}_6\text{H}_4\text{COOH}$	166.18	10, 156			197–199			sl s hot aq
e31	2-Ethoxybenzyl alcohol	$\text{CH}_3\text{CH}_2\text{OC}_6\text{H}_4\text{CH}_2\text{OH}$	152.19	6, 893		1.5321 ²⁰		265		
e32	Ethoxycarbonyl isothiocyanate	$\text{CH}_3\text{CH}_2\text{OC}(=\text{O})\text{NCS}$	131.15	3 ³ , 279	1.112	1.5000 ²⁰		56 ^{18mm}	50	
e33	Ethoxydimethylvinylsilane	$(\text{CH}_3)_2\text{Si}(\text{OC}_2\text{H}_5)\text{-CH=CH}_2$	130.3		0.790 ²⁰ ₄	1.398 ²⁰		99 ^{710mm}		
e34	2-Ethoxyethanol	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{OH}$	90.12	1, 467	0.9295 ²⁰	1.4075 ²⁰	–59	134.8	48	misc aq, alc, eth, acet
e35	2-(2-Ethoxyethoxy)-ethanol	$\text{C}_2\text{H}_5\text{OCH}_2\text{CH}_2\text{OCH}_2\text{-CH}_2\text{OH}$	134.18	1 ² , 520	0.9841 ²⁵ ₄	1.4254 ²⁵	–55	201.9	96	misc aq, alc, bz, chl, acet, pyr
e36	2-(2-Ethoxyethoxy)-ethyl acetate	$\text{C}_2\text{H}_5\text{OCH}_2\text{CH}_2\text{OCH}_2\text{-CH}_2\text{OOCCH}_3$	176.21		1.0096 ²⁰	1.4213 ²⁰	–25	218.5	110	misc aq, alc, eth, oils
e37	2-Ethoxyethyl acetate	$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{-OCH}_2\text{CH}_3$	132.16	2 ² , 155	0.9749 ²⁰ ₄	1.4023 ²⁰	–61.7	156.3	57	29 aq; misc alc, eth
e38	2-Ethoxyethylamine	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{NH}_2$	89.14	4 ² , 718	0.8512 ²⁰ ₄	1.4101 ²⁰		107	21	misc aq, alc, eth
e39	3-Ethoxy-4-hydroxybenzaldehyde	$\text{C}_2\text{H}_5\text{OC}_6\text{H}_3(\text{OH})\text{CHO}$	166.18	8, 256			76–78			s eth, glycols; 50 alc
e40	3-Ethoxymethacrolein	$\text{C}_2\text{H}_5\text{OCH}=\text{C}(\text{CH}_3)\text{CHO}$	114.15	1 ⁴ , 4082	0.960	1.4792 ²⁰		78–81 ^{14mm}	35	
e41	4-Ethoxy-3-methoxybenzaldehyde	$\text{C}_2\text{H}_5\text{OC}_6\text{H}_3(\text{OCH}_3)\text{CHO}$	180.20	8, 256			59–60			s alc, bz, chl, eth
e42	Ethoxymethyldiphenylsilane	$(\text{C}_6\text{H}_5)_2\text{Si}(\text{CH}_3)\text{OC}_2\text{H}_5$	242.4		1.018 ²⁰ ₄	1.544 ²⁰		122 ^{0.3mm}		
e43	Ethoxymethylene-malononitrile	$\text{CH}_3\text{CH}_2\text{OCH}=\text{C}(\text{CN})_2$	122.13	3 ¹ , 162			64–66	160 ^{12mm}		

Eschenmoser's salt, d549
 Estragole, a94
 Ethanal, a4
 Ethanediarnide, o54
 Ethanenitrile, a29

Ethanoic acid, a19
 Ethanolamine, a164
 Ethenyl acetate, v2
 Ethenylbenzene, s19
 4-Ethoxy-*m*-anisaldehyde, e41

1-Ethoxybutane, b449
 Ethoxyethane, d300
 2-Ethoxyethyl ether, b176
 Ethoxyformic anhydride, d326

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e44	1-Ethoxynaphthalene	$C_{10}H_7OCH_2CH_3$	172.23	6, 606	1.060 ₄ ²⁰	1.6040 ²⁰	5.5	280	>112	i aq; v s alc, eth
e45	<i>N</i> -(4-Ethoxyphenyl)-acetamide	$CH_3CH_2OC_6H_4NHCOCH_3$	179.21	13 ² , 244			134–135			0.076 aq; 6.7 alc; 7.1 chl; 1.1 eth; s glyc
e46	<i>trans</i> -2-Ethoxy-5-(1-propenyl)phenol	$C_2H_5OC_6H_3(CH=CH-CH_3)OH$	178.23	6 ² , 918						
e47	3-Ethoxypropylamine	$C_2H_5OCH_2CH_2CH_2NH_2$	103.17	4 ³ , 739	0.861	1.4178 ²⁰		136–138	32	
e48	3-Ethoxysalicylaldehyde	$C_2H_5OC_6H_3(OH)CHO$	166.18	8 ² , 267			86–88	263–264		
e49	2-Ethoxytetrahydrofuran	$C_2H_5O(C_4H_7O)$	116.16	17 ⁴ , 1020	0.908	1.4140 ²⁰		170–172	16	
e50	Ethoxytrimethylsilane	$(CH_3)_3SiOC_2H_5$	118.3		0.7573 ₄ ²⁰	1.3742 ²⁰				
e51	Ethyl acetate	$CH_3COOC_2H_5$	88.11	2, 125	0.9006 ₄ ²⁰	1.3724 ²⁰	–84	77.1	–3	9.7 aq; misc alc, acet, chl, eth
e52	Ethyl acetimidate HCl	$CH_3C(=NH)OC_2H_5 \cdot HCl$	123.58	2, 182			112–114			
e53	Ethyl acetoacetate (enol)	$CH_3COCH=C(OH)OC_2H_5$	130.15	3, 632	1.0119 ¹⁰	1.4480 ¹⁰	–44	180.8	84	1.9 aq; misc alc, chl
e54	Ethyl acetoacetate (keto)	$CH_3COCH_2COOC_2H_5$	130.15	3, 632	1.0368 ¹⁰	1.4224 ¹⁰	–39	180.8	84	12 aq; misc alc, chl
e55	<i>p</i> -Ethylacetophenone	$C_2H_5C_6H_4COCH_3$	148.21	7 ⁴ , 1101	0.993	1.5293 ²⁰	–20.6	114 ^{11mm}	90	
e56	Ethyl acrylate	$CH_2=CHCOOCH_2CH_3$	100.12	2, 399	0.9405 ₄ ²⁰	1.4068 ²⁰	–71.2	99.5	15	1.5 aq; s alc, eth
e57	Ethylaluminum dichloride	$CH_3CH_2AlCl_2$	126.95		1.207 ⁵⁰		32	113 ^{50mm}		
e58	Ethylamine	$CH_3CH_2NH_2$	45.09	4, 87	0.689 ₁₅ ¹⁵		–81.0	16.6	–17	misc aq, alc, eth
e59	Ethyl 2-amino-benzoate	$H_2NC_6H_4COOCH_2CH_3$	165.19	14, 319	1.088 ¹⁵		14	266–268		i aq; s alc, eth

e60	Ethyl 4-amino-benzoate	$\text{H}_2\text{NC}_6\text{H}_4\text{COOCH}_2\text{CH}_3$	165.19	14, 422			88–90	310		0.04 aq; 20 alc; 50 chl; 25 eth; s dil acid
e61	Ethyl 3-amino-crotonate	$\text{CH}_3\text{C}(\text{NH}_2)=\text{CH}-\text{COOCH}_2\text{CH}_3$	129.16	3, 654	1.021 ₄ ²⁰		33–35	210–215		i aq; s alc, bz, eth
e62	2-(Ethylamino)-ethanol	$\text{CH}_3\text{CH}_2\text{NHCH}_2\text{CH}_2\text{OH}$	89.14	4, 282	0.914 ₄ ²⁰	1.4402 ²⁰	–90	170	71	v s aq, alc, eth
e63	N-Ethylaniline	$\text{C}_6\text{H}_5\text{NHCH}_2\text{CH}_3$	121.18	12, 159	0.958 ₂₅ ²⁵	1.5559 ²⁰	–63	204.5	85	i aq; misc alc, eth
e64	2-Ethylaniline	$\text{CH}_3\text{CH}_2\text{C}_6\text{H}_4\text{NH}_2$	121.18	12 ² , 584	0.983 ₄ ²²	1.5590 ²⁰	–44	210	97	sl s aq; v s alc, eth
e65	4-Ethylaniline	$\text{CH}_3\text{CH}_2\text{C}_6\text{H}_4\text{NH}_2$	121.18	12, 1090	0.975 ₄ ²²	1.5542 ²⁰	–5	216	85	sl s aq; v s alc, eth
e66	2-Ethylanthraquinone		236.27	7 ¹ , 425			108–111			
e67	Ethylbenzene- <i>d</i> ₁₀	$\text{C}_6\text{D}_5\text{CD}_2\text{CD}_3$	116.25			1.4920 ²⁰		134.6	31	
e68	Ethylbenzene	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_3$	106.17	5 ² , 274	0.8670 ₄ ²⁰	1.4959 ²⁰	–95.0	136.2	20	0.01 aq; misc alc, bz, chl, eth
e69	Ethyl benzoate	$\text{C}_6\text{H}_5\text{COOCH}_2\text{CH}_3$	150.18	9, 110	1.050 ₄ ²⁵	1.5052 ²⁰	–34.7	212.4	84	0.05 aq; misc alc, chl, bz, eth, PE
e70	Ethyl benzoylacetate	$\text{C}_6\text{H}_5\text{C}(=\text{O})\text{CH}_2-\text{COOCH}_2\text{CH}_3$	192.21	10, 674	1.110	1.5338 ²⁰		265 d	140	i aq; misc alc, eth
e71	Ethyl 2-benzylacetoacetate	$\text{CH}_3\text{COCH}(\text{CH}_2\text{C}_6\text{H}_5)-\text{COOC}_2\text{H}_5$	220.27	10, 674	1.036	1.4996 ²⁰		276	>112	
e72	N-Ethylbenzylamine	$\text{C}_6\text{H}_5\text{CH}_2\text{NHC}_2\text{H}_5$	135.21	12, 1020	0.909	1.5117 ²⁰		194	66	
e73	Ethyl (2-benzyl)-benzoylacetate	$\text{C}_6\text{H}_5\text{COCH}(\text{CH}_2\text{C}_6\text{H}_5)-\text{COOC}_2\text{H}_5$	282.34	10, 764	1.110	1.5567 ²⁰		270 ^{80mm}	>112	

α -Ethoxy- α -phenylacetophenone, b47

3-Ethoxy-1-propene, a90

Ethyl alcohols, e21, e22

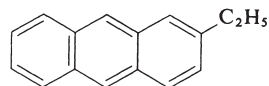
Ethylaldehyde, a4

Ethyl anthranilate, e59

Ethyl benzenecarboxylate, e69

Ethyl 3-benzenepropenoate, e103

α -Ethylbenzyl alcohol, p142



e66

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e74	Ethyl <i>N</i> -benzyl- <i>N</i> -cyclopropyl-carbamate	$C_6H_5CH_2N(C_3H_5)COOCH_2CH_3$	219.28		0.997	1.5104 ²⁰			>112	
e75	Ethyl bromoacetate	$BrCH_2COOCH_2CH_3$	167.01	2, 214	1.506 ²⁰ ₂₀	1.4510 ²⁰		159	47	i aq; misc alc, eth
e76	Ethyl 2-bromo-butyrate	$CH_3CH_2CH(Br)COOCH_2CH_3$	195.06	2 ² , 255	1.329 ²⁰ ₂₀	1.4470 ²⁰		177 d	58	i aq; misc alc, eth
e77	Ethyl 4-bromo-butyrate	$BrCH_2CH_2CH_2COOCH_2CH_3$	195.06	2, 283	1.363	1.4559 ²⁰		82 ^{10mm}	90	
e78	Ethyl 2-bromoiso-butyrate	$(CH_3)_2C(Br)COOCH_2CH_3$	195.06	2, 296	1.329 ²⁰ ₄	1.4446 ²⁰		67 ^{11mm}	60	i aq; misc alc, eth
e79	Ethyl 3-bromo-2-oxo-propionate	$BrCH_2C(=O)COOCH_2CH_3$	195.02	3 ² , 409	1.554	1.4695 ²⁰		100 ^{10mm}	98	
e80	Ethyl 2-bromo-pentanoate	$CH_3(CH_2)_2CH(Br)COOCH_2CH_3$	209.09	2, 302	1.226	1.4486 ²⁰		190–192	77	i aq; misc alc, eth
e81	Ethyl 2-bromopro-pionate	$CH_3CH(Br)COOCH_2CH_3$	181.03	2, 255	1.447 ²⁰ ₂₀	1.4470 ²⁰	159–160	51		i aq; misc alc, eth
e82	Ethyl 3-bromopro-pionate	$BrCH_2CH_2COOCH_2CH_3$	181.03	2, 256	1.4123 ¹⁸ ₄	1.4569 ¹⁸		136 ^{50mm}	79	i aq; misc alc, eth
e83	2-Ethyl-1-butanol	$(C_2H_5)_2CHCH_2OH$	102.18	1, 412	0.8330 ²⁰	1.4224 ²⁰	–114.4	146.5	58	0.63 aq
e84	2-Ethyl-1-butene	$(C_2H_5)_2C=CH_2$	84.16	1 ³ , 814	0.6696 ²⁰ ₄	1.3967 ²⁰	–131.5	64.7		
e85	<i>N</i> -Ethylbutylamine	$CH_3(CH_2)_3NHCH_2CH_3$	101.19	4, 157	0.740 ²⁰ ₄	1.4050 ²⁰		108	18	
e86	2-Ethylbutylamine	$(C_2H_5)_2CHCH_2NH_2$	101.19	4, 192	0.776 ²⁰ ₂₀			121–125	21	s aq, alc, acet, eth
e87	2-Ethylbutyraldehyde	$(C_2H_5)_2CHCHO$	100.16	1, 693	0.8162 ²⁰ ₂₀	1.4018 ²⁰	–89	116.7	21	0.31 aq
e88	Ethyl butyrate	$CH_3CH_2CH_2COOCH_2CH_3$	116.16	2, 270	0.879 ²⁰ ₄	1.3928 ²⁰	–98.0	121.6	29	0.49 aq; misc alc, eth
e89	2-Ethylbutyric acid	$(C_2H_5)_2CHCOOH$	116.16	2, 333	0.9225 ²⁰ ₂₀	1.4133 ²⁰	–15	194.2	99	0.22 aq
e90	Ethyl butyrylacetate	$CH_3(CH_2)_2C(O)CH_2COOC_2H_5$	158.20	3, 684	1.001	1.4295 ²⁰		104 ^{22mm}	78	

e91	Ethyl carbamate	$\text{H}_2\text{NCOOCH}_2\text{CH}_3$	89.09	3, 22	1.056		49–50	182–184		200 aq; 125 alc; 111 chl; 67 eth
e92	Ethyl carbazate	$\text{H}_2\text{NNHCOOCH}_2\text{CH}_3$	104.11	3, 98			44–47	110 ^{22mm}		
e93	<i>N</i> -Ethylcarbazole		195.27	20, 436			66–68			
e94	Ethyl chloroacetate	$\text{ClCH}_2\text{COOCH}_2\text{CH}_3$	122.55	2, 197	1.1498 ₄ ²⁰	1.4227 ²⁰	–26	144–146	65	i aq; misc alc, eth
e95	Ethyl 2-chloroaceto- acetate	$\text{CH}_3\text{C}(=\text{O})\text{CH}(\text{Cl})\text{-COOC}_2\text{H}_5$	164.59	3, 662	1.190	1.4430 ²⁰		107 ^{14mm}	50	i aq; s alc, eth
e96	Ethyl 4-chloroaceto- acetate	$\text{ClCH}_2\text{C}(=\text{O})\text{CH}_2\text{-COOC}_2\text{H}_5$	164.59	3, 663	1.218 ₄ ¹⁷	1.4520 ²⁰		115 ^{14mm}	96	i aq; misc alc, eth
e97	Ethyl 4-chloro- butyrate	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{COOC}_2\text{H}_5$	150.61	2, 278	1.0754 ₄ ²⁰	1.4306 ²⁰		186	51	s alc, acet, eth
e98	Ethyl chloroformate	$\text{ClCOOC}_2\text{H}_5$	108.52	3, 10	1.1403 ₄ ²⁰	1.3941 ²⁰	–81	95	2	misc alc, bz, chl, eth
e99	Ethyl 2-chloropro- pionate	$\text{CH}_3\text{CH}(\text{Cl})\text{COOC}_2\text{H}_5$	136.58	2, 248	1.086 ₄ ²⁰	1.4185 ²⁰		147–148	38	i aq; misc alc, eth
e100	Ethyl 3-chloropro- pionate	$\text{ClCH}_2\text{CH}_2\text{COOC}_2\text{H}_5$	136.58	2, 250	1.1086 ₄ ²⁰	1.4249 ²⁰		163	54	misc alc, eth
e101	Ethyl chlorothio- formate	$\text{ClC}(=\text{O})\text{SCH}_2\text{CH}_3$	124.59	3, 134	1.195	1.4820 ²⁰		132	30	
e102	Ethyl chrysanth- emumate		196.29	9 ² , 45	0.906	1.4600 ²⁰		112 ^{10mm}		

Ethyl benzyl ether, b95
 Ethyl bromide, b277
 Ethyl 2-bromo-2-methylpropanoate, e78
 Ethyl bromopyruvate, e79

Ethyl bromovalerate, e80
 Ethyl butyl ether, b449
 Ethyl butyl ketone, h16
 Ethyl caprate, e113

Ethyl caproate, e142
 Ethyl caprylate, e190
 Ethyl chloride, c102
 Ethyl chloroglyoxylate, e191

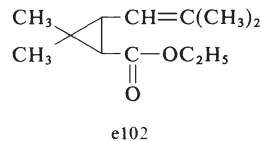
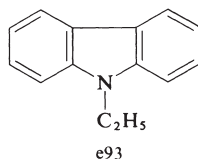


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e103	Ethyl <i>trans</i> -cinnamate	$C_6H_5CH=CHCOOCH_2CH_3$	176.22	9 ² , 385	1.0495 ₄ ²⁰	1.5598 ²⁰	12	271.0		misc alc, eth; i aq
e104	Ethyl crotonate	$CH_3CH=CHCOOCH_2CH_3$	114.14	2, 411	0.9175 ₄ ²⁰	1.4248 ²⁰		138	2	i aq; s alc, eth
e105	Ethyl cyanoacetate	$NCCH_2COOCH_2CH_3$	113.12	2, 585	1.0564 ₄ ²⁵	1.4156 ²⁰	−22.5	206.0	110	i aq; misc alc, eth
e106	Ethyl cyanoformate	$NCCOCH_2CH_3$	99.09	2, 547	1.003 ₄ ²⁰	1.3820 ²⁰		116	24	
e107	Ethyl cyano(hydroxy-imino)acetate	$NCC(=NOH)COOCH_2CH_3$	142.12	3, 775			130–132			
e108	Ethylcyclohexane	$C_6H_{11}CH_2CH_3$	112.22	5, 35	0.7879 ²⁰	1.4330 ²⁰	−111.3	131.8	18	
e109	<i>cis</i> -2-Ethylcyclohexanol	$CH_3CH_2C_6H_{10}OH$	128.22	6 ² , 26	0.927 ₄ ²¹	1.4646 ²⁰		74–79 ^{12mm}	68	i aq
e110	4-Ethylcyclohexanol	$CH_3CH_2C_6H_{10}OH$	128.22	6 ² , 26	0.889	1.4625 ²⁰		84 ^{10mm}	77	
e112	Ethyl cyclohexylacetate	$C_6H_{11}CH_2COOCH_2CH_3$	170.25	9, 14	0.948	1.4439 ²⁰		212	80	
e112	Ethyl cyclopropane-carboxylate	$C_3H_5COOCH_2CH_3$	114.14	9, 4	0.960	1.4197 ²⁰		129–133	18	
e113	Ethyl decanoate	$CH_3(CH_2)_8COOCH_2CH_3$	200.32	2, 356	0.862 ²⁰	1.4248 ²⁰		245	102	misc alc, chl, eth
e114	Ethyl diazoacetate	$N_2CH_2COOCH_2CH_3$	114.10	3 ¹ , 211	1.0852 ₄ ¹⁸	1.4588 ¹⁸	−22	141 ^{720mm}	26	misc alc, bz, eth explodes when heated
e115	Ethyl 2,3-dibromopropionate	$BrCH_2CH(Br)COOCH_2CH_3$	259.94	2, 259	1.788 ₄ ¹⁶	1.4986 ²⁰		214	91	s alc, eth
e116	Ethyl dichlorophosphate	$CH_3CH_2OP(O)Cl_2$	162.94	1, 332	1.373	1.4338 ²⁰		65 ^{10mm}		
e117	Ethyl dichlorothiophosphate	$CH_3CH_2OP(S)Cl_2$	179.01	1, 333	1.353	1.5040 ²⁰		55–68 ^{10mm}		
e118	<i>N</i> -Ethyl diethanolamine	$CH_3CH_2N(CH_2CH_2OH)_2$	133.19	4, 284	1.014	1.4665 ²⁰	−50	246–252	123	
e119	Ethyl diethoxyphosphinylformate	$(C_2H_5O)_2P(O)COOC_2H_5$	210.17	3 ² , 103	1.110	1.4230 ²⁰		135 ^{13mm}		

e120	Ethyl 3-(diethyl-amino)propionate	$(C_2H_5)_2NCH_2CH_2COOC_2H_5$	173.26	4,404	0.881	1.4253 ²⁰		84 ^{12mm}	7	
e121	Ethyl 3,3-dimethylacrylate	$(CH_3)_2C=CHCOOC_2H_5$	128.17	2,433	0.9247 ²⁰ ₄	1.4350 ²⁰		155	33	
e122	Ethyl 2-dimethylaminobenzoate	$(CH_3)_2NC_6H_4COOC_2H_5$	193.25		1.061	1.5425 ²⁰			98	
e123	Ethyl 2,2-dimethylpropionate	$(CH_3)_3CCOOCH_2CH_3$	130.19	2 ² , 280	0.8584 ¹⁸ ₄	1.3922 ¹⁸		118.2		s alc, eth
e124	Ethylene carbonate		88.06	19,100	1.3208 ²⁵	1.4199 ⁴⁰	36.4	238	160	misc aq
e125	Ethylenediamine-N,N,N',N'-tetraacetic acid	$(HOOCCH_2)_2NCH_2CH_2N(CH_2COOH)_2$	292.24				245 d			0.05 aq
e126	Ethylene dinitrate	$O_2NOCH_2CH_2ONO_2$	152.07		1.496 ¹⁵ ₁₅	1.499 ¹⁵	-22	106 ^{19mm}		
e127	2,2'-(Ethylenedioxy)-bisethanol	$HOCH_2CH_2OCH_2CH_2OCH_2CH_2OH$	150.17		1.1274 ¹⁵ ₄	1.4578 ¹⁵	-72	285	166	misc aq, alc, bz
e128	Ethylene glycol	$HOCH_2CH_2OH$	62.07	1,465	1.1135 ²⁰ ₄	1.4319 ²⁰	-13	197.6	110	misc aq, alc, acet, glc, HOAc, pyr; sl s eth; i bz, chl
e129	Ethylene oxide	H_2C-CH_2 O	44.05		0.891 ⁰ ₄	1.3597 ⁷	-112.44	10.6	-18	misc aq; s alc, eth

Ethyl 2-cyano-3-ethoxyacrylate, e132
N-Ethyl-diisopropylamine, d418
 Ethylene bromohydrin, b279
 Ethylene chlorohydrin, c103
 Ethylene cyanohydrin, h169
 Ethylene diacetate, e17

Ethylenediamine, e15
 Ethylene dibromide, d78
 Ethylene dichloride, d177
 (Ethylenedinitrilo)tetraacetic acid, e125
 2,2'-(Ethylenedioxybis (ethanol), t270
 Ethylene glycol, e16

Ethylene glycol *p*-butylphenyl ethers, b475, b476
 Ethylene glycol diacetate, e17
 Ethylene glycol diethyl ether, d252
 Ethylene glycol dimethyl ether, d439
 Ethylene glycol dinitrate, e126

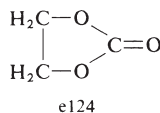


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e130	Ethylene sulfide	$\begin{array}{c} \text{H}_2\text{C}-\text{CH}_2 \\ \\ \text{S} \end{array}$	60.12	17 ² , 12	1.010	1.4935 ²⁰		55–56	10	sl s alc, eth
e131	Ethylenimine	$\begin{array}{c} \text{H}_2\text{C}-\text{CH}_2 \\ \\ \text{NH} \end{array}$	43.07		0.8321 ²⁵ ₄	1.4123 ²⁵	–78.0	56	–24	misc aq; sl s alc
e132	Ethyl (ethoxymethyl-ene)cyanoacetate	$\text{C}_2\text{H}_5\text{OCH}=\text{C}(\text{CN})-\text{COOC}_2\text{H}_5$	169.18	3, 470			51–53	190 ^{30mm}		
e133	Ethyl fluoroacetate	$\text{FCH}_2\text{COOC}_2\text{H}_5$	106.10	2, 193	1.0926 ²¹	1.3755 ²⁰		119 ^{753mm}	30	s aq
e134	Ethyl fluoro-sulfonate	$\text{FSO}_2\text{OC}_2\text{H}_5$	128.12					23–25 ^{12mm}	32	
e135	Ethyl formate	HCOOC_2H_5	74.08	2, 19	0.917 ²⁰ ₄	1.3599 ²⁰	–79.4	54.2	–28	12 aq; misc alc, eth
e136	Ethyl 2-furoate		140.14	18, 275	1.117 ²⁰ ₄		33–36	196	70	i aq; s alc, eth
e137	Ethyl heptafluorobutyrate	$\text{CF}_3\text{CF}_2\text{CF}_2\text{COOC}_2\text{H}_5$	242.09		1.394 ²⁰	1.3030 ²⁰		94–96		
e138	Ethyl heptanoate	$\text{CH}_3(\text{CH}_2)_5\text{COOC}_2\text{H}_5$	158.24	2 ² , 295	0.8685 ²⁰ ₄	1.4144 ¹⁵	–66	187		s alc, eth
e139	Ethyl hexadecanoate	$\text{CH}_3(\text{CH}_2)_{14}\text{COOC}_2\text{H}_5$	284.48	2 ² , 336	0.8577 ²⁵ ₄	1.4347 ³⁴	22	191 ^{10mm}		s alc, eth
e140	3-Ethylhexane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{C}_2\text{H}_5)_2$	114.24	1 ³ , 478	0.7136 ²⁰ ₄	1.4016 ²⁰		118.5		sl s alc; s eth
e141	2-Ethyl-1,3-hexanediol	$\text{C}_3\text{H}_7\text{CH}(\text{OH})\text{CH}(\text{C}_2\text{H}_5)\text{CH}_2\text{OH}$	146.23		0.9325 ²² ₄	1.4530 ²²	–40	244.2	129	0.6 aq; s alc
e142	Ethyl hexanoate	$\text{CH}_3(\text{CH}_2)_4\text{COOC}_2\text{H}_5$	144.21	2, 323	0.871 ²⁰ ₄	1.4075 ²⁰	–67	166–168	49	i aq; misc alc, eth
e143	2-Ethylhexanoic acid	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)-\text{COOH}$	144.21	2, 349	0.9077 ²⁰ ₂₀	1.4241 ²⁰	–118.4	227.6	127	0.25 aq
e144	2-Ethyl-1-hexanol	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)-\text{CH}_2\text{OH}$	130.23		0.9344 ²⁰ ₂₀	1.4231 ²⁰	–76	184.3	77	0.07 aq; s alc, bz, chl
e145	2-Ethylhexanoyl chloride	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)-\text{COCl}$	162.66	2 ² , 304	0.939	1.4335 ²⁰		68 ^{11mm}	69	
e146	2-Ethylhexyl acetate	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)-\text{CH}_2\text{OOCCH}_3$	172.27		0.8718 ²⁰ ₂₀	1.4204 ²⁰	–93	198.6	82	0.03 aq; misc alc

e147	2-Ethylhexylamine	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)\text{-CH}_2\text{NH}_2$	129.31		0.792 ₂₀ ²⁰			165–169	57	i aq; s alc, acet, eth
e148	2-Ethylhexyl vinyl ether	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)\text{-CH}_2\text{OCH=CH}_2$	156.26		0.8102 ₂₀ ²⁰	1.4273 ²⁰	<100 glass	177.7		0.01 aq
e149	Ethyl hydrogen hexanedioate	$\text{HOOC}(\text{CH}_2)_4\text{COOC}_2\text{H}_5$	174.20	2 ¹ , 277		1.4387 ²⁰	28–29	180 ^{18mm}	>112	
e150	Ethyl hydroxyacetate	$\text{HOCH}_2\text{COOC}_2\text{H}_5$	104.11	3, 236	1.087 ₄ ¹⁵			160		v s alc, eth
e151	Ethyl 4-hydroxybenzoate	$\text{HOC}_6\text{H}_4\text{COOC}_2\text{H}_5$	166.18	10, 159			116	297 d		0.07 aq; v s alc, eth
e152	Ethyl 3-hydroxybutyrate	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{COOC}_2\text{H}_5$	132.16	3, 309	1.017 ₄ ²⁰	1.4205 ²⁰		170	64	s aq, alc
e153	Ethyl 2-hydroxyethyl sulfide	$\text{HOCH}_2\text{CH}_2\text{SCH}_2\text{CH}_3$	106.19	1 ² , 525	1.020 ₂₀ ²⁰	1.4869 ²⁰		184.5		s eth
e154	Ethyl 2-hydroxyisobutyrate	$(\text{CH}_3)_2\text{C}(\text{OH})\text{COOC}_2\text{H}_5$	132.16	3, 315	0.965	1.4078 ²⁰		150	44	d hot aq
e155	Ethyl 4-hydroxy-3-methoxyphenylacetate	$\text{HOC}_6\text{H}_3(\text{OCH}_3)\text{CH}_2\text{-COOC}_2\text{H}_5$	210.23	10 ¹ , 198			44–47	180–185 ^{14mm}		

Ethylene glycol monoacetate, h116
 Ethylene glycol monobutyl ether, b410
 Ethylene glycol monoethyl ether, e34
 Ethylene glycol monomethyl ether, m65
 Ethylene glycol monomethyl ether acetate, m68
 Ethylene iodide, d403
 Ethylene iodohydrin, i35

1,8-Ethylenenaphthalene, a2
 Ethylenethiourea, i5
 Ethylene trichloride, t227
 Ethyleneurea, i7
 N-Ethylethanamine, d267
 Ethyl N-ethylcarbamate, e231
 Ethylethylene oxide, e3

Ethyl fluoroide, f17
 2-Ethylhexyl alcohol, e144
 Ethyl homovanillate, e155
 N-Ethyl-N-(2-hydroxyethyl)-3-toluidine, e225
 Ethyl 2-hydroxy-2-methylpropanoate, e154

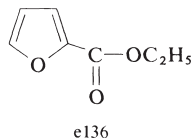


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

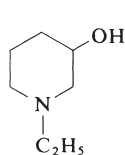
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e156	2-Ethyl-2-(hydroxymethyl)-1,3-propanediol	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_2\text{OH})_3$	134.18	1 ³ , 2349			60–62	159–161 ^{2mm}		
e157	<i>N</i> -Ethyl-3-hydroxypiperidine		129.20		0.970	1.4754 ²⁰		93–95 ^{15mm}	47	
e158	5-Ethylidene-2-norbornene		120.20		0.893	1.4895			38	
e159	2-Ethylimidazole		96.13				79–81			
e160	2-Ethyl-6-isopropylaniline	$(\text{CH}_3)_2\text{CHC}_6\text{H}_3(\text{C}_2\text{H}_5)\text{NH}_2$	163.26		0.949			249		
e161	Ethyl isothiocyanate	$\text{CH}_3\text{CH}_2\text{NCS}$	87.14	4, 123	1.003 ¹⁸ ₄	1.5142 ¹⁸	–6	130–132	32	i aq; misc alc, eth
e162	Ethyl L-(+)-lactate	$\text{CH}_3\text{CH}(\text{OH})\text{COOC}_2\text{H}_5$	118.13	3, 264	1.0328 ²⁰	1.4124 ²⁰	–26	154.5	70	misc aq, alc, eth, esters, PE
e163	Ethyl DL-mandelate	$\text{C}_6\text{H}_5\text{CH}(\text{OH})\text{COOC}_2\text{H}_5$	180.21	10, 202			37	253–255		
e164	Ethyl 2-mercaptoacetate	$\text{HSCH}_2\text{COOC}_2\text{H}_5$	120.17	3, 255	1.0964 ¹⁵	1.4571 ²⁰		54 ^{12mm}	47	s alc, eth
e165	Ethylmercury chloride	$\text{CH}_3\text{CH}_2\text{HgCl}$	165.13		3.5		192	subl		0.78 eth; 2.6 chl
e166	Ethyl methacrylate	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COOC}_2\text{H}_5$	114.14	2, 423	0.909 ²⁵ ₁₅	1.4116 ²⁵		118	49	i aq; s alc, eth
e167	Ethyl 4-methoxyphenylacetate	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}_2\text{COOC}_2\text{H}_5$	194.23	10 ¹ , 83	1.097	1.5075 ²⁰		138 ^{7mm}	46	
e168	Ethyl 2-methylacetoacetate	$\text{CH}_3\text{C}(=\text{O})\text{CH}(\text{CH}_3)\text{COOC}_2\text{H}_5$	144.17	3, 679	1.019 ²⁰ ₄	1.4182 ²⁰		187	62	i aq; s alc, eth
e169	<i>N</i> -Ethyl- <i>N</i> -methylaniline	$\text{C}_6\text{H}_5\text{N}(\text{CH}_3)\text{C}_2\text{H}_5$	135.21	12, 162	0.9193 ⁵⁵ ₄	1.5474 ²⁰		203–205		i aq; misc alc, eth
e170	Ethyl 3-methylbutyrate	$(\text{CH}_3)_2\text{CHCH}_2\text{COOC}_2\text{H}_5$	130.19	2 ² , 275	0.868 ²⁰ ₂₀	1.3962 ²⁰	–99.3	134.7	26	0.2 aq; misc alc, bz
e171	Ethyl methyl ether	$\text{CH}_3\text{CH}_2\text{OCH}_3$	60.09	1, 314	0.725 ⁰ ₀			10.8		s aq; misc alc, eth

e172	2-Ethyl-4-methylimidazole		110.16	23 ² , 72	0.975	1.4995 ²⁰		292–295	137	
e173	Ethyl 4-methyl-5-imidazolecarboxylate		154.17	25 ¹ , 534			204–206			
e174	3-Ethyl-2-methylpentane	(C ₂ H ₅) ₂ CHCH(CH ₃) ₂	114.24	1 ³ , 489	0.7193 ²⁰ ₄	1.4040 ²⁰	–115.0	115.7		i aq; sl s alc; s eth
e175	3-Ethyl-3-methylpentane	(C ₂ H ₅) ₃ CCH ₃	114.24		0.7274 ²⁰ ₄	1.4078 ²⁰	–90.9	118.3		i aq; s eth
e176	Ethyl 3-methyl-3-phenylglycidate		206.24		1.091 ⁵ ₄	1.508 ²⁰				
e177	Ethyl 1-methyl-2-piperidinecarboxylate		171.24	22 ¹ , 485	0.975	1.4519 ²⁰		92–96 ^{11mm}	73	

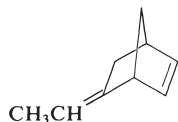
Ethyl 2-hydroxypropionate, e162
Ethylidene bromide, d77
Ethylidene chloride, d176
Ethylidene dimethyl ether, d438
Ethylidene fluoride, d346
2,2'-Ethyliminodiethanol, e118
Ethyl iodide, i34

Ethyl isonicotinate, e216
Ethyl isonipicotate, e206
Ethyl isopropylacetate, e170
Ethyl isothiocyanatoformate, e32
Ethyl isovalerate, e170
Ethyl levulinate, e195
Ethyl linoleate, e188

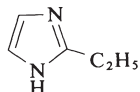
Ethyl mercaptan, e20
Ethyl 3-methylcrotonate, e121
Ethyl methyl ketone, b393
Ethyl 1-methylnipicotate, e177
Ethyl 2-methyl-4-oxo-2-cyclohexene-1-carboxylate, c9
Ethyl 1-methylpipercolinate, e178



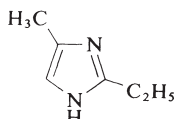
e157



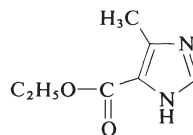
e158



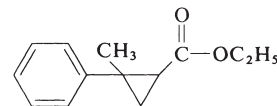
e159



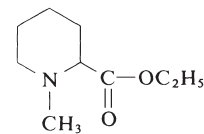
e172



e173



e176



e177

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

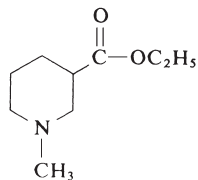
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e178	Ethyl 1-methyl-3-piperidinecarboxylate		171.24		0.954	1.4510 ²⁰		89 ^{11mm}		
e179	2-Ethyl-2-methyl-1,3-propanediol	HOCH ₂ C(C ₂ H ₅)(CH ₃)CH ₂ OH	118.18	1, 487			41–44	226		
e180	3-Ethyl-4-methylpyridine	C ₂ H ₅ (CH ₃)C ₅ H ₃ N	121.18	20 ² , 163	0.9286 ¹⁷			198		s alc, eth; sl s aq
e181	5-Ethyl-2-methylpyridine	C ₂ H ₅ (CH ₃)C ₅ H ₃ N	121.18	20, 248	0.9184 ²³	1.4974 ²⁰		178	66	s alc, bz, eth, acid
e182	Ethyl methyl sulfide	CH ₃ CH ₂ SCH ₃	76.15	1, 343	0.8422 ²⁰	1.4403 ²⁰	–105.9	66.7	49	i aq; misc alc, eth
e183	Ethyl (methylthio)acetate	CH ₃ SCH ₂ COOC ₂ H ₅	134.20		1.043	1.4587 ²⁰			59	
e184	<i>N</i> -Ethylmorpholine		115.18	27 ¹ , 203	0.916 ²⁰ ₂₀	1.4410 ²⁰	–63	139	27	misc aq, alc, eth
e185	Ethyl nitrate	CH ₃ CH ₂ ONO ₂	91.13	1, 329	1.100 ²⁵ ₄	1.3849 ²²	–94.6	87.7	27 flam- mable	l aq; misc alc, eth
e186	Ethyl nitrite	CH ₃ CH ₂ ONO	75.07	1, 329	0.90 ¹⁵ ₁₅			17		misc alc, eth
e187	4-Ethylnitrobenzene	C ₂ H ₅ C ₆ H ₄ NO ₂	151.17	5, 358	1.118	1.5445 ²⁰	–32	245–246	> 112	v s alc, eth
e188	Ethyl (<i>Z,Z</i>)-9,12-octadecadienoic acid	H(CH ₂) ₅ CH=CHCH ₂ -CH=CH(CH ₂) ₇ COOC ₂ H ₅	308.51	2 ² , 461	0.8846 ¹⁶ ₄	1.4675 ²⁰		193 ^{6mm}	> 112	misc DMF, oils
e189	Ethyl <i>cis</i> -9-octadecenoate	CH ₃ (CH ₂) ₇ CH=CH(CH ₂) ₇ COOC ₂ H ₅	310.52	2, 467	0.869 ²⁰ ₄	1.445 ²⁵	< –15	216 ^{15mm}		i aq; misc alc, eth
e190	Ethyl octanoate	CH ₃ (CH ₂) ₆ COOC ₂ H ₅	172.27	2, 348	0.878 ¹⁷	1.4166 ²⁰	–47	206–208	75	i aq; misc alc, eth
e191	Ethyl oxalyl chloride	CH ₃ CH ₂ OC(=O)COCl	136.53	2, 541	1.2223 ²⁰ ₄	1.4164 ²⁰		135	41	d aq, alc; s bz, eth
e192	Ethyl oxamate	CH ₃ CH ₂ OC(=O)CONH ₂	117.10	2, 544			114–116			s aq, eth; i bz
e193	2-Ethyl-2-oxazoline		99.13		0.982	1.4370 ²⁰	–62	128.4	29	

e194	Ethyl 2-oxocyclopentanecarboxylate	$(O=)C_5H_7COOC_2H_5$	156.18		1.054	1.4485 ²⁰		102 ^{11mm}	>112	
e195	Ethyl 4-oxopentanoate	$CH_3C(=O)CH_2CH_2COOC_2H_5$	144.17	3, 675	1.012 ²⁰ ₂₀	1.4222 ²⁰		205–206		v s aq; misc alc
e196	Ethyl 2-oxopropionate	$CH_3C(=O)COOC_2H_5$	116.12	3, 616	1.060 ¹⁶ ₄	1.408 ¹⁶		144	45	sl s aq; misc alc, eth
e197	3-Ethylpentane	$(C_2H_5)_3CH$	100.20	1 ³ , 441	0.6982 ²⁰ ₄	1.3934 ²⁰	–118.6	93.5		i aq; s alc, eth
e198	Ethyl pentanoate	$CH_3(CH_2)_3COOC_2H_5$	130.19	2, 301	0.877 ²⁰ ₄	1.3732 ²⁰	–91.3	145.5		0.2 aq; misc alc, eth
e199	4-Ethylphenol	$CH_3CH_2C_6H_4OH$	122.17	6, 472	1.011 ²⁵ ₄	1.5239	47.0	218–219		i aq; misc alc, eth
e200	Ethyl phenylacetate	$C_6H_5CH_2COOC_2H_5$	164.20	9, 434	1.0333 ²⁰ ₄	1.4980 ²⁰		226	77	i aq; misc alc, eth
e201	Ethyl N-piperazinecarboxylate		158.20	23 ² , 9	1.080	1.4765 ²⁰		273	>112	
e202	1-Ethylpiperidine		113.20	20, 17	0.8237 ²⁰ ₄	1.4440 ²⁰		131	18	
e203	2-Ethylpiperidine		113.20	20, 104	0.850	1.4510 ²⁰		143	31	s aq
e204	Ethyl 2-piperidinecarboxylate		157.21	22, 7	1.006	1.4562 ²⁰		216–217	46	
e205	Ethyl 3-piperidinecarboxylate		157.21		1.012	1.4601 ²⁰		104 ^{7mm}	90	

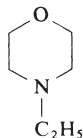
Ethyl nicotinate, e215
 Ethyl nipecotate, e205
 Ethyl oleate, e189

Ethyl pentyl ketone, o35
 Ethyl phenyl ether, e28
 Ethyl picolinate, e214

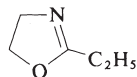
Ethyl pipercolinate, e204
 Ethylpiperidinol, e157



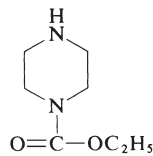
e178



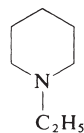
e184



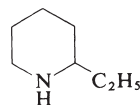
e193



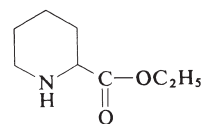
e201



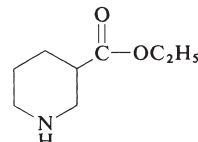
e202



e203



e204



e205

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

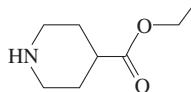
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e206	Ethyl 4-piperidine-carboxylate		157.21		1.010	1.4591 ²⁰		204	80	s aq, alc, bz, eth
e207	Ethyl <i>N</i> -piperidine-propionate		185.27	20, 62	0.927	1.4545 ²⁰		217–219	87	
e208	Ethyl propionate	CH ₃ CH ₂ COOC ₂ H ₅	102.13	2, 240	0.891 ₄ ²⁰	1.3839 ²⁰	−73.9	99.1	12	2 aq; misc alc, eth
e209	Ethyl propyl ether	CH ₃ CH ₂ OCH ₂ CH ₂ CH ₃	88.15	1, 354	0.739 ₄ ²⁰	1.3695 ²⁰	−79	62–63	32	sl s aq; misc alc, eth
e210	Ethyl propyl sulfide	CH ₃ CH ₂ SCH ₂ CH ₂ CH ₃	104.21	1 ³ , 1432	0.8270 ₄ ²⁰	1.4462 ²⁰	−117.0	118.5		s alc
e211	2-Ethylpyridine	CH ₃ CH ₂ C ₅ H ₄ N	107.16	20, 241	0.937	1.4964 ²⁰		149	29	sl s aq; s alc, eth
e212	3-Ethylpyridine	CH ₃ CH ₂ C ₅ H ₄ N	107.16	20, 242	0.954	1.5015 ²⁰		162–165	48	v s alc, eth; sl s aq
e213	4-Ethylpyridine	CH ₃ CH ₂ C ₅ H ₄ N	107.16	20, 243	0.9404 ₄ ²²	1.5009 ²⁰		168	47	sl s aq; s alc, eth
e214	Ethyl 2-pyridine-carboxylate		151.17	22, 35	1.1194 ²⁰	1.5088 ²⁰	2	240–241	107	misc aq, alc, eth
e215	Ethyl 3-pyridine-carboxylate		151.17	22, 39	1.1070 ²⁰	1.5040 ²⁰	8–9	23–224	93	v s aq, alc, eth; s bz
e216	Ethyl 4-pyridine-carboxylate		151.17	22 ² , 37	1.009 ₄ ¹⁵	1.5009 ²⁰	23	220	87	i aq; s alc, bz, chl
e217	1-Ethyl-2-pyrrolidinone		113.16		0.992	1.4652 ²⁰		97 ^{20mm}	76	
e218	Ethyl salicylate	C ₆ H ₄ (OH)COOC ₂ H ₅	166.18	10, 73	1.131 ₄ ²⁰	1.5219 ²⁰	2–3	231–234	107	misc alc, eth; sl s aq
e219	Ethyl sorbate	CH ₃ CH=CHCH=CH-COOC ₂ H ₅	140.18	2, 484	0.959	1.4942 ²⁰		195.5	69	
e220	<i>S</i> -Ethyl thioacetate	CH ₃ C(=O)SCH ₂ CH ₃	104.16	2, 232	0.976 ₄ ²⁸	1.4503 ²⁸		116–117		i aq; v s alc, eth
e221	3-Ethylthio-1,2-propanediol	C ₂ H ₅ SCH ₂ CH(OH)CH ₂ OH	136.21		1.095	1.5065 ²⁰			>112	
e222	Ethyl 4-toluene-sulfonate	CH ₃ C ₆ H ₄ SO ₂ OC ₂ H ₅	200.26	11, 99	1.166 ₄ ⁴⁵	1.5110 ²⁰	33	173 ^{15mm}	157	i aq; s alc, eth
e223	<i>N</i> -Ethyl- <i>m</i> -toluidine	CH ₃ C ₆ H ₄ NHC ₂ H ₅	135.21	12, 857	0.957	1.5451 ²⁰		221	89	

e224	6-Ethyl- <i>o</i> -toluidine	$\text{CH}_3\text{CH}_2\text{C}_6\text{H}_3(\text{CH}_3)\text{NH}_2$	135.21		0.968	1.5525^{20}	−33	231	89	
e225	2-(<i>N</i> -Ethyl- <i>m</i> -toluidino)ethanol	$\text{CH}_3\text{C}_6\text{H}_4\text{N}(\text{C}_2\text{H}_5)\text{CH}_2\text{CH}_2\text{OH}$	179.26		1.019	1.5540^{20}		$115^{1\text{mm}}$		
e226	Ethyl trichloroacetate	$\text{Cl}_3\text{CCOOC}_2\text{H}_5$	191.44	2, 209	1.3834^{20}	1.4447^{20}		168	65	i aq; s alc, eth
e227	Ethyl trifluoroacetate	$\text{F}_3\text{CCOOC}_2\text{H}_5$	142.08	2^2 , 186	1.194	1.3068^{20}		60–62	−1	
e228	Ethyl (trimethylsilyl)acetate	$(\text{CH}_3)_3\text{SiCH}_2\text{COOC}_2\text{H}_5$	160.29		0.876	1.4153^{20}		156–159	35	
e229	Ethyl undecanoate	$\text{CH}_3(\text{CH}_2)_9\text{COOC}_2\text{H}_5$	214.35	2, 358	0.859	1.4280^{20}		$105^{4\text{mm}}$	>112	i aq; s org solv
e230	Ethylurea	$\text{CH}_3\text{CH}_2\text{NHC}(=\text{O})\text{NH}_2$	88.11	4, 115	1.213^{18}		93–96			v s aq; 80 alc; i eth
e231	<i>N</i> -Ethylurethane	$\text{CH}_3\text{CH}_2\text{NHCOOC}_2\text{H}_5$	117.15	4, 114	0.9814^{20}	1.4211^{20}		$85^{20\text{mm}}$	75	63 aq
e232	Ethyl vinyl ether	$\text{CH}_3\text{CH}_2\text{OCH}=\text{CH}_2$	72.11	1, 433	0.7531^{20}	1.3754^{20}	−115.8	35.7	−17	0.9 aq
e233	<i>N</i> -Ethyl-2,3-xylidine	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{NHC}_2\text{H}_5$	149.24	12, 1101	0.917	1.5468^{20}		227–228	71	
e234	1-Ethynyl-1-cyclohexanol	$\text{C}_6\text{H}_{10}(\text{C}\equiv\text{CH})\text{OH}$	124.18	6^2 , 100	0.967^{20}_{20}		30–31	180	62	2.4 aq; misc alc, bz, acet, ketones, PE

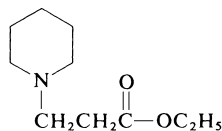
Ethyl pivalate, e123
 1-Ethyl-1-propanol, p39
 Ethyl propenoate, e56
 1-Ethylpropylamine, a252

Ethyl pyruvate, e196
 2-(Ethylthio)ethanol, e153
 Ethyl thioglycolate, e164
 Ethyltriethoxysilane, t261

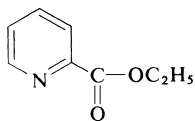
Ethyl trimethylacetate, e123
 Ethyl vanillin, e39
 Ethyne, a41
 Ethynylbenzene, p82



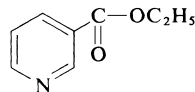
e206



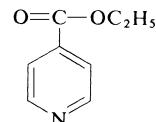
e207



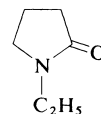
e214



e215



e216



e217

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
e235	1-Ethynylcyclohexylamine	$C_6H_{10}(C\equiv CH)NH_2$	123.30		0.913	1.4817 ²⁰		66 ^{20mm}	42	
f1	Fluoranthene		202.26	5, 685	1.252 ₄ ⁰		107–110	384		sl s alc; s bz, eth
f2	Fluorene		166.22	5, 625	1.203 ₄ ⁰		114.8	295		v s HOAc; s bz, eth
f3	9-Fluorenone		180.21	7, 465	1.1300 ₄ ⁹⁹	1.6369 ⁹⁹	82–85	342		s alc, bz; v s eth
f4	Fluorescein		332.31	19, 222			314 d			s hot alc, hot HOAc, alk; i bz, chl, eth
f5	Fluoroacetamide	$FCH_2C(O)NH_2$	77.06	2, 193			107 subl			v s aq; s acet
f6	Fluoroacetic acid	FCH_2COOH	78.04	2, 193			33	165		sl s aq, alc
f7	Fluoroacetone	$CH_3C(O)CH_2F$	76.07		1.054	1.3700		75	7	
f8	<i>p</i> -Fluoroacetophenone	$FC_6H_4COCH_3$	138.14		1.138	1.5110 ²⁰		196	71	
f9	<i>p</i> -Fluoroaniline	$FC_6H_4NH_2$	111.12	12, 597	1.1725 ₄ ²⁰	1.5395 ²⁰	–1.9	187	73	sl s aq; s alc, eth
f10	<i>o</i> -Fluorobenzaldehyde	FC_6H_4CHO	124.11	7 ¹ , 132	1.178	1.5220 ²⁰	–44.5	91 ^{46mm}	55	
f11	Fluorobenzene	C_6H_5F	96.11	5, 198	1.0240 ₄ ²⁰	1.4657 ²⁰	–42.2	84.7	–12	0.15 aq; misc alc
f12	<i>o</i> -Fluorobenzoic acid	FC_6H_4COOH	140.11	9, 333	1.460 ₄ ²⁵		123–125			sl s aq; s alc, eth
f13	<i>p</i> -Fluorobenzoic acid	FC_6H_4COOH	140.11	9, 333	1.479 ₄ ²⁵		182.6			0.1 aq; s alc, eth
f14	<i>p</i> -Fluorobenzoyl chloride	FC_6H_4COCl	158.56	9 ¹ , 137	1.342	1.5296 ²⁰	9	82 ^{20mm}	82	
f15	<i>o</i> -Fluorobenzyl alcohol	$FC_6H_4CH_2OH$	126.13	6 ¹ , 222	1.173	1.5136 ²⁰			90	
f16	<i>p</i> -Fluorobenzyl chloride	$FC_6H_4CH_2Cl$	144.58		1.207	1.5130 ²⁰		82 ^{26mm}	60	
f17	Fluoroethane	CH_3CH_2F	48.06	1, 82	0.00220 ⁰		–143.2	–37.7		198 mL aq; v s alc, eth

f18	Fluoromethane	CH ₃ F	34.04	1, 59	1.1951 g·L		−141.8	−78.4		166 mL aq; v s alc, eth
f19	4-Fluoro-1-methoxy- benzene	FC ₆ H ₄ OCH ₃	126.13	6 ¹ , 98	1.114	1.4877 ²⁰	−45	157	43	s eth
f20	2-Fluoro-2-methyl- propane	(CH ₃) ₃ CF	76.11	1 ⁴ , 286			−77	12.1	−12	
f21	1-Fluoro-4-nitro- benzene	FC ₆ H ₄ NO ₂	141.10	5, 241	1.3300 ²⁰ ₄	1.5312 ²⁰	21	205	83	i aq; s alc, eth
f22	4-Fluorophenol	FC ₆ H ₄ OH	112.10	6, 183			46–48	185	68	
f23	2-Fluoropyridine	FC ₅ H ₄ N	97.09	20 ¹ , 80	1.128	1.4680 ²⁰		126	28	
f24	<i>o</i> -Fluorotoluene	FC ₆ H ₄ CH ₃	110.13	5, 290	1.0014 ¹⁷	1.4716 ¹⁷	−62.0	114.4	12	v s alc, eth
f25	<i>m</i> -Fluorotoluene	FC ₆ H ₄ CH ₃	110.13	5, 290	0.9974 ²⁰	1.4691 ²⁰	−87.7	116.5	9	s alc, eth
f26	<i>p</i> -Fluorotoluene	FC ₆ H ₄ CH ₃	110.13	5, 290	0.9975 ²⁰	1.4688 ²⁰	−56.7	116.6	40	s alc, eth
f27	Formaldehyde	H ₂ C=O	30.03	1, 558	0.815 ²⁰ ₄	0.8153 ^{−20}	−92	−19.5		122 aq; s alc, eth
f28	Formamide	HC(=O)NH ₂	45.04	2, 26	1.1334 ²⁰ ₄	1.4475 ²⁰	2.6	111 ^{20mm}	154	misc aq, alc, acet
f29	Formamidine acetate	HC(=NH)NH ₂ ·HOOCCH ₃	104.11				158 d			
f30	Formamidinesulfinic acid	H ₂ NC(=NH)S(O)OH	108.12	3 ¹ , 36			126 d			

Eugenol, m99

Fenchone, t351

Fenchyl alcohol, t350

Ferulic acid, h136

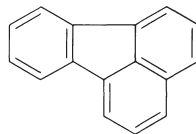
2,7-Fluorenediamine, d38

N-9H-2-(2-Fluorenyl)acetamide, a13

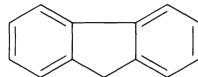
Fluorotrichloromethane, t232

Fluothane, b258

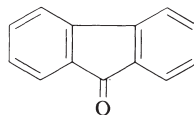
Formic acid hydrazide, f34



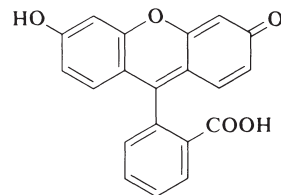
f1



f2



f3



f4

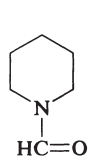
TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
f31	Formanilide	C_6H_5NHCHO	121.14	12, 230	1.144		47	271		2.5 aq
f32	Formic acid	$HCOOH$	46.03	2, 8	1.220 ₄ ²⁰	1.3714 ²⁰	8.5	100.8	68	misc aq, alc, eth
f33	2-Formylbenzoic acid	$C_6H_4(HCO)COOH$	150.13	10, 666	1.404		98			s aq; v s alc, eth
f34	Formylhydrazine	$HC(=O)NHNH_2$	60.06	2, 93			54–56			v s alc, chl, eth; s bz
f35	<i>N</i> -Formylpiperidine		113.16	20, 45	1.019	1.4780 ²⁰		222	91	
f36	D-(–)-Fructose		180.16	31, 321						v s aq; 6.7 alc; s pyr
f37	Fumaric acid	$HOOCCH=CHCOOH$	116.07	2, 737	1.635 ₄ ²⁰		287	subl 200		0.6 aq; 9 alc; 0.7 eth
f38	Fumaroyl dichloride	$ClC(=O)CH=CH-C(=O)Cl$	152.96	2, 743	1.408 ²⁰	1.4988 ²⁰		161–164	73	d aq, alc
f39	2-Furaldehyde		96.09	17 ² , 305	1.1598 ₄ ²⁰	1.5262 ²⁰	–36.5	161.8	68	8 aq; misc alc, eth
f40	Furan		68.07	17, 27	0.9371 ₄ ²⁰	1.4214 ²⁰	–85.6	31.4	–35	1 aq; misc alc, eth
f41	2-Furanacrylic acid		138.12	18, 300			141	286		0.2 aq; 1.1 bz; s alc, eth, HOAc
f42	2-Furancarboxylic acid		112.08	18, 272			133–134	230–232		4 aq; s alc; v s eth
f43	2,5-Furandimethanol		128.13	17 ¹ , 90			74–76			
f44	2-Furanmethanethiol		114.17	17 ² , 116	1.132	1.5304 ²⁰		155	45	
f45	Furfuryl acetate		140.14	17 ² , 115	1.1175 ₄ ²⁰	1.4618 ²⁰		175–177	65	i aq; s alc, eth
f46	Furfuryl alcohol		98.10	17, 112	1.1285 ₄ ²⁰	1.4868 ²⁰	–14.6	170.0	65	misc aq(d); v s alc
f47	Furfurylamine		97.12	18, 584	1.0995 ₄ ²⁰	1.4900 ²⁰	–70	145–146	45	misc aq; s alc, eth
f48	2-Furoyl chloride		130.53	18, 276	1.324	1.5310 ²⁰	–2	170	85	d aq, alc; s eth
g1	D-(+)-Galactose		180.16	31, 295			167			200 aq; s pyr; sl s alc
g2	Geraniol	$(CH_3)_2C=CHCH_2CH_2-C(CH_3)=CHCH_2OH$	154.25	1, 457	0.8894 ₄ ²⁰	1.4760 ²⁰		230	76	i aq; misc alc, eth
g3	α-D-Glucoheptonic acid γ-lactone		208.17				145–148			s aq

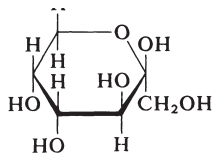
Formylamide, f28
 Formylphenols, h94, h95, h96
 1-Formylpiperazine, p180
 Formylpyridines, p251, p256, p253
 Freon-11, t232
 Freon-12, d170
 Freon-12B2, d75
 Freon-21, d183
 Freon-22, c85

Freon-114, d227
 2,5-Furandione, m2
 2-Furanmethanol, f46
 Furfural, f39
 2-Furfuraldehyde, f39
 Furfuryl mercaptan, f44
 Furoic acid, f42
 Furylacrylic acid, f41
 2-Furyl methyl ketone, a44

Galactaric acid, t84
 Galactitol, d738
 Gallic acid, t306
 Gallusic acid, t306
 Gentisic acid, d384
 Geranial, d562
 D-Glucitol, s5

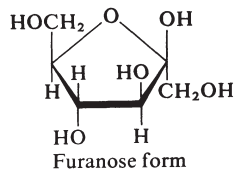


f35

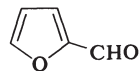


Pyranose form

f36



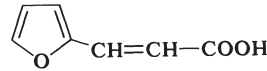
Furanose form



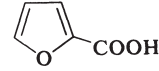
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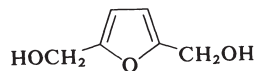
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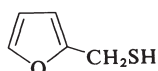
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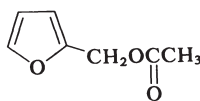
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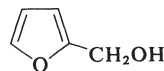
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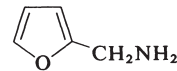
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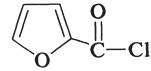
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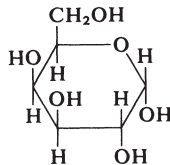
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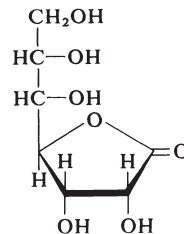
f47



f48



g1



g3

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
g4	D-Gluconic acid		196.16	3, 542			131			v s aq; sl s alc; i eth
g5	D-Glucosamine		179.17	1, 902			88(α)			v s aq; i chl, eth
g6	α -D-(+)-Glucose		180.16	31, 83	1.5620 ₄ ¹⁸		146			91 aq; 0.83 MeOH; s pyr
g7	α -D-Glucose penta-acetate		390.34	31, 119			109–111			0.15 aq; 1.3 alc; 3 eth
g8	D-Glucurono-3,6-lactone		176.12				176–178			27 aq; 2.8 MeOH
g9	L-Glutamic acid		147.13	4, 488	1.538 ₄ ²⁰		d 247	subl 200		0.8 aq; i alc, eth
g10	L-Glutamine		146.15	4, 491			d 185			4 aq; 0.0035 MeOH; i bz, chl, eth, acet
g11	Glutaric acid	HOOCCH ₂ CH ₂ CH ₂ COOH	132.12	2, 631	1.429 ₄ ²⁰	1.4188 ¹⁰⁶	97.5	200 ^{20mm}		64 aq; v s alc, eth; s bz, chl; sl s PE
g12	Glutaric anhydride		114.10	17, 411			52–55	150 ^{10mm}		
g13	Glutaric dialdehyde	OCHCH ₂ CH ₂ CH ₂ CHO	100.12	1, 776		1.3730 ²⁰	–6	187–189 d		misc aq, alc
g14	Glutaronitrile	NCCH ₂ CH ₂ CH ₂ CN	94.12	2, 635	0.9888 ²³	1.4345 ²⁰	–29	286	112	s aq, alc, chl; i eth
g15	Glutaryl dichloride	ClC(=O)CH ₂ CH ₂ CH ₂ -C(=O)Cl	169.01	2, 634	1.324	1.4720 ²⁰		216–218	106	d aq, alc; s eth
g16	Glycerol	HOCH ₂ CH(OH)CH ₂ OH	92.09	1, 502	1.2613 ²⁰	1.4746 ²⁰	18.18	182 ^{20mm}		misc aq, alc; 0.2 eth
g17	Glyceryl 1,2-diacetate	HOCH ₂ CH(OOCCH ₃)-CH ₂ OOCCH ₃	176.17	2, 147	1.184 ₄ ¹⁶	1.1173 ¹⁵	40	172 ^{40mm}		s aq, alc, bz, eth
g18	Glyceryl 1,3-diacetate	CH ₃ COOCH ₂ CH(OH)-CH ₂ OOCCH ₃	176.17	2, 290	1.179 ¹⁵	1.4395 ²⁰	42	172 ^{40mm}		s aq, alc, bz, chl
g19	Glyceryl tris-(butyrate)		302.37	2, 273	1.032 ₄ ²⁰	1.4359 ²⁰	–75	305–310	173	i aq; v s alc, eth
g20	Glyceryl tris-(dodecanoate)		639.02	2, 363	0.894 ₄ ⁶⁰	1.4404 ⁶⁰	46			v s bz, eth; sl s alc

g21	Glyceryl tris-(nitrate)	$\text{O}_2\text{NOCH}_2\text{CH}(\text{ONO}_2)\text{-CH}_2\text{ONO}_2$	227.09	1, 516	1.594_4^{20}	1.4786^{12}	13.3	$160^{5\text{mm}}$	expl 270	0.18 aq; 54 alc; misc eth
g22	Glyceryl tris-(oleate)		885.46	4, 468	0.915_4^{15}	1.4621^{40}	-4 to -5	$235^{15\text{mm}}$		s chl, eth, CCl_4
g23	Glyceryl tris-(palmitate)		807.35	2, 373	0.8663_4^{80}	1.4381^{80}	65-66	310-320		v s bz, chl, eth
g24	Glyceryl tris-(tetradecanoate)		723.18	2, 367	0.885_4^{60}	1.4428^{60}	57			v s alc, bz, chl

Glutaraldehyde, g13

Glyceraldehyde, d398

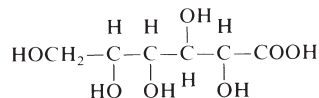
Glycerol dichlorohydrin, d220

Glycerol α -monochlorohydrin, c212

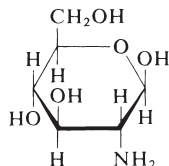
Glyceryl triacetate, p201

Glyceryl tris(laurate), g20

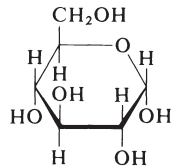
Glyceryl tris(myristate), g24



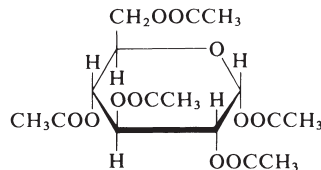
g4



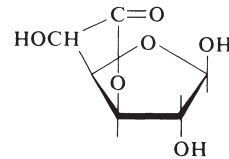
g5



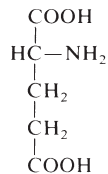
g6



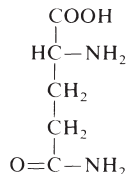
g7



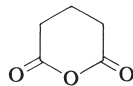
g8



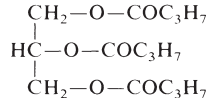
g9



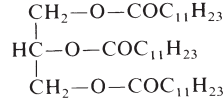
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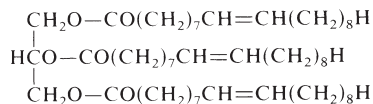
g12



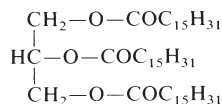
g19



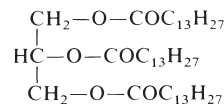
g20



g22



g23



g24

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

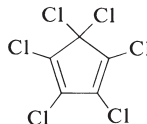
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
g25	Glycine	$\text{H}_2\text{NCH}_2\text{COOH}$	75.07	4, 333	1.1607		d 233			25 aq; 0.6 pyr; i eth
g26	<i>N</i> -Glycylglycine	$\text{H}_2\text{NCH}_2\text{C}(=\text{O})\text{NHCH}_2\text{COOH}$	132.12	4, 371			d 262			s hot aq; sl s alc
g27	Glyoxal	$\text{HC}(=\text{O})\text{CHO}$	58.04	1, 759	1.29_4^{20}	1.3826^{20}	15	51		violent reaction aq; s anhyd solv; mixtures with air may explode
g28	Glyoxylic acid	$\text{HC}(=\text{O})\text{COOH}$	74.04	3, 594			98			v s aq; sl s alc, eth
g29	Guanidine	$\text{H}_2\text{NC}(=\text{NH})\text{NH}_2$	59.07	3, 82			~60	d 160		v s aq, alc
h1	Heptadecane	$\text{CH}_3(\text{CH}_2)_{15}\text{CH}_3$	140.41	1, 173	0.7767^{22}	1.4360^{25}	22.0	302.2	148	s eth; sl s alc
h2	Heptafluorobutyric acid	$\text{CF}_3\text{CF}_2\text{CF}_2\text{COOH}$	214.04		1.645			120		
h3	Heptafluoro-2,3,3-trichlorobutane	$\text{CF}_3\text{CCl}_2\text{CF}(\text{Cl})\text{CF}_3$	287.5		1.7484^{20}	1.3530^{20}	4	98		
h4	2,2,4,4,6,8,8-Heptamethylnonane	$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{C}(\text{CH}_3)_3$	226.45		0.793	1.4391^{20}		240		
h5	Heptanal	$\text{CH}_3(\text{CH}_2)_5\text{CHO}$	114.19	1 ² , 750	0.8216_4^{15}	1.4285^{20}	-43	153	35	misc alc, eth; sl s aq
h6	Heptane	$\text{CH}_3(\text{CH}_2)_5\text{CH}_3$	100.21	1, 154	0.6838_4^{20}	1.3877^{20}	-90.6	98.4	-1	s alc, chl, eth
h7	1,7-Heptanediamine	$\text{H}_2\text{N}(\text{CH}_2)_7\text{NH}_2$	130.24	4, 271			27-29	147-149	87	
h8	Heptanedioic acid	$\text{HOOC}(\text{CH}_2)_5\text{COOH}$	160.17	2, 670	1.329^{15}		105.8	212 ^{10mm}		5 aq; v s alc, eth
h9	1-Heptanethiol	$\text{CH}_3(\text{CH}_2)_6\text{SH}$	132.27	1, 415			-43.2	176.9	46	i aq
h10	Heptanoic acid	$\text{CH}_3(\text{CH}_2)_5\text{COOH}$	130.19	2, 338	0.9181_4^{20}	1.4221^{20}	-7.5	223.0	>112	0.25 aq; s alc, eth
h11	Heptanoic anhydride	$[\text{CH}_3(\text{CH}_2)_5\text{CO}]_2\text{O}$	242.36	2, 340	0.932_4^{20}	1.4332^{20}	-12.4	268	>112	i aq; s alc, eth
h12	1-Heptanol	$\text{CH}_3(\text{CH}_2)_6\text{OH}$	116.20	1, 414	0.8219_4^{20}	1.4242^{20}	-34.6	175.8	73	misc alc, eth
h13	2-Heptanol	$\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{OH})\text{CH}_3$	116.20	1, 415	0.8193_4^{20}	1.4210^{20}		160	41	0.35 aq; s alc, bz, eth

h14	3-Heptanol	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{OH})\text{-CH}_2\text{CH}_3$	116.20	1 ¹ , 205	0.818	1.4214 ²⁰		66 ^{20mm}	54	sl s aq
h15	2-Heptanone	$\text{CH}_3(\text{CH}_2)_4\text{COCH}_3$	114.19	1, 699	0.8197 ¹⁵ ₄	1.4116 ¹⁵	−35	151	47	s alc, eth
h16	3-Heptanone	$\text{CH}_3(\text{CH}_2)_3\text{C(=O)-CH}_2\text{CH}_3$	114.19	1, 699	0.8197 ²⁰ ₂₀	1.4085 ²⁰	−36.7	147.8	41	0.43 aq; s alc, eth
h17	4-Heptanone	$\text{CH}_3\text{CH}_2\text{CH}_2(\text{O})\text{CH}_2\text{-CH}_2\text{CH}_3$	114.19	1, 699	0.821 ¹⁵ ₄	1.4068 ²⁰	−32.1	143.7	48	0.53 aq; misc alc, eth
h18	Heptanoyl chloride	$\text{CH}_3(\text{CH}_2)_5\text{COCl}$	148.63	2, 340	0.960 ²⁰	1.4300 ²⁰		173	57	d aq, alc; s eth
h19	1-Heptene	$\text{CH}_3(\text{CH}_2)_4\text{CH=CH}_2$	98.90	1, 219	0.6970 ²⁰	1.3999 ²⁰	−118.9	93.6	−1	0.1 aq; s alc, eth
h20	1-Heptylamine	$\text{CH}_3(\text{CH}_2)_6\text{NH}_2$	115.22	4, 193	0.777	1.4243 ²⁰	−23	154–156	35	s alc, acet, eth, PE
h21	Heptyltrichlorosilane	$\text{CH}_3(\text{CH}_2)_6\text{SiCl}_3$	233.7		1.087 ²⁰ ₄	1.4439 ²⁵		211–212		
h22	1-Heptyne	$\text{CH}_3(\text{CH}_2)_4\text{C}\equiv\text{CH}$	96.17	1, 256	0.733	1.4075 ²⁰	−81	99–100	22	
h23	Hexachloroacetone	$\text{Cl}_3\text{CC(=O)CCl}_3$	264.75	1, 657	1.743	1.5112 ²⁰	−30	66 ^{6mm}	none	sl s aq; s acet
h24	Hexachlorobenzene	C_6Cl_6	284.78	5, 205	2.044 ²⁴		231	323–326		s bz, chl, eth
h25	Hexachloro-1,3-butadiene	$\text{Cl}_2\text{C=CClCCl=CCl}_2$	260.76	1, 250	1.655	1.5550 ²⁰	−19	210–220	none	s alc, eth
h26	1,2,3,4,5,6-Hexachlorocyclohexane	$\text{C}_6\text{H}_6\text{Cl}_6$	290.83	5 ² , 11	1.87 ²⁰		113			s bz, chl
h27	Hexachlorocyclo-1,3-pentadiene		272.77		1.701 ²⁵ ₄	1.5644 ²⁰	−10	239	none	

Glycidol, e11
 Glycidyl methacrylate, e12
 Glycinonitrile, a106
 Glycolaldehyde, h86
 Glycolaldehyde diethyl acetal, d253
 Glycolic acid, h87
 Glycol methacrylate, h121

Glyoxaline, 14
 Guaiacol, m87
 Heliotropin, m239
 Heliotropyl alcohol, m242
 Hemimellitene, t333
 Hemimellitic acid, b28
 Heptaldehyde, h5

sec-Heptyl alcohol, h13
 Heptyl bromide, b291
 Heptyl chloride, c128
 Heptyl iodide, i37
 Heptyl mercaptan, h9
 Hexachloro-2-propanone, h23



h27

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h28	Hexachlorodisiloxane	$\text{Cl}_3\text{SiOSiCl}_3$	284.9				−35	137		s alc, bz, chl, eth
h29	Hexachloroethane	Cl_3CCCl_3	236.74	1, 87	2.091 ₄ ²⁰		187–188			
h30	1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-dicarboxylic anhydride		370.83				235–239			
h31	Hexachloropropene	$\text{Cl}_3\text{CC}(\text{Cl})=\text{CCl}_2$	248.75	1, 200	1.765	1.5480 ²⁰		210	none	misc eth
h32	Hexadecane	$\text{CH}_3(\text{CH}_2)_{14}\text{CH}_3$	226.45	1, 172	0.7733 ₄ ²⁰	1.4345 ²⁰	18.2	286.8	135	
h33	1,2-Hexadecanediol	$\text{CH}_3(\text{CH}_2)_{13}\text{CH}(\text{OH})\text{CH}_2\text{OH}$	258.45	1 ³ , 2244			72–74			
h34	1-Hexadecanethiol	$\text{CH}_3(\text{CH}_2)_{15}\text{SH}$	258.51	1, 430	0.840	1.4720 ²⁰	18–20	184 ^{7mm}	101	sl s alc; s eth
h35	Hexadecanoic acid	$\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$	256.43	2, 370	0.852 ₄ ⁶²	1.4273 ⁸⁰	63–64	215 ^{15mm}		s hot alc, chl, eth
h36	1-Hexadecanol	$\text{CH}_3(\text{CH}_2)_{15}\text{OH}$	242.45	1, 429	0.8116 ⁶⁰	1.4355 ⁶⁰	49.3	344	135	s alc, chl, eth
h37	1-Hexadecene	$\text{CH}_3(\text{CH}_2)_{13}\text{CH}=\text{CH}_2$	224.43	1, 226	0.783 ₄ ²⁰	1.4401	4.1	274	132	s alc, eth, PE
h38	1-Hexadecylamine	$\text{CH}_3(\text{CH}_2)_{15}\text{NH}_2$	241.46	4, 202			40–42	330	140	v s alc, eth; s bz, chl
h39	4-Hexadecylaniline	$\text{CH}_3(\text{CH}_2)_{15}\text{C}_6\text{H}_4\text{NH}_2$	317.56	12, 1186			51–52	254–255 ^{15mm}		
h40	2,4-Hexadienal	$\text{CH}_3\text{CH}=\text{CHCH}=\text{CHCHO}$	96.13	1 ² , 809	0.898 ²⁰	1.5386 ²⁰		76 ^{30mm}	67	
h41	1,5-Hexadiene	$\text{H}_2\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2$	82.15	1, 253	0.6923 ₄ ²⁰	1.4042 ²⁰	−140.7	59.5	<1	s alc, eth
h42	2,4-Hexadienoic acid	$\text{CH}_3\text{CH}=\text{CHCH}=\text{CHCOOH}$	112.13	2, 483			134.5	119 ^{10mm}	127	0.2 aq; 13 alc; 9 acet; 2.3 bz; 11 diox; 1 CCl_4
h43	Hexafluorobenzene	C_6F_6	186.05		1.6182 ²⁰	1.3781 ²⁰	5.1	80.3	10	
h44	Hexafluoroethane	F_3CCF_3	138.01	1 ³ , 132	1.590 ^{−78}		−100.1	−78.3		sl s alc, eth
h45	1,1,1,3,3,3-Hexafluoro-2-propanol	$(\text{CF}_3)_2\text{CHOH}$	168.04		1.596 ²⁵	1.2750 ²⁰	−3	58.2	4	s aq, bz, CCl_4
h46	cis-Hexahydroindane		124.23	5, 82	0.876	1.4702	−53	167	23	s eth
h47	Hexamethylbenzene	$\text{C}_6(\text{CH}_3)_6$	162.28	5, 450			165.6	264		v s bz; s acet, eth

h48	Hexamethylcyclotri-siloxane	[—Si(CH ₃) ₂ O—] ₃	222.48	4 ³ , 1884			64	133–135	35	
h49	1,1,1,3,3,3-Hexamethyltrisilazane	(CH ₃) ₃ SiNHSi(CH ₃) ₃	161.40		0.774 ₄ ²⁰	1.4071 ²⁰		126	22	
h50	Hexamethyldi-siloxane	(CH ₃) ₃ SiOSi(CH ₃) ₃	162.38		0.764 ₄ ²⁰	1.3775 ²⁰	–67	101	–1	
h51	Hexamethyleneimine		99.18	20, 94	0.880	1.4631 ²⁰		138 ^{749mm}	18	
h52	Hexamethylene-tetramine		140.19	1, 583	1.331 ^{–5}	subl 263			250	67 aq; 8 alc; 10 chl
h53	Hexamethylphosphor-amide	[(CH ₃) ₂ N] ₃ P(O)	179.20		1.027 ²⁰	1.4588 ²⁰	7.2	233	105	misc aq
h54	Hexanal	CH ₃ (CH ₂) ₄ CHO	100.16	1 ² , 745	0.8335 ₄ ²⁰	1.4035 ²⁰		131	32	v s alc, eth; sl s aq
h55	Hexane	CH ₃ (CH ₂) ₄ CH ₃	86.18	1, 142	0.6594 ₄ ²⁰	1.3749 ²⁰	–95.4	68.7	–23	misc alc, chl, eth
h56	1,6-Hexanediamine	H ₂ N(CH ₂) ₆ NH ₂	116.21	4, 269			42	205	81	v s aq; sl s alc, bz
h57	1,6-Hexanedioic acid	HOOC(CH ₂) ₄ COOH	146.14	2, 649	1.360 ₄ ²⁵		152	337.5	196	1.4 aq; v s alc; s acet

$\alpha,\alpha,\alpha',\alpha'$ -Hexachloro-*p*-xylene, b202

Hexadecyl mercaptan, h34

$\alpha,\alpha,\alpha',\alpha',\alpha'$ -Hexafluoro-3,5-xylidine, b205

Hexahydroaniline, c334

Hexahydro-2*H*-azepin-2-one, o57

Hexahydrobenzaldehyde, c315

Hexahydrobenzoic acid, c317

Hexahydrobenzylamine, c324

Hexahydrophthalic acid, c320

Hexahydropyridine, p183

Hexamethylenediamine, h56

Hexamethylene diisocyanate, d410

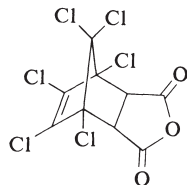
Hexamethylene, glycol, h59

Hexamethylene oxide, o47

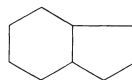
Hexamethylethane, t100

2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexene, s8

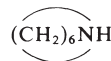
2,6,10,15,19,23-Hexamethyltetracosane, s7



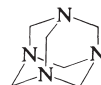
h30



h46



h51



h52

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h58	DL-Hexanediol	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{OH})\text{CH}_2\text{OH}$	118.18	1 ¹ , 251	0.951	1.4425 ²⁰		223–234	>112	
h59	1,6-Hexanediol	$\text{HO}(\text{CH}_2)_6\text{OH}$	118.18	1, 484	0.958	1.4579 ²⁵	42.8	243–250	101	v s aq, alc
h60	2,5-Hexanediol	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$	118.18	1, 485	0.9617 ⁴⁵ ₁₆	1.4465 ²⁰	–50 glass	220.8	101	s aq, alc, eth
h61	2,5-Hexanedione	$\text{CH}_3\text{COCH}_2\text{CH}_2\text{COCH}_3$	114.14	1, 788	0.973	1.4260 ²⁰	–6	191.4	70	misc aq, alc, eth
h62	Hexanedioyl dichloride	$\text{ClC}(=\text{O})(\text{CH}_2)_4\text{COCl}$	183.03	2, 653	1.259	1.4706 ²⁰		105 ^{2mm}	>112	
h63	Hexanenitrile	$\text{CH}_3(\text{CH}_2)_4\text{CN}$	97.16	2, 324	0.8052 ²⁰	1.4069 ²⁰	–80.3	163.6	43	i aq; s alc, eth
h64	1-Hexanethiol	$\text{CH}_3(\text{CH}_2)_5\text{SH}$	118.24	1 ³ , 1659	0.8424 ²⁰ ₄	1.4496 ²⁰	–80.5	152.7	20	i aq; v s alc, eth
h65	1,2,6-Hexanetriol	$\text{HOCH}_2\text{CH}(\text{OH})(\text{CH}_2)_3\text{CH}_2\text{OH}$	134.17		1.1063 ²⁰ ₂₀	1.4771	–32.8	178 ^{5mm}	79	misc alc, acet; i bz
h66	Hexanoic acid	$\text{CH}_3(\text{CH}_2)_4\text{COOH}$	116.16	2, 321	0.9265 ²⁰ ₄	1.4168 ²⁰	–4.0	205.7	104	1.1 aq; v s alc, eth
h67	Hexanoic anhydride	$[\text{CH}_3(\text{CH}_2)_4\text{C}(=\text{O})]_2\text{O}$	214.31	2, 324	0.926	1.4280 ²⁰	–41	246–248	>112	s alc
h68	1-Hexanol	$\text{CH}_3(\text{CH}_2)_5\text{OH}$	102.18	1, 407	0.8186 ²⁰ ₄	1.4182 ²⁰	–51.6	157.5	60	8 aq; misc bz, eth; s alc
h69	2-Hexanol	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{OH})\text{CH}_3$	102.18	1, 408	0.8108 ²⁵ ₄	1.4128 ²⁵	–47	139.9	41	sl s aq; s alc, eth
h70	3-Hexanol	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$	102.18	1, 408	0.8193 ²⁰ ₄	1.4160 ²⁰		135	41	
h71	6-Hexanolactone		114.14	17 ² , 290	1.030	1.4630 ²⁰		97 ^{15mm}	109	
h72	2-Hexanone	$\text{CH}_3(\text{CH}_2)_3\text{COCH}_3$	100.16	1, 689	0.8209 ²⁰ ₄	1.4024 ²⁰	–56.9	127.2	35	v s alc, eth
h73	Hexanoyl chloride	$\text{CH}_3(\text{CH}_2)_4\text{COCl}$	134.61	2, 324	0.9754 ²⁰ ₄	1.4263 ²⁰	–87	153	79	d aq, alc; s eth
h74	1,4,7,10,13,16-Hexaoxacyclooctadecane		264.32				40			
h75	1-Hexene	$\text{CH}_3(\text{CH}_2)_3\text{CH}=\text{CH}_2$	84.16	1, 215	0.6732 ²⁰	1.3879 ²⁰	–139.8	63.5	–26	0.005 aq
h76	<i>trans</i> -3-Hexenoic acid	$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2\text{COOH}$	114.14	2, 435	0.963	1.4398 ²⁰	11–12	119 ^{22mm}	>112	
h77	<i>trans</i> -2-Hexen-1-ol	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_2\text{OH}$	100.16	1 ² , 486	0.849	1.4343 ²⁰		158–160	54	

h78	5-Hexen-2-one	$\text{H}_2\text{C}=\text{CHCH}_2\text{CH}_2\text{COCH}_3$	98.15	1,734	0.847	1.4197 ²⁰		128–129	23	
h79	Hexyl acetate	$\text{CH}_3(\text{CH}_2)_5\text{OOCCH}_3$	144.21	2,132	0.860 ²⁰ ₂₀	1.4090 ²⁰	–80	168–170	37	0.13 aq; v s alc, eth
h80	Hexylamine	$\text{CH}_3(\text{CH}_2)_5\text{NH}_2$	101.19	4,188	0.763 ²⁵ ₄	1.4180 ²⁰	–23	131–132	8	sl s aq; misc alc, eth
h81	4-Hexylaniline	$\text{CH}_3(\text{CH}_2)_5\text{C}_6\text{H}_4\text{NH}_2$	177.29	12 ³ , 2759				146–148 ^{17mm}		
h82	1-Hexyne	$\text{H}(\text{CH}_2)_4\text{C}\equiv\text{CH}$	82.14	1 ³ , 977	0.7152 ²⁰ ₄	1.3989 ²⁰	–131.9	71.3		i aq; s alc, eth
h83	L-Histidine		155.16	25, 513			d 285			41 aq; v sl s alc
h84	Hydantoin		100.08	24, 242			220			s alc, alk; sl s eth
h85	Hydrindantin		322.27	8 ¹ , 631			100	d 252		v sl s aq
h86	Hydroxyacetaldehyde	HOCH_2CHO	60.05	1,817	1.366 ¹⁰⁰		93–94	110 ^{12mm}		v s aq, alc; sl s eth
h87	Hydroxyacetic acid	HOCH_2COOH	76.05	3, 228			80			

D-*erythro*-Hex-2-enoic acid γ -lactone, 159

Hexyl alcohol, h68

sec-Hexyl alcohol, e83

sec-Hexylamine, m353a

Hexylbenzene, p117

Hexyl bromide, b294

Hexyl chloride, c129

Hexylene glycol, m338

Hexyl iodide, i39

Hexyl methyl ketone, o34

Hexyl propyl ketone, d16

Hippuric acid, b71

Histamine, i8

Homocysteine, a204

Homopiperidine, h51

Homoserines, a188, a189

Homoveratric acid, d447

Homoveratrylamine, d451

Hydracrylonitrile, h169

2-Hydrazinoethanol, h120

Hydrazobenzene, d673

Hydrindene, i13

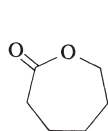
Hydrocinnamic acid, p146

Hydroquinone, d379

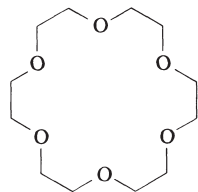
Hydroquinone dimethyl ether, d433

Hydroquinonesulfonic acid, d382

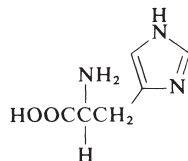
Hydroxyacetanilides, a15, a16, a17



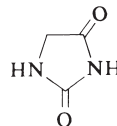
h71



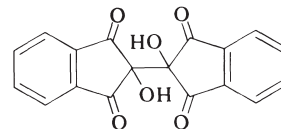
h74



h83



h84



h85

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h88	1'-Hydroxy-2'-aceto-naphthone	$C_{10}H_6(OH)COCH_3$	186.21	8, 149			98–100	325 sl d		i aq; v s bz; s HOAc
h89	Hydroxyacetone	$HOCH_2COCH_3$	74.08	1 ¹ , 84	1.082	1.4315 ²⁰	–17	145–146	56	misc aq, alc, eth
h90	<i>o</i> -Hydroxyacetophenone	$HOC_6H_4COCH_3$	136.15	8, 85	1.131 ₄ ²¹	1.5584 ²⁰	4–6	213 ^{717mm}	>112	misc alc, eth; sl s aq
h91	<i>m</i> -Hydroxyacetophenone	$HOC_6H_4COCH_3$	136.15	8, 86	1.100 ¹⁰⁰	1.535 ¹⁰⁰	87–88	296		s aq; v s alc, bz, eth
h92	<i>p</i> -Hydroxyacetophenone	$HOC_6H_4COCH_3$	136.15	8, 87	1.109 ¹⁰⁰		106–107	147 ^{3mm}		v s alc, eth; sl s aq
h93	1-Hydroxyanthraquinone		224.22	8, 338			196–198			
h94	2-Hydroxybenzaldehyde	$C_6H_4(OH)CHO$	122.12	8, 31	1.167 ₄ ²⁰	1.5718 ²⁰	–7	196.7	76	1.7 aq ⁸⁶ ; s alc, eth
h95	3-Hydroxybenzaldehyde	$C_6H_4(OH)CHO$	122.12	8, 58			100–102	191 ^{50mm}		s alc, bz, eth; sl s aq
h96	4-Hydroxybenzaldehyde	HOC_6H_4CHO	122.12	8, 64	1.129 ₄ ¹³⁰		117–119	subl		1 aq; 70 acet; 4 bz; v s alc, eth
h97	2-Hydroxybenzaldehyde oxime	$C_6H_4(OH)CH=NOH$	137.14	8, 49			57	d		v s alc, bz, eth, acid
h98	2-Hydroxybenzamide	$C_6H_4(OH)CONH_2$	137.14	10, 87			140	d 270		0.2 aq; s alc, chl, eth
h99	2-Hydroxybenzoic acid	$C_6H_4(OH)COOH$	138.12	10, 43	1.443 ₄ ²⁰		157–159	211 ^{20mm}		0.2 aq; 37 alc; 33 eth; 33 acet; 2 chl; 0.7 bz
h100	3-Hydroxybenzoic acid	$C_6H_4(OH)COOH$	138.12	10, 134	1.473		201–203			0.8 aq; 10 eth
h101	4-Hydroxybenzoic acid	HOC_6H_4COOH	138.12	10, 149	1.468 ⁴		214–215			0.2 aq; v s alc; 23 eth

h102	<i>p</i> -Hydroxybenzo-phenone	$\text{HOC}_6\text{H}_4\text{COC}_6\text{H}_5$	198.22	8 ² , 184			132–135			v s alc, eth; sl s aq
h103	1-Hydroxybenzo-triazole		135.13	26, 41			155–158			
h104	6-Hydroxy-1,3-benz-oxathiol-2-one		168.17	19 ⁴ , 2508			158–160			
h105	2-Hydroxybenzyl alcohol	$\text{HOC}_6\text{H}_4\text{CH}_2\text{OH}$	124.13	6, 891	1.161 ²⁵		86–87	subl 100		6.6 aq; v s alc, chl, eth; s bz
h106	3-Hydroxy-2-butanone	$\text{CH}_3\text{COCH}(\text{OH})\text{CH}_3$	88.10	1, 827	0.997	1.4171 ²⁰	15	148	50	misc aq, alc; sl s eth
h107	<i>p</i> -Hydroxycinnamic acid	$\text{HOC}_6\text{H}_4\text{CH}=\text{CHCOOH}$	164.16	10, 297			210–213			s alc, eth; sl s aq
h108	4-Hydroxycoumarin		162.14	17, 488			213 d			s aq, alc, eth
h109	7-Hydroxycoumarin		162.14	18, 27			226–228	subl		v s alc, chl, alk, HOAc
h110	1-Hydroxy-1-cyclohexanecarbonitrile	$\text{C}_6\text{H}_{10}(\text{OH})\text{CN}$	125.17	10, 5	1.031	1.4576 ²⁰	29		60	
h111	2-Hydroxy-3,5-diiodobenzoic acid	$\text{I}_2\text{C}_6\text{H}_2(\text{OH})\text{COOH}$	389.91	10, 113			235 d			v s alc, eth; i bz, chl
h112	2'-Hydroxy-4',6'-dimethylacetophenone	$(\text{CH}_3)_2\text{C}_6\text{H}_2(\text{OH})\text{COCH}_3$	164.20				53–57			

2-Hydroxybenzenemethanol, h105
m-Hydroxybenzotrifluoride, t290

2-Hydroxybiphenyl, p131
 4-Hydroxybiphenyl, p132

Hydroxybutanedioic acids, h180, h181

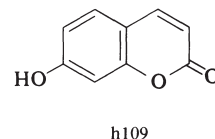
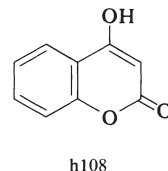
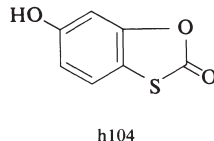
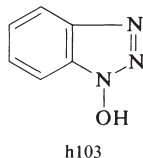
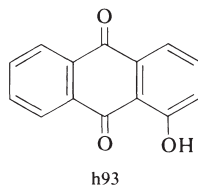


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h113	2-Hydroxydiphenylmethane	$\text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_4\text{OH}$	184.24	6, 675			20.6	312		s alc, chl, eth, alk
h114	2-Hydroxyethanesulfonic acid, Na salt	$\text{HOCH}_2\text{CH}_2\text{SO}_3^- \text{Na}^+$	148.11	4 ³ , 42			191–194			v s aq
h115	<i>N</i> -(2-Hydroxyethyl)-acetamide	$\text{HOCH}_2\text{CH}_2\text{NHCOCH}_3$	103.12	4 ¹ , 430	1.1233 ²⁰ ₂₀	1.4575 ²⁰	63–65	d	176	misc aq; sl s bz
h116	2-Hydroxyethyl acetate	$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{OH}$	104.11	2, 141	1.108 ¹⁵			181–186	102	misc aq, alc, chl, eth
h117	3-(α -Hydroxyethyl)-aniline	$\text{CH}_3\text{CH}(\text{OH})\text{C}_6\text{H}_4\text{NH}_2$	137.18	13 ³ , 1654			68–71			
h118	2-Hydroxyethyl disulfide	$\text{HOCH}_2\text{CH}_2\text{SSCH}_2\text{CH}_2\text{OH}$	154.25	1, 471	1.261	1.5655 ²⁰	25–27	158 ^{3.5mm}		
h119	<i>N</i> -(2-Hydroxyethyl)-ethylenediamine- <i>N,N,N'</i> -triacetic acid	$\text{HOOCCH}_2\text{N}(\text{CH}_2\text{CH}_2\text{OH})\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{COOH})_2$	278.26				212 d			
h120	2-Hydroxyethylhydrazine	$\text{HOCH}_2\text{CH}_2\text{NHNH}_2$	76.10	4 ¹ , 562	1.119		–70	220	73	misc aq; s alc
h121	2-Hydroxyethyl methacrylate	$\text{HOCH}_2\text{CH}_2\text{OOC}-\text{C}(\text{CH}_3)=\text{CH}_2$	130.14		1.034	1.4515 ²⁰		67 ^{3.5mm}	97	
h122	<i>N</i> -(β -Hydroxyethyl)-morpholine		131.18	27, 7	1.083	1.4760 ²⁰		227	99	misc aq
h123	<i>N</i> -(β -Hydroxyethyl)-piperazine		130.19	23 ² , 6	1.061	1.5065 ²⁰		246	>112	
h124	<i>N</i> -(2-Hydroxyethyl)-piperazine- <i>N'</i> -ethanesulfonic acid		238.31				234 d			

h125	4'-(2-Hydroxyethyl)-piperidine		129.20	21 ² , 10	1.0059 ¹⁵		199–202		
h126	2'-(2-Hydroxyethyl)-pyridine	HOCH ₂ CH ₂ C ₅ H ₄ N	123.16	21, 50	1.093	1.5368 ²⁰	116 ^{9mm}	92	v s aq, alc, chl
h127	2-Hydroxyisobutyric acid	(CH ₃) ₂ C(OH)COOH	104.11	3, 313			77–80	84 ^{1.5mm}	v s aq, alc, eth
h128	4-Hydroxy-2-mercapto-6-methylpyrimidine		142.18	24 ³ , 1289			330 d		
h129	4-Hydroxy-2-mercapto-6-propylpyrimidine		170.23				219–221		0.1 aq; 1.7 alc; 1.7 acet; v s alk; i bz
h130	2-Hydroxy-3-methoxybenzaldehyde	CH ₃ OC ₆ H ₃ (OH)CHO	152.15	8, 240			40–42	265–266	v s alc, eth; sl s aq
h131	4-Hydroxy-3-methoxybenzaldehyde	CH ₃ OC ₆ H ₃ (OH)CHO	152.15	8, 247	1.056		80–81	285	1 aq; s alc, chl, pyr
h132	4-Hydroxy-3-methoxybenzoic acid	CH ₃ OC ₆ H ₃ (OH)COOH	168.15	10, 392			210		0.12 aq; v s alc

Hydroxyethanal, h86

3-(α -Hydroxyethyl)aniline, a261

N-(2-Hydroxyethyl)-3-aza-1,5-pentanediol, t264

N-(2-Hydroxyethyl)ethyleneimine, a321

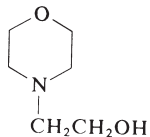
N-(2-Hydroxyethyl)piperidine, p185

2-(2-Hydroxyethyl)piperidine, p186

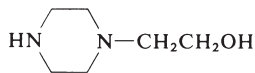
O-Hydroxyethylresorcinol, h159

2-Hydroxyisobutyronitrile, h145

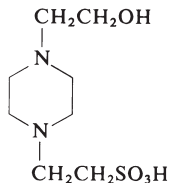
2-Hydroxy-3-methyl-2-cyclopenten-1-one, m214



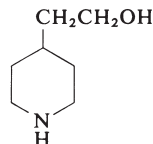
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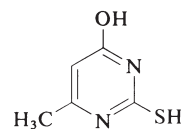
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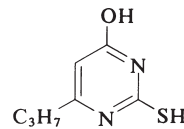
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h125



h128



h129

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

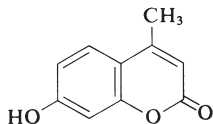
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h133	4-Hydroxy-3-methoxybenzonitrile	$\text{CH}_3\text{OC}_6\text{H}_3(\text{OH})\text{CN}$	149.15	10, 398			85–87			
h134	2-Hydroxy-4-methoxybenzophenone	$\text{CH}_3\text{OC}_6\text{H}_3(\text{OH})\text{COC}_6\text{H}_5$	228.25	8, 312			66	155 ^{5mm}		v s alc, chl, eth
h135	4-Hydroxy-3-methoxybenzyl alcohol	$\text{CH}_3\text{OC}_6\text{H}_3(\text{OH})\text{CH}_2\text{OH}$	154.17	6, 1113			113–115			
h136	4-Hydroxy-3-methoxycinnamic acid	$\text{CH}_3\text{OC}_6\text{H}_3(\text{OH})\text{CH}=\text{CH}-\text{COOH}$	194.19	10, 436			174			s hot aq, alc, eth, EtAc; sl s bz, PE
h137	2-Hydroxy-3-methylbenzoic acid	$\text{CH}_3\text{C}_6\text{H}_3(\text{OH})\text{COOH}$	152.15	10, 220			165–166			s alc, chl, eth, alk
h138	2-Hydroxy-4-methylbenzoic acid	$\text{CH}_3\text{C}_6\text{H}_3(\text{OH})\text{COOH}$	152.15	10, 233			177			s alc, chl, eth, alk
h139	4-Hydroxy-3-methyl-2-butanone	$\text{HOCH}_2\text{CH}(\text{CH}_3)\text{COCH}_3$	102.13	1 ¹ , 422	0.993	1.4340 ²⁰		92 ^{15mm}	78	
h140	7-Hydroxy-4-methylcoumarin		176.17	18, 31			194–195			s alc, HOAc; sl s eth
h141	2-Hydroxymethyl-2-methyl-1,3-propanediol	$\text{HOCH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{OH})_2$	120.09	1, 520			199–203			
h142	4-Hydroxy-4-methyl-2-pentanone	$(\text{CH}_3)_2\text{C}(\text{OH})\text{CH}_2\text{COCH}_3$	116.16		0.9385 ²⁰	1.4235 ²⁰	–42.8	169	12	misc aq
h143	<i>N</i> -(Hydroxymethyl)phthalimide		177.16	21, 475			142–145			sl s aq, alc, bz
h144	4-Hydroxy- <i>N</i> -methylpiperidine		115.18	21 ¹ , 188		1.4775 ²⁰	29–31	200	>112	
h145	2-Hydroxy-2-methylpropanenitrile	$(\text{CH}_3)_2\text{C}(\text{OH})\text{CN}$	85.10	3, 316	0.9267 ²⁵ ₄	1.3992 ²⁰	–19	95	63	s aq, alc, chl, eth

h146	3-Hydroxy-2-methyl-4-pyrone		126.11			161–162		1.2 aq; v s hot aq; s alc, alk; sl s bz, eth
h147	2-Hydroxy-1-naphthaldehyde	$C_{10}H_6(OH)CHO$	172.18	8, 143		82–85	192 ^{27mm}	
h148	1-Hydroxy-2-naphthalenecarboxylic acid	$C_{10}H_6(OH)COOH$	188.18	10, 331		191–192		v s alc, bz, eth, alk
h149	3-Hydroxy-2-naphthalenecarboxylic acid	$C_{10}H_6(OH)COOH$	188.18	10, 333		222–223		v s alc, eth; s bz, chl
h150	2-Hydroxy-3,6-naphthalenedisulfonic acid, disodium salt	$C_{10}H_5(OH)(SO_3^-Na^+)_2$	348.25	11, 288				v s aq, alc; i eth
h151	4-Hydroxy-2,7-naphthalenedisulfonic acid, disodium salt	$C_{10}H_5(OH)(SO_3^-Na^+)_2$	348.25	11, 227		> 300		
h152	2-Hydroxy-1,4-naphthoquinone		174.16	8, 300		d 185		s HOAc

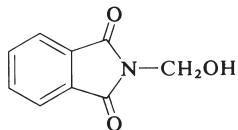
3-Hydroxymethylpiperidine, p187

1-Hydroxy-2-naphthoic acid, h148

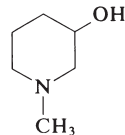
3-Hydroxy-2-naphthoic acid, h149



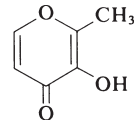
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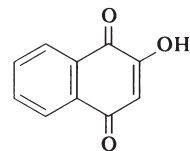
h143



h144



h146



h152

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

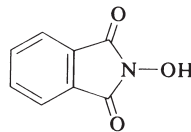
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h153	4-Hydroxy-3-nitrobenzenearsonic acid	$\text{HOC}_6\text{H}_3(\text{NO}_2)\text{-AsO}(\text{OH})_2$	263.04	16 ¹ , 456			>300			v s alc, acet, HOAc, alk; sl s aq; i eth
h154	3-Hydroxy-4-nitrobenzoic acid	$\text{HOC}_6\text{H}_3(\text{NO}_2)\text{COOH}$	183.12	10, 146			229–231			
h155	2-Hydroxy-5-nitrobenzyl bromide	$\text{HOC}_6\text{H}_3(\text{NO}_2)\text{CH}_2\text{Br}$	232.04	6, 367			147–149			
h156	5-Hydroxy-1-pentanal	$\text{HO}(\text{CH}_2)_4\text{CHO}$	102.13		1.055	1.4530 ²⁰		115 ^{15mm}	>112	s aq
h157	5-Hydroxy-2-pentanone	$\text{CH}_3\text{COCH}_2\text{CH}_2\text{CH}_2\text{OH}$	102.13	1, 831	1.007 ₄ ²⁰	1.4372 ²⁰		144 ^{100mm}	93	misc aq; s alc, eth
h158	4-Hydroxy-3-penten-2-one acetate	$\text{CH}_3\text{COOC}(\text{CH}_3)=\text{CH-COCH}_3$	142.15			1.4525 ²⁰		195	75	
h159	2-(<i>m</i> -Hydroxyphenoxy)ethanol	$\text{HOC}_6\text{H}_4\text{OCH}_2\text{CH}_2\text{OH}$	154.17				83–86			
h160	4-Hydroxyphenylacetic acid	$\text{HOC}_6\text{H}_4\text{CH}_2\text{COOH}$	152.15	10, 190			149–151	subl		v s alc, eth; sl s aq
h161	2-Hydroxy- <i>N</i> -phenylbenzamide	$\text{HOC}_6\text{H}_4\text{CONHC}_6\text{H}_5$	213.14	12, 500			136			v s alc, bz, chl, eth
h162	4-(<i>p</i> -Hydroxyphenyl)-2-butanone	$\text{HOC}_6\text{H}_4\text{CH}_2\text{CH}_2\text{COCH}_3$	164.20				82–83			
h163	D-(–)- <i>p</i> -Hydroxyphenylglycine	$\text{HOC}_6\text{H}_4\text{CH}(\text{NH}_2)\text{COOH}$	167.16	14 ¹ , 659			240 d			sl s aq, alc, bz, acet
h164	<i>N</i> -(<i>p</i> -Hydroxyphenyl)glycine	$\text{HOC}_6\text{H}_4\text{NHCH}_2\text{COOH}$	167.16	13, 488			220–248 d			s alk, acid; v sl s aq, alc, acet, bz, chl, eth
h165	1-(3-Hydroxyphenyl)-urea	$\text{HOC}_6\text{H}_4\text{NHCONH}_2$	152.15	13, 417			182–184			

h166	<i>N</i> -Hydroxyphthalimide		163.13	21, 500			233 d			
h167	<i>N</i> -Hydroxypiperidine		101.15	20, 80			37–40	111 ^{55mm}		
h168	2-Hydroxypropionitrile	CH ₃ CH(OH)CN	71.08	3 ² , 209	0.9834 ²⁵	1.4027 ²⁵	–34	103 ^{50mm}	77	misc aq, alc; s eth
h169	3-Hydroxypropionitrile	HOCH ₂ CH ₂ CN	71.08	3, 298	1.0404 ²⁵ ₄	1.4256 ²⁰	–46	228	>112	misc aq, alc, acet; 2.3 eth; i bz, PE
h170	<i>o</i> -Hydroxypropio-phenone	HOC ₆ H ₄ COCH ₂ CH ₃	150.18	8, 102	1.094	1.5480 ²⁰		115 ^{15mm}	>112	v s alc, eth; sl s aq
h171	<i>p</i> -Hydroxypropio-phenone	HOC ₆ H ₄ COCH ₂ CH ₃	150.18	8, 102			148			v s alc, eth; sl s aq
h172	1-(2-Hydroxy-1-propoxy)-2-propanol	CH ₃ CH(OH)CH ₂ OCH ₂ -CH(OH)CH ₃	134.18		1.0252 ²⁰ ₂₀	1.4440 ²⁰		231.8	138	misc aq, alc
h173	2-Hydroxypyridine	HOC ₅ H ₄ N	95.10	21, 43			105–107	280–281		s aq, alc, bz; sl s eth
h174	3-Hydroxypyridine	HOC ₅ H ₄ N	95.10	21, 46			126–129	151 ^{3mm}		v s aq, alc; sl s eth
h175	4-Hydroxypyridine	HOC ₅ H ₄ N	95.10	21, 48				230 ^{12mm}		v s aq; i alc, bz, eth
h176	2-Hydroxypyridine-5-carboxylic acid	HO(C ₅ H ₃ N)COOH	139.11	22, 215			>300			sl s aq, alc, eth

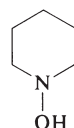
6-Hydroxynicotinic acid, h176
 α -Hydroxy- α -phenylacetophenone, b46
3-(*p*-Hydroxyphenyl)alanine, t437

2-Hydroxy-2-phenylbenzeneacetic acid, b36
3-Hydroxy-1-propanesulfonic acid γ -sultone, p198

2-Hydroxypropanoic acids, L1, L2
1-Hydroxy-2-propanone, h89
3-Hydroxypropionitrile, c290



h166



h167

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

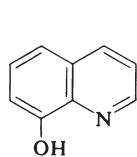
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
h177	3-Hydroxypyridine- <i>N</i> -oxide	(HO)C ₅ H ₄ N=O	111.10				190–192			
h178	8-Hydroxyquinoline		145.16	21, 91			76	267		v s alc, acet, bz, chl
h179	8-Hydroxyquinoline-5-sulfonic acid		225.22	22, 407			213 d			v s aq; sl s alc, eth
h180	DL-Hydroxysuccinic acid	HOOCCH(OH)CH ₂ COOH	134.09	3, 435			131–133			56 aq; 45 EtOH; 18 acet; 0.8 eth; 23 diox; i bz
h181	L-Hydroxysuccinic acid	HOOCCH(OH)CH ₂ COOH	134.09	3, 419			100			36 aq; 87 EtOH; 2.7 eth; 61 acet; 75 diox
h182	<i>N</i> -Hydroxy-succinimide		115.09	21, 380			93–95			v s aq
h183	6-Hydroxytetrahydropyran-2-carboxylic acid lactone		128.13		1.226	1.4593 ²⁰				
h184	3-Hydroxy-3,7,11-trimethyl-1,6,10-dodecatriene	H ₂ C=CHC(OH)(CH ₃)-CH ₂ CH ₂ CH=C(CH ₃)-CH ₂ CH ₂ CH=C(CH ₃) ₂	222.37		0.8760 ²⁵	1.4769 ²⁵		114 ^{1mm}	96	s abs alc
h185	3-Hydroxy-2,2,4-trimethyl-3-pentenoic acid β -lactone		140.18		0.947	1.4380 ²⁰	–18	170	62	
h186	Hypoxanthine		136.11	26, 416			d 150			0.25 aq; s alk, acid
i1	1 <i>H</i> ,1 <i>H</i> ,11 <i>H</i> -Icosafluoro-1-undecanol	HCF ₂ (CF ₂) ₉ CH ₂ OH	531.1				95–97	181 ^{200mm}		
i2	Icosane	CH ₃ (CH ₂) ₁₈ CH ₃	282.56	1, 174	0.7777 ³⁷	1.4346 ⁴⁰	36.4	343.8	>112	
i3	1-Icosene	CH ₃ (CH ₂) ₁₇ CH=CH ₂	280.54	1 ³ , 881			28.7	342.4		

i4	Imidazole		68.08	23, 45			90–91	257	145	v s aq, alc, chl, eth
i5	2-Imidazolidinethione		102.16	24, 4			203–204			2 aq; s alc, pyr; i bz, acet, chl, eth
i6	Imidazolidinetrione		114.06				230	subl 100		5 aq; s alc
i7	2-Imidazolidone		86.09	24, 16			131			v s aq, hot alc
i8	2-(4-Imidazolyl)ethylamine		111.15	25, 315			83–84	209 ^{18mm}		v s aq, alc, hot chl
i9	3,3'-Iminobispropylamine	$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{CH}_2\text{NH}_2$	131.22		0.938	1.4810 ²⁰	–14	151 ^{50mm}	118	
i10	Iminodiacetic acid	$\text{HOOCCH}_2\text{NHCH}_2\text{COOH}$	133.10	4, 365			243 d			2 aq; v sl s bz, eth
i11	Iminodiacetonitrile	$\text{NCCH}_2\text{NHCH}_2\text{CN}$	95.11	4, 367			77			s aq, alc: sl s eth
i12	Iminodibenzyl		195.27				105–108			
i13	Indan		118.18		0.9639 ²⁰ ₄	1.5360 ²⁰	–51.4	176.5	50	s alc, chl, eth; i aq
i14	5-Indanol		134.18	6, 575			51–53	255		v s alc, eth; sl s aq
i15	1-Indanone		132.16	7, 360	1.1090 ⁴⁵ ₄	1.561 ⁴⁵	40–42	243–245		s alc, eth; sl s aq

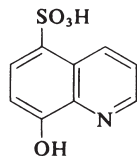
5-Hydroxyvaleraldehyde, h156
Imidodicarbonic diamide, b215

Indalone, b445

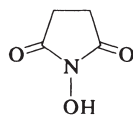
Indanamines, a199, a200



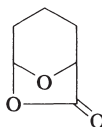
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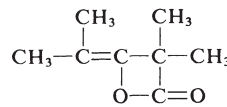
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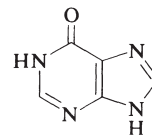
h182



h183



h185



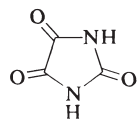
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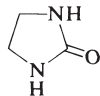
i4



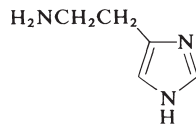
i5



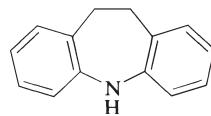
i6



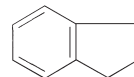
i7



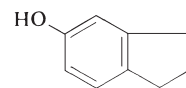
i8



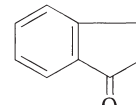
i12



i13



i14



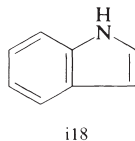
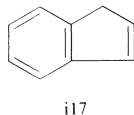
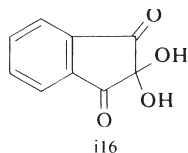
i15

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

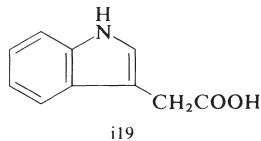
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
i16	1,2,3-Indantrione hydrate		178.14				d 241			
i17	Indene		116.16	5, 515	0.9968 ₄ ²⁰	1.5762 ²⁰	−1.8	181.6	78	misc alc, bz, chl, eth
i18	Indole		117.15	20, 304	1.0643	1.609 ⁶⁰	52	253		s hot aq, bz, eth
i19	Indole-3-acetic acid		175.19	22, 66			168–170			v s alc; s acet, eth
i20	Indole-3-carbaldehyde		145.16	21, 313			195–198			
i21	Indole-2,3-dione		147.13	21, 432			203.5 d			s hot aq, hot alc, alk
i22	Indoline		119.17	20, 257	1.063	1.5906 ²⁰		221	92	sl s aq
i23	Inositol		180.16	6 ² , 1157	1.752		225–227			14 aq; sl s aq; i eth
i24	Iodoacetamide	ICH ₂ CONH ₂	184.96	2, 223			91–93			s hot aq
i25	Iodoacetic acid	ICH ₂ COOH	185.95	2, 222			82–83			s aq, alc; v sl s eth
i26	3-Iodoaniline	IC ₆ H ₄ NH ₂	219.03	12, 670	1.821	1.6820 ²⁰	25	146 ^{15mm}	>112	i aq; s alc, eth
i27	Iodobenzene	C ₆ H ₅ I	204.01	5, 215	1.8383 ₄ ²⁵	1.621 ¹⁸	−30	188.3	74	misc alc, chl, eth
i28	Iodobenzene diacetate	C ₆ H ₅ I(OOCCH ₃) ₂	322.10				163–165			
i29	2-Iodobenzoic acid	IC ₆ H ₄ COOH	248.02	9, 363	2.249 ₄ ²⁵		162			s alc, eth; sl s aq
i30	1-Iodobutane	CH ₃ CH ₂ CH ₂ CH ₂ I	184.02	1, 123	1.616 ₄ ²⁰	1.4999 ²⁰	−103.5	129–130	33	i aq; s alc, eth
i31	2-Iodobutane	CH ₃ CH ₂ CH(I)CH ₃	184.02		1.592 ₄ ²⁰	1.4991 ²⁰	−104.0	118–120	28	i aq; s alc, eth
i32	Iodocyclohexane	C ₆ H ₁₁ I	210.06	5 ² , 13	1.626 ₁₅ ¹⁵	1.5472 ²⁰		180		i aq; s eth
i33	1-Iododecane	CH ₃ (CH ₂) ₉ I	268.18	1, 168	1.257 ₄ ²⁰	1.4827 ²⁰		132 ^{15mm}		i aq; s alc, eth
i34	Iodoethane	CH ₃ CH ₂ I	155.97	1, 96	1.9358 ²⁰	1.5137	−110.9	72.4	none	0.4 aq; misc alc, bz, chl, eth
i35	2-Iodoethanol	ICH ₂ CH ₂ OH	171.97	1, 339	2.2197 ₄ ²⁰	1.5694 ²⁰		75 ^{5mm}	65	s aq; v s alc, eth
i36	Iodoform	CHI ₃	393.73	1, 73	4.008		120–123		none	1.4 alc; 10 chl; 13 eth; v s bz, acet
i37	1-Iodoheptane	CH ₃ (CH ₂) ₆ I	226.10	1, 155	1.373 ₄ ²⁰	1.4900 ²⁰	−48.2	204	78	i aq; s alc, eth
i38	1-Iodohexadecane	CH ₃ (CH ₂) ₁₅ I	352.35	1, 172	1.121	1.4806 ²⁰		206–207 ^{10mm}		

i39	1-Iodoheptane	$\text{CH}_3(\text{CH}_2)_5\text{I}$	212.08	1, 146	1.437^{20}_4	1.4926^{20}		179.5	61	i aq
i40	Iodomethane	CH_3I	141.94	1, 69	2.2789^{20}_4	1.5308^{20}	-66.5	42.4	none	1.4 aq; misc alc, eth
i41	4-Iodomethoxybenzene	$\text{IC}_6\text{H}_4\text{OCH}_3$	234.04	6, 208			48-50	$237^{726\text{mm}}$		s hot alc, eth
i42	1-Iodo-3-methylbutane	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{I}$	198.06	1 ³ , 367	1.509^{20}_4	1.4939^{20}		147.5		misc alc, eth; sl s aq
i43	1-Iodo-2-methylpropane	$(\text{CH}_3)_2\text{CHCH}_2\text{I}$	184.02	1, 128	1.603^{20}_4		-93.5	119		i aq; misc alc, eth
i44	2-Iodo-2-methylpropane	$(\text{CH}_3)_3\text{CI}$	184.02	1 ³ , 326	1.571^0_0	1.4918^{20}	-38.2			d aq; misc alc, eth
i45	1-Iodo-3-nitrobenzene	$\text{IC}_6\text{H}_4\text{NO}_2$	249.01	5, 253	1.9477^{50}_{24}		36-38	280		i aq; s alc, eth
i46	1-Iodooctane	$\text{CH}_3(\text{CH}_2)_7\text{I}$	240.13	1, 160	1.330^{20}_{24}	1.4889^{20}	-45.9	221		s alc, eth
i47	1-Iodopentane	$\text{CH}_3(\text{CH}_2)_4\text{I}$	198.06	1, 133	1.512^{20}_{24}	1.4954^{20}	-85.6	154.5	79	sl s aq; s alc, eth
i48	1-Iodopropane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{I}$	169.99	1, 113	1.7489^{20}_{20}	1.5058^{20}	-101	102.5	none	0.1 aq; misc alc, eth

Indonaphthene, i17



4-Iodoanisole, i41



5-Iodoanthranilic acid, a203

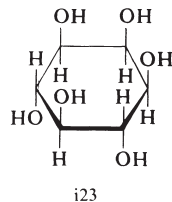
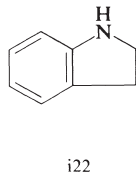
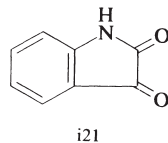
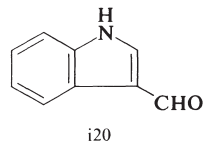


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
i49	2-Iodopropane	$(\text{CH}_3)_2\text{CHI}$	169.99	1, 114	1.7025 ₄ ²⁰	1.4992 ²⁰	−90.0	89.5	none	0.14 aq; misc alc, bz, chl, eth
i50	3-Iodo-1-propene	$\text{ICH}_2\text{CH}=\text{CH}_2$	167.97	1 ³ , 114	1.845 ₄ ²²	1.5540 ²¹	−99	1–3		misc alc, chl, eth
i51	5-Iodosalicylic acid	$\text{IC}_6\text{H}_3(\text{OH})\text{COOH}$	264.02	10, 112			189–191			v s alc; i bz, chl
i52	2-Iodothiophene		210.04	17, 34	1.902	1.6520 ²⁰	−40	73 ^{15mm}	71	v s eth
i53	2-Iodotoluene	$\text{IC}_6\text{H}_4\text{CH}_3$	218.04	5, 310	1.713	1.6079 ²⁰		211	90	i aq; s alc, eth
i54	3-Iodotoluene	$\text{IC}_6\text{H}_4\text{CH}_3$	218.04	5, 311	1.698	1.6040 ²⁰		80 ^{10mm}	82	i aq; misc alc, eth
i55	Iodotrimethylsilane	$(\text{CH}_3)_3\text{SiI}$	200.10		1.406 ₄ ²⁰	1.4710 ²⁰		106	< 1	
i56	α -Ionone		192.30	7, 168	0.932 ²⁰	1.4980 ²⁰		124 ^{11mm}	104	s alc, bz, chl, eth
i57	β -Ionone		192.30	7, 167	0.946 ¹⁷	1.521 ¹⁷		140 ^{18mm}	> 112	s alc, bz, chl, eth
i58	Isatoic anhydride		163.13	27, 264			233 d			sl s aq, hot alc, acet
i59	D-(−)-Isoascrobic acid		176.12				169 d			s aq, alc, acet, pyr
i60	DL-Isoborneol		154.25	6 ² , 80			212	subl		v s alc, chl, eth
i61	2-Isobutoxy-1-isobutoxycarbonyl-1,2-dihydroquinoline		303.40		1.022	1.5230 ²⁰		140 ^{0.2mm}	> 112	
i62	Isobutyl acetate	$(\text{CH}_3)_2\text{CHCH}_2\text{OOCCH}_3$	116.16	2, 131	0.8745 ²⁰	1.3902 ²⁰	−98.9	118.0	25	0.7 aq; v s alc
i63	Isobutylamine	$(\text{CH}_3)_2\text{CHCH}_2\text{NH}_2$	73.14	4, 163	0.724 ₄ ²⁰	1.3972 ²⁰	−84.6	67.7	−26	misc aq, alc, acet, eth
i64	Isobutylbenzene	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}(\text{CH}_3)_2$	134.22	5, 414	0.8673 ₄ ²⁰	1.4855 ²⁰	−51.5	172.8	55	misc alc, eth
i65	Isobutyl chloroformate	$\text{ClCOOCH}_2\text{CH}(\text{CH}_3)_2$	136.58	3, 12	1.053	1.4070 ²⁰		128.8	26	misc bz, chl, eth
i66	Isobutyl formate	$\text{HCOOCH}_2\text{CH}(\text{CH}_3)_2$	102.13	2, 21	0.8854 ₄ ²⁰	1.3855 ²⁰	−94.5	98.4	10	1 aq; misc alc, eth
i67	Isobutyl isobutyrate	$(\text{CH}_3)_2\text{CHCH}_2\text{OOCCH}(\text{CH}_3)_2$	144.22	2, 291	0.8542 ²⁰	1.3999 ²⁰	−80.7	147.5		0.5 aq; misc alc
i68	Isobutyl lactate	$\text{CH}_3\text{CH}(\text{OH})\text{COOCH}_2\text{CH}(\text{CH}_3)_2$	146.19	3 ² , 188	0.971 ₂₀ ²⁰	1.4181 ²⁵		96 ^{40mm}		

i69	Isobutyl methacrylate	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COOCH}_2\text{-CH}(\text{CH}_3)_2$	142.19			0.882_{15}^{25}	1.4170^{25}		155	45	misc alc, eth
i70	Isobutyl nitrate	$(\text{CH}_3)_2\text{CHCH}_2\text{ONO}_2$	119.12			1.015_{44}^{20}	1.4028^{20}		123–125		i aq; misc alc, eth
i71	Isobutyl nitrite	$(\text{CH}_3)_2\text{CHCH}_2\text{ONO}$	103.12	1, 377		0.870_{44}^{22}	1.3715^{22}		67	4	misc alc; sl s aq(d)
i72	Isobutyl vinyl ether	$(\text{CH}_3)_2\text{CHCH}_2\text{OCH}=\text{CH}_2$	100.16			0.7702_{20}^{20}	1.3961^{20}	–132.3	83.4		0.2 aq
i73	Isobutyraldehyde	$(\text{CH}_3)_2\text{CHCHO}$	72.11	1, 671		0.7988_{44}^{20}	1.3723^{20}	–65.9	63–64	–40	11 aq; misc alc, bz, acet, chl, eth
i74	Isobutyramide	$(\text{CH}_3)_2\text{CHCONH}_2$	87.12	2, 293		1.013	127–129	216–220			
i75	Isobutyric acid	$(\text{CH}_3)_2\text{CHCOOH}$	88.11	2, 288		0.950_{44}^{20}	1.3925^{20}	–46	154	55	17 aq; misc alc, chl, eth

Isatin, i21

Isethionic acid, h114

Isoamyl acetate, i80

Isoamyl alcohol, m155

sec-Isoamyl alcohol, m156

Isoamyl bromide, b305

Isoamyl iodide, i42

Isoamyl nitrite, i81

Isobutane, m375

Isobutene, m383

α -Isobutoxy- α -phenylacetophenone, b48

Isobutylacetylene, m352

Isobutyl alcohol, m381

Isobutyl bromide, b310

Isobutyl chloride, c161

Isobutyl chlorocarbonate, i65

Isobutyl 1,2-dihydro-2-isobutoxy-1-quinolinecarboxylate, i61

Isobutyl ether, d407

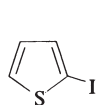
Isobutyl heptyl ketone, t349

Isobutyl mercaptan, m379

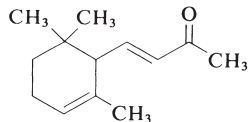
Isobutyraldehyde, m374

Isobutyramide, m388

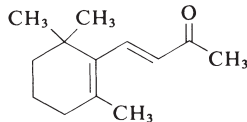
Isobutyric acid, m390



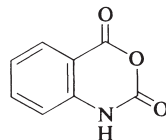
i52



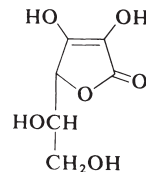
i56



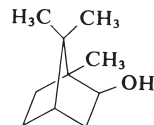
i57



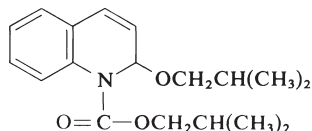
i58



i59



i60



i61

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
i76	Isobutyronitrile	$(\text{CH}_3)_2\text{CHCN}$	69.11	2, 294	0.7704 ²⁰	1.3734 ²⁰	−71.5	103.8	3	v s alc, eth; sl s aq
i77	Isobutyrophenone	$\text{C}_6\text{H}_5\text{COCH}(\text{CH}_3)_2$	148.21	7, 316	0.988 ²⁰	1.5172		217	84	
i78	Isobutryl chloride	$(\text{CH}_3)_2\text{CHCOCl}$	106.55	2, 293	1.017	1.4073 ²⁰	−90	91–93	1	d aq, d alc; s eth
i79	L-Isoleucine	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{NH}_2)\text{COOH}$	131.18	4, 454			d 284	subl 168		4 aq; sl s hot alc
i80	Isopentyl acetate	$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$	130.19	2, 132	0.876 ¹⁵	1.4007 ²⁰	−78.5	142.0	25	0.25 aq; misc alc, eth
i81	Isopentyl nitrite	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{ONO}$	117.15	1, 402	0.872	1.3860 ²⁰		99	10	misc alc, eth; sl s aq
i82	Isophorone		138.21	7, 65	0.923	1.4759 ²⁰	−8.1	215.2	84	1.2 aq
i83	DL-Isopinocampheol		154.25	6, 67			35–36	217		
i84	Isopropenyl acetate	$\text{CH}_3\text{COOC}(\text{CH}_3)=\text{CH}_2$	100.12	2 ² , 278	0.909	1.4005 ²⁰		94	18	
i85	2-Isopropoxyphenol	$(\text{CH}_3)_2\text{CHOC}_6\text{H}_4\text{OH}$	152.19	6 ³ , 4209	1.030	1.5157 ²⁰		100–102 ^{11mm}		
i86	1-Isopropoxy-2-propanol	$\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{OCH}(\text{CH}_3)_2$	118.1		0.879 ²⁵	1.407 ²⁵		47.9	49	
i87	Isopropyl acetate	$(\text{CH}_3)_2\text{CHOOCC}_2\text{H}_5$	102.13	2, 130	0.870 ²⁰	1.3773 ²⁰	−73.4	88.2	16	3 aq; misc alc, eth
i88	Isopropylamine	$(\text{CH}_3)_2\text{CHNH}_2$	59.11	4, 152	0.686 ²⁵	1.3711 ²⁵	−101	32.4	−17	misc aq, alc, eth
i89	2-Isopropylamino-ethanol	$(\text{CH}_3)_2\text{CHNHCH}_2\text{CH}_2\text{OH}$	103.17	4, 282	0.8970 ²⁰	1.4395 ²⁰		75 ^{11mm}		misc aq, alc, eth
i90	2-Isopropylaniline	$(\text{CH}_3)_2\text{CHC}_6\text{H}_4\text{NH}_2$	135.2		0.966			222		
i91	Isopropylbenzene	$\text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2$	120.20	5, 393	0.864 ²⁰	1.4915 ²⁰	−96.0	152.4	46	s alc, bz, eth
i92	4-Isopropylbenzyl alcohol	$(\text{CH}_3)_2\text{CHC}_6\text{H}_4\text{CH}_2\text{OH}$	150.22	6 ³ , 1911	0.982 ¹⁵	1.5206 ²⁰	28	248.4	>112	misc alc, eth; i aq
i93	N-Isopropylbenzylamine	$\text{C}_6\text{H}_5\text{CH}_2\text{NHCH}(\text{CH}_3)_2$	149.24		0.892	1.5025 ²⁰		200	87	
i94	Isopropylcyclohexane	$\text{C}_6\text{H}_{11}\text{CH}(\text{CH}_3)_2$	126.24	5, 41	0.8023 ²⁰	1.4399 ²⁰	−90	155	35	v s alc, eth
i95	N-Isopropylcyclohexylamine	$\text{C}_6\text{H}_{11}\text{NHCH}(\text{CH}_3)_2$	141.26		0.859	1.4480 ²⁰		60 ^{12mm}	33	

i96	4,4'-Isopropylidene-bis[2-(2,6-dibromophenoxy)-ethanol]	$(\text{CH}_3)_2\text{C}[\text{C}_6\text{H}_2(\text{Br})_2\text{OCH}_2\text{CH}_2\text{OH}]_2$	632.01				107			
i97	4,4'-Isopropylidene-diphenol	$(\text{CH}_3)_2\text{C}[\text{C}_6\text{H}_4\text{OH}]_2$	228.29	6, 1011			153–156	220 ^{4mm}		
i98	Isopropyl isocyanate	$(\text{CH}_3)_2\text{CHCNO}$	85.11	4, 155	0.866	1.3825 ²⁰		74–75	–2	
i99	Isopropyl S-(–)-lactate	$(\text{CH}_3)_2\text{CHOOC-CH(OH)CH}_3$	132.16	3, 282	0.998 ²⁰	1.4082 ²⁵		166–168		s aq, alc, eth

Isocapronitrile, m339
 Isocinchomeric acid, p260
 Isocrotonic acid, b401
 Isodurene, t98
 Isoeugenol, m98
 Isohexane, m336
 Isoleucinol, a216
 Isoniazid, p258
 Isonicotinaldehyde, p253
 Isonicotine acid, p257
 Isonicotinic acid hydrazide, p258
 Isonicotinonitrile, c297
 Isooctane, t354

Isopentane, m149
 Isopentyl alcohol, m155
 Isopentyl isovalerate, m170
 Isophorone, t340
 Isophthalic acid, b16
 Isophthalonitrile, d237
 Isophthaloyl dichloride, b14
 Isoprene, m147
 Isopropanolamine, a269
 Isopropenyl acetate, p208
 Isopropenylacetylene, m166
 4-Isopropenyl-1-cyclohexene-1-carbaldehyde, p58

Isopropenyl methyl ether, m96
 Isopropylacetylene, m171
 Isopropylacrylic acid, m349
 Isopropyl alcohol, p203
 Isopropyl chloride, c211
 Isopropyl cyanide, i76
 Isopropyl ether, d417
 Isopropylethylene, m160
 Isopropylidone acetone, m350
 Isopropyl iodide, i49

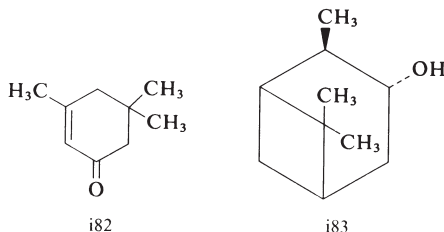


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
i100	2-Isopropyl-1-methylbenzene	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}(\text{CH}_3)_2$	134.21	5, 419	0.8766^{20}_4	1.5006^{20}	−71.5	178.2		misc alc, eth
i101	3-Isopropyl-1-methylbenzene	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}(\text{CH}_3)_2$	134.21	5, 419	0.8610^{20}_4	1.4930^{20}	−63.75	175.1		misc alc, eth
i102	4-Isopropyl-1-methylbenzene	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}(\text{CH}_3)_2$	134.21	5, 420	0.8573^{20}_4	1.4909^{20}	−67.9	177.1	47	misc alc, eth
i102a	2-Isopropyl-5-methylphenol	$\text{CH}_3\text{C}_6\text{H}_3(\text{OH})\text{CH}(\text{CH}_3)_2$	150.22	6, 532	0.925^{80}_4		49–51	232		i aq; v s alc, chl, eth
i103	<i>N</i> ¹ -Isopropyl-2-methyl-1,2-propanediamine	$(\text{CH}_3)_2\text{C}(\text{NH}_2)\text{CH}_2\text{NHCH}(\text{CH}_3)_2$	130.24		0.822	1.4269^{20}		147–149	90	
i104	Isopropyl methyl sulfide	$(\text{CH}_3)_2\text{CHSCH}_3$	90.18	1, 367			−101.5	84.7		
i105	Isopropyl nitrate	$(\text{CH}_3)_2\text{CHONO}_2$	105.09	1 ³ , 1465	1.036^{19}_{19}	1.3912^{16}		102.1		
i106	2-Isopropylphenol	$(\text{CH}_3)_2\text{CHC}_6\text{H}_4\text{OH}$	136.19	6, 504	1.012^{20}	1.5259^{20}	15–16	212–213	107	misc alc, eth
i107	4-Isopropylphenol	$(\text{CH}_3)_2\text{CHC}_6\text{H}_4\text{OH}$	136.19	6, 505	0.990^{20}		59–61	212		316 alc; 350 eth
i108	Isopropyl vinyl ether	$(\text{CH}_3)_2\text{CHOCH}=\text{CH}_2$	86.13		0.753^{20}_4	1.3849^{20}	−140	5–6		
i109	Isopulegol		154.25	6, 65	0.911	1.4725^{20}		91 ^{12mm}	78	v sl s aq
i110	Isoquinoline		129.16	20, 380	1.0910^{30}_4	1.6208^{30}	26.5	243.2	107	sl s aq; s acid
k1	Ketene	$\text{H}_2\text{C}=\text{C}=\text{O}$	42.04	1, 724			−151	−41		s acet, eth; d aq
L1	DL-Lactic acid	$\text{CH}_3\text{CH}(\text{OH})\text{COOH}$	90.08	3, 268	1.249^{15}_4		16.8	122 ^{14mm}		s aq, alc; i chl
L2	L-(+)-Lactic acid	$\text{CH}_3\text{CH}(\text{OH})\text{COOH}$	90.08	3, 261	1.2060^{25}_4	1.4392^{20}	53	119 ^{12mm}	>112	v s aq, alc, eth
L3	α-Lactose		342.30	31, 408	1.525^{20}		219 d			17 aq; i alc, eth
L4	DL-Leucine	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{NH}_2)\text{COOH}$	131.18	4, 447			d 332	subl 293		1 aq; 0.13 alc; i eth
L5	L-Leucine	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{NH}_2)\text{COOH}$	131.18	4, 437	1.293^{18}		d 293	subl 145		2.4 aq; 0.07 alc; 1 HOAc; i eth

L6	(+)-Limonene		136.24	5, 133	0.8411 ²⁰ ₄	1.4715	−96.5	175–176	53	misc alc, eth
L7	(−)-Limonene		136.24	5, 136	0.844	1.4706 ²⁰	−96.5	175–176	48	misc alc, eth
L8	(+)-Limonene oxide		152.24	17, 44	0.929	1.4661 ²⁰		114 ^{50mm}	65	
L9	Linalool		154.25	1, 462	0.865 ¹⁵	1.4615 ²⁰		199	76	misc alc, eth
L10	Linalyl acetate		196.29	2, 141	0.895 ²⁰	1.451		220 d	84	misc alc, eth
L11	<i>N</i> -Lithiohexamethyl- disilazane	(CH ₃) ₃ SiN(Li)Si(CH ₃) ₃	167.3				70–72	115		

Isopropyl mercaptan, p200

1-Isopropyl-4-methyl-1,3-cyclohexadiene, t5

1-Isopropyl-4-methyl-1,4-cyclohexadiene, t6

Isopropyl methyl ketone, m157

Isopropyltolueness, i100, i101, i102

Isopseudocumenol, t358

Isovaleraldehyde, m174

Isovaleric acid, m177

Isovaleronitrile, m178

Isovaleryl chloride, m179

Itaconic acid, m245

Keto compounds, *see* Oxo

2-Ketobutyric acid, o56

5-Keto-1,7,7-trimethylnorcamphane, c3

4-Ketovaleric acid, o58

Koshland's reagent I, h155

Lactonitrile, h168

Lauraldehyde, d731

Lauric acid, d726

Lauroitrile, d724

Lauroyl chloride, d728

Lauryl alcohol, d727

Laurylamine, d732

Lauryl bromide, b275

Lauryl mercaptan, d725

Lauryl sulfate, d735

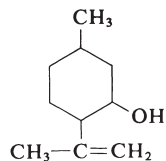
Lepidine, m408

Leucinol, a217

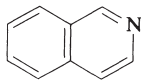
Levulinic acid, o58

Linoleic acid, o1

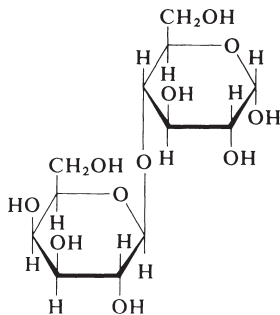
Linolenic acid, o7



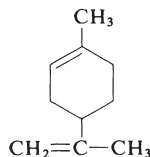
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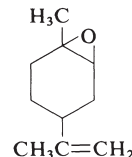
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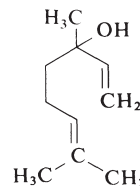
L3



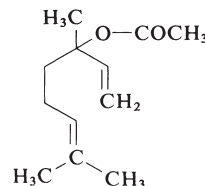
L6, L7



L8



L9



L10

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
L12	L-(+)-Lysine	$\text{H}_2\text{N}(\text{CH}_2)_4\text{-CH}(\text{NH}_2)\text{COOH}$	146.19	4, 435			d 224			v s aq; sl s alc; i eth
m1	Maleic acid	$\text{HOOCCH}=\text{CHCOOH}$	116.07	2, 748	1.590		138–139			79 aq; 70 alc; 8 eth
m2	Maleic anhydride		98.06	17, 432	1.48		52.8	202.0	103	s aq (to acid), alc (to ester); 227 acet; 53 chl; 50 bz; 112 EtAc
m3	Malonic acid	$\text{HOOCCH}_2\text{COOH}$	104.06	2, 566	1.63		135 d			154 aq; 42 alc; 8 eth
m4	Malonodiamide	$\text{H}_2\text{NCOCH}_2\text{CONH}_2$	102.09	2, 582			168–170			9 aq; i alc, eth
m5	Malononitrile	NCCH_2CN	66.06	2, 589	1.049		32–34	220	112	13 aq; 40 alc; 20 eth
m6	Malonyl dichloride	$\text{ClCOCH}_2\text{COCl}$	140.95	2 ¹ , 252	1.4486 ₄ ¹⁹	1.4620 ²⁰		53 ¹⁹ mm	47	d hot aq; s eth
m7	D-(+)-Maltose hydrate		342.30	31, 386	1.540 ¹⁷		102–103	d 130		v s aq; sl s alc; i eth
m8	D-Mandelic acid	$\text{C}_6\text{H}_5\text{CH}(\text{OH})\text{COOH}$	152.15	10, 197	1.300 ₄ ²⁰		119	d		16 aq; 100 alc; s eth
m9	Mandelonitrile	$\text{C}_6\text{H}_5\text{CH}(\text{OH})\text{CN}$	133.15	10, 193	1.117	1.5315 ²⁰	–10	d 170		v s alc, chl, eth; i aq
m10	Mannitol		182.17	1, 534	1.52 ²⁰		166–168	290 ^{3.5} mm		18 aq; 1.2 alc; i eth
m11	D-(+)-Mannose		180.16	31, 284	1.54 ²⁰		128–130			250 aq; 28 pyr; 0.8 alc
m12	L-Menthol		156.27	6, 28	0.890 ₁₅ ¹⁵	1.458 ²⁵	43–45	212	93	v s alc, chl, eth, PE
m13	L-Menthone		154.25	7, 38	0.895 ₄ ²⁰	1.4510 ²⁰	–6	207	69	misc alc, eth; sl s aq
m14	Mercaptoacetic acid	HSCH_2COOH	92.12	3, 245	1.325	1.5030 ²⁰	–16.5	96 ⁵ mm	>112	misc aq, alc, bz, eth
m15	2-Mercaptobenzimidazole		150.20	24, 119			303–304			sl s aq; s alc

m16	o-Mercaptobenzoic acid	$\text{HSC}_6\text{H}_4\text{COOH}$	154.19	10, 125			164–165		v s alc, HOAc
m17	2-Mercaptobenzo-thiazole		167.25	27, 185	1.42_4^{20}		180–181	d	2 alc; 1 eth; 10 acet; 1 bz; s alk; i aq
m18	2-Mercaptoethanol	$\text{HSCH}_2\text{CH}_2\text{OH}$	78.13	1, 470	1.1143_4^{20}	1.5006^{20}		156.9	73 misc aq, alc, bz, eth
m19	2-Mercaptoethyltri-ethoxysilane	$\text{HSCH}_2\text{CH}_2\text{Si}(\text{OC}_2\text{H}_5)_3$	224.38		0.988_4^{20}	1.432^{20}		210	104

Luminol, a153

2,6-Lupetidine, d591

β -Lutidine, e212

Lutidines, d604, d605, d606, d607

Maleic hydrazide, d400

Malic acids, h180, h181

Malonaldehyde bis(dimethyl acetal), t91

Malonamide nitrile, c286

Malonic acid diamide, m4

Malonylurea, b1

Melamine, t198

Mellitic acid, b19

MEM chloride, m67

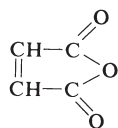
Menadione, m310

1,8-Mentanediamine, d41

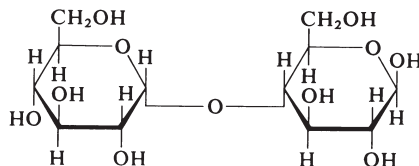
p-Mentha-1,8-diene, d649

p-Mentha-6,8-dien-2-one, c20

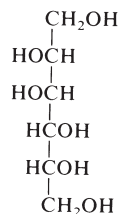
Mercaptobenzene, t159



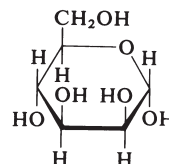
m2



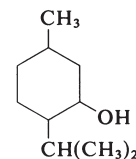
m7



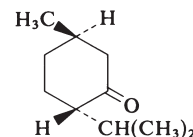
m10



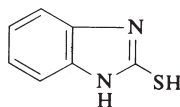
m11



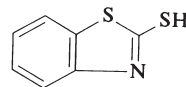
m12



m13



m15



m17

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m20	3-Mercapto-1,2-propanediol	$\text{HSCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$	108.16	1, 519	1.295 ₄ ¹⁴	1.5243 ²⁰		118 ^{5mm}	>112	misc alc; v s acet
m21	2-Mercaptopropionic acid	$\text{CH}_3\text{CH}(\text{SH})\text{COOH}$	106.14	3, 289	1.220 ₄ ¹⁵	1.4809 ²⁰	10	117 ^{16mm}	87	misc aq, alc, eth, acet
m22	(3-Mercaptopropyl)-trimethoxysilane	$\text{HS}(\text{CH}_2)_3\text{Si}(\text{OCH}_3)_3$	196.34		1.039 ₄ ²⁰	1.4416 ²⁰		93 ^{40mm}	48	
m23	Mercaptosuccinic acid	$\text{HOOCCH}_2\text{CH}(\text{SH})\text{COOH}$	150.15	3, 439			152–154			50 aq; 50 alc; s eth
m24	Methacrylaldehyde	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{CHO}$	70.09	1, 731	0.8304 ₄ ²⁰	1.4160 ²⁰	–81	69	–15	6 aq; misc alc, eth s alc; sl s eth
m25	Methacrylamide	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{CONH}_2$	85.11	2 ² , 399			109–111			
m26	Methacrylic acid	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COOH}$	86.09	2, 421	1.0153 ₄ ²⁰	1.4314 ²⁰	16	163	76	9 aq; misc alc, eth
m27	Methacrylonitrile	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{CN}$	67.91	2, 423	0.8001 ₄ ²⁰	1.4007 ²⁰	–35.8	90.3	12	2.6 aq; misc acet, bz
m28	Methacryloyl chloride	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COCl}$	104.54	2 ² , 394	1.070	1.4447 ²⁰		95–96	2	
m29	Methane	CH_4	16.04	1, 56	0.4240 ^{bp} 0.7168 g/L		–182.5	–161.5		3.3 mL aq; 47 mL alc
m30	Methanesulfonic acid	$\text{CH}_3\text{SO}_3\text{H}$	96.10	4, 4	1.4812 ₄ ¹⁸	1.4303 ²⁰	20	167 ^{10mm}	>112	1.5 bz; misc aq
m31	Methanesulfonic anhydride	$(\text{CH}_3\text{SO}_2)_2\text{O}$	174.19				71	138 ^{10mm}		v s aq(d)
m32	Methanesulfonyl chloride	$\text{CH}_3\text{SO}_2\text{Cl}$	114.55	4, 5	1.4805 ₄ ¹⁸	1.4518 ²⁰	–32	161	110	s alc, eth
m33	Methanethiol	CH_3SH	48.11	1, 288	0.8665 ₄ ²⁰		–123.0	6.0		2.3 aq; v s alc, eth
m34	Methanol	CH_3OH	32.04	1, 273	0.7913 ₄ ²⁰	1.3284 ²⁰	–97.7	64.7	11	misc aq, alc, bz, chl, eth

m35	Methanol- <i>d</i>	CH ₃ OD	33.05	1 ³ , 1186	0.8127 ²⁰ ₄	1.3270 ²⁰	−110	65.5	11	misc aq, alc, eth
m36	Methanol- <i>d</i> ₄	CD ₃ OD	36.07	1 ³ , 1187	0.888	1.3256 ²⁰		65.4	11	misc aq, alc, eth
m37	DL-Methionine	CH ₃ SCH ₂ CH ₂ - CH(NH ₂)COOH	149.21	4 ² , 938	1.340		281 d			3 aq; i eth; v sl s alc
m38	Methoxyacetic acid	CH ₃ OCH ₂ COOH	90.08	3, 232	1.174	1.4158 ²⁰		202–204	>112	misc aq, alc, eth
m39	<i>o</i> -Methoxyaceto- phenone	CH ₃ OC ₆ H ₄ COCH ₃	150.18	8, 85	1.090 ²⁰ ₄	1.5393 ²⁰		131 ^{18mm}	108	
m40	<i>m</i> -Methoxyaceto- phenone	CH ₃ OC ₆ H ₄ COCH ₃	150.18	8, 86	1.094	1.5410 ²⁰		239–241	110	s aq
m41	<i>p</i> -Methoxyaceto- phenone	CH ₃ OC ₆ H ₄ COCH ₃	150.18	8, 87	1.082 ⁴¹ ₄	1.5335 ²⁰	36–38	154 ^{26mm}		v s alc, eth
m42	2-Methoxyaniline	CH ₃ OC ₆ H ₄ NH ₂	123.16	13, 358	1.098 ¹⁵ ₁₅	1.5730 ²⁰	5	225	98	i aq; misc alc, eth
m43	3-Methoxyaniline	CH ₃ OC ₆ H ₄ NH ₂	123.16	13, 404	1.096	1.5794 ²⁰	1	251	>112	s alc, acid; sl s aq
m44	4-Methoxyaniline	CH ₃ OC ₆ H ₄ NH ₂	123.16	13, 435	1.087		60	243		v s alc; sl s aq
m45	2-Methoxybenz- aldehyde	CH ₃ OC ₆ H ₄ CHO	136.15	8, 43	1.127	1.560 ²⁰	35–36	236	117	sl s alc, bz; i eth
m46	4-Methoxybenz- aldehyde	CH ₃ OC ₆ H ₄ CHO	136.15	8, 67	1.119	1.5713 ²⁰	−1	248	108	misc alc
m47	4-Methoxybenzamide	CH ₃ OC ₆ H ₄ CONH ₂	151.17	10 ² , 100			164–167	295		s aq; v s alc; sl s eth
m48	Methoxybenzene	C ₆ H ₅ OCH ₃	108.14	6, 138	0.9942 ²⁰	1.5170 ²⁰	−37.5	153.8	51	1 aq; misc alc, eth
m49	4-Methoxybenzene- sulfonyl chloride	CH ₃ OC ₆ H ₄ SO ₂ Cl	206.65	11, 243			40–43			d aq; s alc, eth
m50	2-Methoxybenzoic acid	CH ₃ OC ₆ H ₄ COOH	152.15	10, 64	1.180		100	200		0.5 aq; v s alc, eth

MES, m451

Mesidine, t330

Mesitol, t362

Mesitylene, t335

Mesityl oxide, m350

Mesoxylurea, a79

Mesyl chloride, m32

Metanilic acid, a119

Methacholine chloride, a49

Methacrolein, m24

Methallyl alcohol, m385

Methallyl chloride, c164

Methanal, f27

Methanoic acid, f32

Methenamine, h52

Methone, d508

4-Methoxy-2-butanone dimethyl acetal, t321

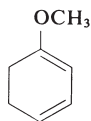
TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m51	3-Methoxybenzoic acid	$\text{CH}_3\text{OC}_6\text{H}_4\text{COOH}$	152.15	10, 137			104	172 ^{10mm}		s hot aq, alc, eth
m52	4-Methoxybenzoic acid	$\text{CH}_3\text{OC}_6\text{H}_4\text{COOH}$	152.15	10, 154	1.385 ⁴		185	275–280		0.04 aq; v s alc, chl
m53	4-Methoxybenzoyl chloride	$\text{CH}_3\text{OC}_6\text{H}_4\text{COCl}$	170.60	10, 163		1.5810 ²⁰	22	145 ^{14mm}	87	i aq(d); s alc(d); s bz, acet
m54	4-Methoxybenzyl alcohol	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}_2\text{OH}$	138.17	6, 897	1.109 ²⁵ ₄	1.5442 ²⁰	23–25	259	>112	i aq; s alc, eth
m55	4-Methoxybenzylamine	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}_2\text{NH}_2$	137.18	13, 606	1.050 ¹⁵	1.5462 ²⁰		236–237	>112	v s aq, alc, eth
m56	2-Methoxybiphenyl	$\text{CH}_3\text{OC}_6\text{H}_4\text{C}_6\text{H}_5$	184.24	6, 672	1.023	1.6105 ²⁰		274	>112	
m57	3-Methoxy-1-butanol	$\text{CH}_3\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{OH}$	104.15		0.9229 ²⁰ ₂₀	1.4145 ²⁰	–85	161.1	46	misc aq
m58	4-Methoxy-3-buten-2-one	$\text{CH}_3\text{OCH}=\text{CHCOCH}_3$	100.12		0.982	1.4660 ²⁰		200	63	
m59	1-Methoxy-1-buten-3-yne	$\text{CH}_3\text{OCH}=\text{CHC}\equiv\text{CH}$	82.10		0.906 ²⁰ ₄	1.4818 ²⁰		122–125	8	v s org solv
m60	4-Methoxycinnamic acid	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}=\text{CHCOOH}$	178.19	10, 298			172–187			s CCl_4
m61	1-Methoxy-1,3-cyclohexadiene		110.16	6 ³ , 367	0.929	1.4885 ²⁰		40 ^{15mm}	26	
m62	1-Methoxy-1,4-cyclohexadiene		110.16	6 ³ , 367	0.940	1.4819 ²⁰		148–150	36	
m63	7-Methoxy-3,7-dimethyloctanal	$(\text{CH}_3)_2\text{C}(\text{OCH}_3)\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CHO}$	186.30		0.877	1.4374 ²⁰		60 ^{0.45mm}	98	
m64	2-Methoxy-1,3-dioxolane		104.11	19 ⁴ , 617	1.092	1.4091 ²⁰		129–130	31	
m65	2-Methoxyethanol	$\text{CH}_3\text{OCH}_2\text{CH}_2\text{OH}$	76.10	1, 467	0.9646 ²⁰	1.4021 ²⁰	–85.1	124.6	46	misc aq

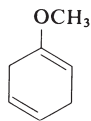
m66	2-(2-Methoxyethoxy)-ethanol	$\text{CH}_3\text{OCH}_2\text{CH}_2\text{OCH}_2\text{-CH}_2\text{OH}$	120.15		1.035 ²⁰	1.4264 ²⁰	-50	194.1	83	misc aq, alc, bz, eth, ketones
m67	2-Methoxyethoxy-methyl chloride	$\text{CH}_3\text{OCH}_2\text{CH}_2\text{OCH}_2\text{Cl}$	124.57		1.091	1.4270 ²⁰		50 ^{13mm}	>112	
m68	2-Methoxyethyl acetate	$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{OCH}_3$	118.13	2, 141	1.0049 ²⁰	1.4022 ²⁰	-65.1	144.5	43	misc aq
m69	2-Methoxyethylamine	$\text{CH}_3\text{OCH}_2\text{CH}_2\text{NH}_2$	75.11	4 ² , 718	0.864	1.4054 ²⁰		95	9	v s aq, alc
m70	1-Methoxy-2-indanol		164.20	6, 970		1.5482 ²⁰		146 ^{11mm}	>112	
m71	2-Methoxy-5-methylaniline	$\text{CH}_3\text{OC}_6\text{H}_3(\text{CH}_3)\text{NH}_2$	137.18	13 ² , 388			52-54	235		s aq; v s alc, bz, eth
m72	3-Methoxy-4-methylaniline	$\text{CH}_3\text{OC}_6\text{H}_3(\text{CH}_3)\text{NH}_2$	137.18	13, 574			51-54	250-252		
m73	4-Methoxy-2-methylaniline	$\text{CH}_3\text{OC}_6\text{H}_3(\text{CH}_3)\text{NH}_2$	137.18	13 ² , 330	1.065	1.5647 ²⁰	13-14	248-249	>112	s alc
m74	(4 <i>S</i> ,5 <i>S</i>)-(-)-4-Methoxymethyl-2-methyl-5-phenyl-2-oxazoline		205.26			1.5155 ²⁰		79 ^{0.05mm}		
m75	4-Methoxy-4-methyl-2-pentanone	$(\text{CH}_3)_2\text{C}(\text{OCH}_3)\text{CH}_2\text{-COCH}_3$	130.18		0.906	1.4181 ²⁵			61	misc aq
m76	1-Methoxynaphthalene	$\text{C}_{10}\text{H}_7\text{OCH}_3$	158.20	6, 606	1.090	1.6220 ²⁰		135 ^{12mm}	>112	

Methoxyethane, e171

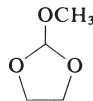
2-Methoxyethoxychloromethane, m67



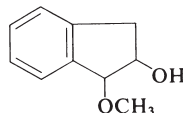
m61



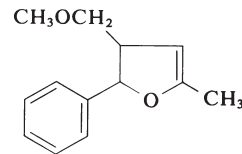
m62



m64



m70



m74

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

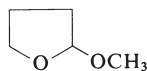
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m77	2-Methoxynaphthalene	$C_{10}H_7OCH_3$	158.20	6, 640			72	272		s bz, eth, CS_2
m78	2-methoxy-4-nitroaniline	$CH_3OC_6H_3(NO_2)NH_2$	168.15	13, 390			138–140			
m79	2-Methoxy-5-nitroaniline	$CH_3OC_6H_3(NO_2)NH_2$	168.15	13, 389	1.207 ¹⁵⁶		117–119			s alc, hot bz, HOAc
m80	4-Methoxy-2-nitroaniline	$CH_3OC_6H_3(NO_2)NH_2$	168.15	13, 521			123–126			sl s aq; s alc, eth
m81	2-Methoxynitrobenzene	$CH_3OC_6H_4NO_2$	153.14	6, 217	1.2527 ₄ ²⁰	1.5619 ²⁰	9.4	277	> 112	0.17 aq; s alc, eth
m82	4-Methoxynitrobenzene	$CH_3OC_6H_4NO_2$	153.14	6, 230	1.233		54	260		i aq; v s alc, eth
m83	4-Methoxy-3-nitrobenzoic acid	$CH_3OC_6H_3(NO_2)COOH$	197.15	10, 181			186–189			
m84	2-Methoxy-5-nitropyridine	$CH_3OC_5H_3N(NO_2)$	154.13	21 ² , 33			108–109			
m85	4-Methoxy-2-nitrotoluene	$CH_3OC_6H_3(NO_2)CH_3$	167.16	6, 411	1.207	1.5525 ²⁰	17	267	> 112	
m86	p-Methoxyphenethylamine	$CH_3OC_6H_4CH_2CH_2NH_2$	151.21	13, 626		1.5379 ²⁰		138 ^{20mm}		
m87	2-Methoxyphenol	$CH_3OC_6H_4OH$	124.14	6, 768	1.112 (liquid)	1.5429	28	205	82	1.5 aq; misc alc, eth
m88	3-Methoxyphenol	$CH_3OC_6H_4OH$	124.14	6, 813	1.131	1.5510 ²⁰	< -17.5	115 ^{5mm}	> 112	misc alc, eth; sl s aq
m89	4-Methoxyphenol	$CH_3OC_6H_4OH$	124.14	6, 843			55–57	243		v s bz; s alk
m90	3-(4-Methoxyphenoxy)-1,2-propanediol	$CH_3OC_6H_4OCH_2CH(OH)CH_2OH$	198.22	6 ³ , 4411			76–80			

m91	4-Methoxyphenyl-acetic acid	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}_2\text{COOH}$	166.18	10, 190			86–88	140 ^{3mm}		i aq; v s alc; s eth
m92	<i>o</i> -Methoxyphenyl-acetone	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}_2\text{COCH}_3$	164.20	8 ³ , 397	1.054	1.5250 ²⁰		130 ^{10mm}	>112	s alc, eth
m93	(<i>o</i> -Methoxyphenyl)-acetonitrile	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}_2\text{CN}$	147.18	10, 188			65–68	143 ^{15mm}		s hot bz
m94	2-Methoxy- <i>p</i> -phenylenediamine sulfate	$\text{CH}_3\text{OC}_6\text{H}_3(\text{NH}_2)_2 \cdot \text{H}_2\text{SO}_4$	236.26	13 ³ , 1349			283 d			
m95	1-Methoxy-2-propanol	$\text{CH}_3\text{OCH}_2\text{CH}(\text{OH})\text{CH}_3$	90.1		0.919 ²⁰ ₂₀	1.4021 ²⁰	–97	120.1	38	misc aq, acet, bz, eth
m96	2-Methoxypropene	$\text{CH}_3\text{C}(\text{OCH}_3)=\text{CH}_2$	72.11	1, 435	0.753	1.3820 ²⁰		34–36	–18	
m97	<i>trans</i> -1-Methoxy-4-(1-propenyl)benzene	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}=\text{CHCH}_3$	148.21	6, 566	0.9883 ²⁰ ₄	1.5615 ²⁰	21.4	237	90	misc chl, eth; 50 alc; s bz, EtAc
m98	2-Methoxy-4-propenylphenol	$\text{CH}_3\text{OC}_6\text{H}_3(\text{OH})-\text{CH}=\text{CHCH}_3$	164.20	6, 955	1.087 ²⁰ ₄	1.5748 ²⁰	–10	266	>112	misc alc, eth; sl s aq
m99	2-Methoxy-4-(2-propenyl)phenol	$\text{CH}_3\text{OC}_6\text{H}_3(\text{OH})-\text{CH}_2\text{CH}=\text{CH}_2$	164.20	6, 961	1.0664 ²⁰ ₄	1.5408 ²⁰	–9.2	255	>112	misc alc, chl, eth; s HOAc, alk; i aq
m100	<i>p</i> -Methoxyprop-iophenone	$\text{CH}_3\text{OC}_6\text{H}_4\text{COCH}_2\text{CH}_3$	164.20	8, 103	1.071	1.5465 ²⁰	27–29	273–275	>112	
m101	2-Methoxypyridine	$\text{CH}_3\text{OC}_5\text{H}_4\text{N}$	109.13	21, 44	1.038	1.5029 ²⁹		142	32	misc aq
m102	2-Methoxytetrahydrofuran		102.13	17 ⁴ , 1019	0.972	1.4119 ²⁰		105–107	7	

α -Methoxy- α -phenylacetophenone, b49

6-Methoxytetralin, m103

Methoxy-1-tetralone, d358



m102

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m103	6-Methoxy-1,2,3,4-tetrahydro-naphthalene		162.23	6 ² , 537		1.5402 ²⁰		90 ^{1mm}	>112	
m104	6-Methoxy-1-tetralone		176.22	9 ² , 889			77–79	171 ^{11mm}		
m105	2-Methoxytoluene	CH ₃ OC ₆ H ₄ CH ₃	122.17	6, 352	0.9851 ¹⁵ ₁₅	1.5161 ²⁰		170–172	51	i aq; v s alc, eth
m106	3-Methoxytoluene	CH ₃ OC ₆ H ₄ CH ₃	122.17	6, 376	0.9697 ²⁵ ₂₅	1.5131 ²⁰		175–176	54	s alc, bz, eth; i aq
m107	4-Methoxytoluene	CH ₃ OC ₆ H ₄ CH ₃	122.17	6, 392	0.969 ²⁵ ₂₅	1.5112 ²⁰		174	53	s alc, eth; i aq
m108	Methoxytrimethylsilane	CH ₃ OSi(CH ₃) ₃	104.2		0.7560 ²⁰ ₄	1.3678 ²⁰		57–58		
m109	Methoxytripropylsilane	CH ₃ OSi(C ₃ H ₇) ₃	188.4		0.822 ²⁰ ₄	1.428 ²⁰		83 ^{12mm}		
m110	<i>N</i> -Methylacetamide	CH ₃ CONHCH ₃	73.10	4, 58	0.9460 ³⁵	1.4253 ³⁵	30.6	206		s aq
m111	Methyl acetate	CH ₃ COOCH ₃	74.08	2, 224	0.9342 ²⁰ ₄	1.3619 ²⁰	–98.1	56.3	–16	24 aq; misc alc, eth
m112	Methyl acetoacetate	CH ₃ COCH ₂ COOCH ₃	116.12	3, 632	1.0747 ²⁰	1.4186 ²⁰	–80	171.7	70	50 aq; misc alc
m113	<i>p</i> -Methylacetophenone	CH ₃ C ₆ H ₄ COCH ₃	134.18	7, 307	1.0051	1.5328 ²⁰	22–24	226	92	i aq; v s alc, eth
m114	Methyl acrylate	H ₂ C=CHCOOCH ₃	86.09	2, 399	0.9561 ²⁰ ₄	1.4117 ¹⁸	–76.5	80.2	6	6 aq; s alc, eth
m115	Methylamine	CH ₃ NH ₂	31.06	4, 32	0.699 ¹¹ ₄		–93.5	–6.3	0	959 mL aq; 10.5 bz; s alc; misc eth
m116	Methyl 2-amino-benzoate	H ₂ NC ₆ H ₄ COOCH ₃	151.17	14, 317	1.68 ¹⁹ ₄	1.5820 ²⁰	24	256	104	sl s aq; v s alc, eth
m117	2-(<i>N</i> -Methylamino)-benzoic acid	CH ₃ NHC ₆ H ₄ COOH	151.17	14, 323			170–172			0.2 aq; s alc, eth
m118	Methyl 3-amino-crotonate	CH ₃ C(NH ₂)=CHCOOCH ₃	115.13	3, 632			81–83			

m119	2-(Methylamino)-ethanol	$\text{CH}_3\text{NHCH}_2\text{CH}_2\text{OH}$	75.11	4, 276	0.937 ²⁰	1.4387 ²⁰		155–156	72	misc aq, alc, eth
m120	4-Methylamino-phenol sulfate	$(\text{CH}_3\text{NHC}_6\text{H}_4\text{OH})_2 \cdot \text{H}_2\text{SO}_4$	344.39	13, 442			260 d			4 aq; sl s alc; i eth
m121	2-(Methylamino)-pyridine	$\text{CH}_3\text{NHC}_5\text{H}_4\text{N}$	108.14	22 ¹ , 629	1.052 ²⁹ ₂₉	1.5785 ²⁰	15	201	87	s aq; v s alc, eth
m122	<i>N</i> -Methylaniline	$\text{C}_6\text{H}_5\text{NHCH}_3$	107.16	12, 135	0.989 ²⁰ ₄	1.5704 ²⁰	–57	196	73	sl s aq; s alc, eth
m123	<i>N</i> -Methylanilinium trifluoroacetate	$\text{C}_6\text{H}_5\text{NHCH}_3 \cdot \text{HOOC}\text{CF}_3$	221.18				65–66			
m124	2-Methylanthraquinone		222.24	7, 809			177	subl		v s bz; s alc, eth
m125	Methylarsonic acid	$\text{CH}_3\text{AsO}(\text{OH})_2$	139.96	4, 613			161			v s aq; s alc
m126	4-Methylbenzaldehyde	$\text{CH}_3\text{C}_6\text{H}_4\text{CHO}$	120.15	7, 297	1.0194 ¹⁷ ₄	1.5447 ²⁰		205	80	misc alc, eth; sl s aq
m127	Methyl benzenesulfonate	$\text{C}_6\text{H}_5\text{SO}_2\text{OCH}_3$	172.20	11 ² , 20	1.2889 ⁰ ₄	1.5151 ²⁰	–4	154 ^{20mm}		v s alc, chl, eth
m128	2-Methylbenzimidazole		132.17	23, 145			176–177			s alk, hot aq; sl s alc
m129	Methyl benzoate	$\text{C}_6\text{H}_5\text{COOCH}_3$	136.15	9, 109	1.0933 ¹⁵ ₄	1.5205 ¹⁵	–12.1	199.5	82	0.2 aq; misc alc, eth

Methylal, d441

Methyl alcohol, m34

Methylaminoacetaldehyde dimethyl acetal, d442

α -(1-Methylaminoethyl)benzyl alcohols, e1, e2

2-Methyl-*p*-anisidine, m71

4-Methyl-*m*-anisidine, m72

5-Methyl-*o*-anisidine, m73

Methylanisoles, m105, m106, m107

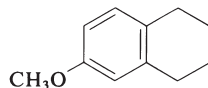
Methyl anthranilate, m116

Methylantranilic acids, a211, a212

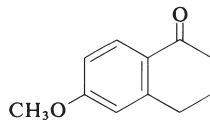
N-Methylantranilic acid, m117

Methylbenzene, t167

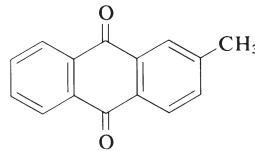
4-Methylbenzenesulfonic acid, t176



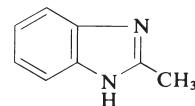
m103



m104



m124



m128

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m130	2-Methylbenzoic acid	$\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	136.15	9, 462	1.062		107–108	258–259		sl s aq; v s alc
m131	3-Methylbenzoic acid	$\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	136.15	9, 475	1.054		111–113	263		0.09 aq; v s alc
m132	4-Methylbenzoic acid	$\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	136.15	9, 483			180–182	274–275		v s alc, eth
m133	2-Methylbenzophenone	$\text{CH}_3\text{C}_6\text{H}_4\text{COC}_6\text{H}_5$	196.25	7, 439	1.083	1.5958 ²⁰	< –18	309–311	> 112	v s alc, org solv
m134	4-Methylbenzophenone	$\text{CH}_3\text{C}_6\text{H}_4\text{COC}_6\text{H}_5$	196.25	7, 440			59–60	326		v s bz, eth
m135	2-Methylbenzothiazole		149.22	27, 46	1.173	1.6170 ²⁰	12–14	238	102	s alc, HOAc; i aq
m136	5-Methyl-1 <i>H</i> -benzotriazole		133.15	26, 58			80–82	210–212 ^{12mm}		
m137	2-Methylbenzoxazole		133.15	27, 46	1.121	1.5497 ²⁰	8.5–10	178	75	
m138	α -Methylbenzyl alcohol	$\text{C}_6\text{H}_5\text{CH}(\text{CH}_3)\text{OH}$	122.17	6, 475	1.0191 ¹³	1.5211 ²⁰	21	204	85	v s alc; s bz, chl
m139	3-Methylbenzyl alcohol	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}_2\text{OH}$	122.17	6, 494	0.916 ¹⁷	1.5334 ²⁰	< –20	217		5 aq; s alc, eth
m140	4-Methylbenzyl alcohol	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}_2\text{OH}$	122.17	6, 498			59–61	217		s alc, eth; sl s aq
m141	DL- α -Methylbenzylamine	$\text{C}_6\text{H}_5\text{CH}(\text{CH}_3)\text{NH}_2$	121.18	12, 1094	0.940	1.5254 ²⁰		185	79	
m142	4-Methylbenzylamine	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}_2\text{NH}_2$	121.18	12, 1141	0.952	1.5340 ²⁰	12–13	195	75	
m143	Methyl bromoacetate	$\text{BrCH}_2\text{COOCH}_3$	152.98	2, 213	1.616	1.4586 ²⁰		52 ^{15mm}	62	s alc
m144	DL-Methyl-2-bromobutyrate	$\text{CH}_3\text{CH}_2\text{CH}(\text{Br})\text{COOCH}_3$	181.04	2, 282	1.573			137–138 ^{50mm}		

m145	Methyl 4-bromo- crotonate	$\text{BrCH}_2\text{CH}=\text{CHCOOCH}_3$	179.02		1.522	1.4980 ²⁰		85 ^{13mm}	91	
m146	Methyl 2-bromo- propionate	$\text{CH}_3\text{CH}(\text{Br})\text{COOCH}_3$	167.01	2, 253	1.497	1.5420 ²⁰		51 ^{19mm}	51	s alc
m147	2-Methyl-1,3- butadiene	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2$	68.12	1, 252	0.681 ²⁰ ₄	1.4216 ²⁰	−145.9	34. 1	−53	misc alc, eth
m148	3-Methyl-1,2- butadiene	$\text{CH}_3\text{C}(\text{CH}_3)=\text{C}=\text{CH}_2$	68.12	1, 252	0.694 ²⁰ ₄	1.4179 ²⁰	−113.6	40.9	−12	
m149	2-Methylbutane	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)_2$	72.15	1, 134	0.6197 ²⁰	1.3537 ²⁰	−159.9	27.9	−56	0.005 aq; misc alc
m150	2-Methyl-1- butanethiol	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{SH}$	104.22	1 ² , 421	0.848	1.4465 ²⁰		119.0	19	s alc, eth; i aq
m151	2-Methyl-2- butanethiol	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{SH}$	104.22	1 ¹ , 196	0.842	1.4385 ²⁰	−103.9	99.1	−1	s alc, eth; i aq
m152	3-Methyl-1- butanethiol	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{SH}$	104.22	1, 405	0.835 ²⁰ ₄	1.4432 ²⁰	−133.5	118.4	18	misc alc, chl, eth
m153	2-Methyl-1- butanol	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{OH}$	88.15	1, 388	0.816 ²⁰ ₄	1.4100 ²⁰	< −70	128	50	3 aq; misc alc, eth
m154	2-Methyl-2- butanol	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{OH}$	88.15	1, 388	0.8090 ²⁰	1.4050 ²⁰	−9.0	102.0	21	11 aq; misc alc, bz, chl, eth
m155	3-Methyl-1- butanol	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{OH}$	88.15	1, 392	0.8129 ¹⁵ ₄	1.4085 ¹⁵	−117.2	132.0	45	2 aq; misc alc, bz, chl, eth, PE, HOAc

α -Methylbenzyl alcohol, p112
N-Methylbenzylamine, b103
Methylbenzyl bromides, b368, b369

Methylbenzyl chlorides, c258, c259, c260
Methylbis(2-chloroethoxy)silane, b157
N-Methylbis(2-chloroethyl)amine, b159

Methyl bromide, b300
3-Methyl-1-buten-1-carboxylic acid, m349

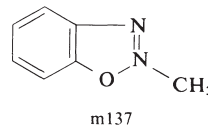
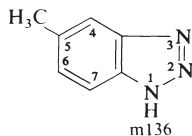
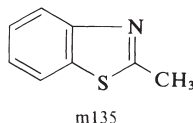


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m156	3-Methyl-2-butanol	$(\text{CH}_3)_2\text{CHCH}(\text{OH})\text{CH}_3$	88.15	1, 391	0.8179 ²⁰	1.4096 ²⁰		111.5	26	2.8 aq; misc alc, eth
m157	3-Methyl-2-butanone	$(\text{CH}_3)_2\text{CHCOCH}_3$	86.13	1, 682	0.802 ²⁰ ₄	1.3890	92	94–95		misc alc, eth
m158	2-Methyl-1-butene	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$	70.14	1, 211	0.6504 ²⁰ ₄	1.3777 ²⁰	–137.6	31.2		misc alc, eth
m159	2-Methyl-2-butene	$\text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2$	70.14	1, 211	0.6620 ²⁰ ₄	1.3878 ²⁰	–133.8	38.6	–45	misc alc, eth; i aq
m160	3-Methyl-1-butene	$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2$	70.14	1 ³ , 797	0.6272 ²⁰ ₄	1.3638 ²⁰	–168.5	20.1		misc alc, eth
m161	(E)-2-Methyl-2-butenic acid	$\text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{COOH}$	100.12	2, 430	0.969	1.4342 ⁸¹	64	198.5		s alc, eth; v s hot aq
m162	(Z)-2-Methyl-2-butenic acid	$\text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{COOH}$	100.12	2, 428	0.983 ⁴⁷ ₄	1.4437 ⁴⁷	45	185		s alc, eth; v s hot aq
m163	3-Methyl-2-butenic acid	$(\text{CH}_3)_2\text{C}=\text{CHCOOH}$	100.12	2, 432	1.006 ²⁴		69	194–195		s aq, alc, eth
m164	2-Methyl-3-buten-2-ol	$(\text{CH}_3)_2\text{C}(\text{OH})\text{CH}=\text{CH}_2$	86.13	1, 444	0.8672 ²⁰ ₂₀	1.4160 ²⁰	2.6	98–99	13	
m165	3-Methyl-3-buten-1-ol	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{OH}$	86.13		0.853	1.4337 ²⁰			36	
m166	2-Methyl-1-buten-3-yne	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{C}\equiv\text{CH}$	66.10	1 ¹ , 126		1.4140 ²⁰	–113	32	–6	
m167	N-Methylbutylamine	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NHCH}_3$	87.17	4, 157	0.736	1.3995 ²⁰	–75	91	<1	
m168	1-Methylbutylamine	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{NH}_2$	87.17	4, 177	0.7384 ²⁰ ₄	1.4029 ²⁰		91	35	misc aq, alc, eth
m169	2-Methylbutylamine	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{NH}_2$	87.17	4 ³ , 342	0.738	1.4116 ²⁰		94–97	3	
m170	3-Methylbutyl-3-methylbutyrate	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{OOC}-\text{CH}_2\text{CH}(\text{CH}_3)_2$	172.27	2, 312	0.8541 ²⁵	1.4100 ²⁵		194.0		misc alc, eth
m171	3-Methyl-1-butyne	$(\text{CH}_3)_2\text{CHC}\equiv\text{CH}$	68.12	1, 251	0.666 ²⁰ ₄	1.3740 ²⁰	–89.8	26.4		misc alc, eth
m172	2-Methyl-3-butyne-2-ol	$(\text{CH}_3)_2\text{C}(\text{OH})\text{C}\equiv\text{CH}$	84.12	1 ¹ , 235	0.8672 ²⁰ ₂₀	1.4209 ²⁰	2.6	104–105	25	misc aq, acet, bz

m173	2-Methylbutyr-aldehyde	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CHO}$	86.13	1 ¹ , 352	0.804	1.3919 ²⁰		90–92	4	
m174	3-Methylbutyr-aldehyde	$(\text{CH}_3)_2\text{CHCH}_2\text{CHO}$	86.13	1, 684	0.785 ²⁰ ₂₀	1.3882 ²⁰	–51	92–93	19	misc alc, eth; sl s aq
m175	Methyl butyrate	$\text{CH}_3\text{CH}_2\text{CH}_2\text{COOCH}_3$	102.13	2 ⁴ , 786	0.898 ²⁰ ₄	1.3879 ²⁰	–85	102	14	1.4 aq; misc alc, eth
m176	2-Methylbutyric acid	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{COOH}$	102.13	2 ⁴ , 888	0.936	1.4055 ²⁰		176.5	>112	
m177	3-Methylbutyric acid	$(\text{CH}_3)_2\text{CHCH}_2\text{COOH}$	102.13	2, 309	0.9308 ²⁰ ₄	1.4033 ²⁰	–30.0	176.5	70	4 aq; s alc, chl, eth
m178	3-Methylbutyro-nitrile	$(\text{CH}_3)_2\text{CHCH}_2\text{CN}$	83.13	2 ² , 278	0.7925 ¹⁹ ₄	1.3927 ²⁰	–101	129		misc alc, eth
m179	3-Methylbutyryl chloride	$(\text{CH}_3)_2\text{CHCH}_2\text{COCl}$	120.58	2, 315	0.985 ²⁰ ₄	1.4161 ²⁰		115–117	18	d aq, alc; s eth
m180	1-(3-Methylbutyryl)-pyrrolidine		155.24		0.938	1.4710 ²⁰			104	
m181	Methyl carbamate	$\text{H}_2\text{NCOOCH}_3$	75.07	3, 21	1.136 ⁵⁶ ₄		52–54	177		220 aq; 73 alc; s eth
m182	Methyl chloro-acetate	$\text{ClCH}_2\text{COOCH}_3$	108.52	2, 197	1.238 ²⁰ ₂₀	1.4220 ²⁰	–33	130–132	57	i aq; misc alc, eth

(Z)-2-Methyl-2-butenedioic acid, c270
Methyl 2-buten-1-oate, m192
3-Methylbutyl acetate, i80
2-Methylbutylamine, a251
Methyl *tert*-butyl ether, b460
Methyl *tert*-butyl ketone, h72

2-Methylbutyl isovalerate, m170
Methyl caprate, m218
Methyl caproate, m265
Methyl carprylate, m329
Methyl carbazate, m271
Methyl carbitol, m66

4-Methylcatechol, d389
Methyl Cellosolve, m65
Methyl Cellosolve acetate, m68
β-Methylchalcone, d658
Methyl chlorocarbonate, m187

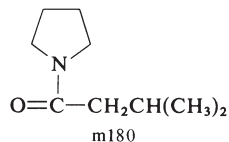


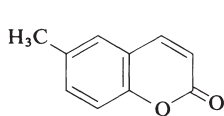
TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m183	Methyl 2-chloro-acetoacetate	$\text{CH}_3\text{COCH}(\text{Cl})\text{COOCH}_3$	150.56		1.236	1.4465 ²⁰	−32.7	137	71	
m184	Methyl <i>m</i> -chloro-benzoate	$\text{ClC}_6\text{H}_4\text{COOCH}_3$	170.60	9, 338		1.4923 ²⁰	21	101 ^{12mm}		
m185	Methyl <i>p</i> -chloro-benzoate	$\text{ClC}_6\text{H}_4\text{COOCH}_3$	170.60	9, 340	1.382 ²⁰		44			s alc
m186	Methyl 4-chloro-butyrat	$\text{ClCH}_2\text{CH}_2\text{CH}_2\text{COOCH}_3$	136.58	2, 278	1.1268 ¹⁴	1.4321 ²⁰		176	59	v s eth; s alc, acet
m187	Methyl chloro-formate	ClCOOCH_3	94.50	3, 9	1.223 ²⁰	1.3865 ²⁰		71	< 1	misc alc, bz, chl, eth
m188	Methyl 3-(chloro-formyl)propionate	$\text{CH}_3\text{OOCCH}_2\text{CH}_2\text{COCl}$	150.56	2 ² , 553	1.223	1.4402 ²⁰		65 ^{3mm}	73	
m189	Methyl 2-chloro-propionate	$\text{CH}_3\text{CH}(\text{Cl})\text{COOCH}_3$	122.55	2, 248	1.075	1.4193 ²⁰		132–133	36	s alc
m190	2-Methylcinnamaldehyde	$\text{C}_6\text{H}_5\text{CH}=\text{C}(\text{CH}_3)\text{CHO}$	146.19	7, 369	1.047 ¹⁷	1.6045 ²⁰		149 ^{27mm}	79	
m191	6-Methylcoumarin		160.17	17, 337			75–76	303 ^{725mm}		
m192	Methyl crotonate	$\text{CH}_3\text{CH}=\text{CHCOOCH}_3$	100.12	2, 410	0.9444 ²⁰	1.4242 ²⁰		121	4	v s alc, eth; i aq
m193	Methyl cyanoacetate	$\text{NCCH}_2\text{COOCH}_3$	99.09	2, 584	1.1225 ²⁵	1.4166 ²⁵	−13.1	205.1	110	misc alc, eth
m194	Methylcyclohexane	$\text{C}_6\text{H}_{11}\text{CH}_3$	98.19	5, 29	0.7694 ²⁰	1.4231 ²⁰	−126.6	100.9	−3	
m195	Methyl cyclohexanecarboxylate	$\text{C}_6\text{H}_{11}\text{COOCH}_3$	142.20	9 ¹ , 5	0.9954 ¹⁶	1.4445 ²⁰		183	60	i aq; s alc, eth
m196	4-Methyl-1,2-cyclohexanedicarboxylic anhydride		168.19		1.162	1.4774 ²⁰				
m197	1-Methylcyclohexanol	$\text{C}_6\text{H}_{10}(\text{CH}_3)\text{OH}$	114.19	6, 11	0.9251 ²⁵	1.4587 ²⁵	26	168	67	i aq; s bz, chl
m198	(<i>Z</i>)-2-Methylcyclohexanol	$\text{C}_6\text{H}_{10}(\text{CH}_3)\text{OH}$	114.19	6 ² , 17	0.9340 ²⁰	1.4654 ²⁰	7	165	58	misc alc, eth

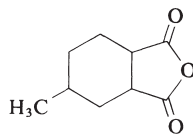
m199	(<i>E</i>)-2-Methylcyclohexanol	$C_6H_{10}(CH_3)OH$	114.19	6, 11	0.9247^{20}_4	1.4616^{20}	-4	165.5	58	misc alc; s eth
m200	(<i>Z</i>)-3-Methylcyclohexanol	$C_6H_{10}(CH_3)OH$	114.19	6, 12	0.9155^{20}	1.4572^{20}	-6	94	62	misc alc, eth
m201	(<i>E</i>)-3-Methylcyclohexanol	$C_6H_{10}(CH_3)OH$	114.19	6, 12	0.9214^{20}	1.4580^{20}	-1	84	62	
m202	(<i>Z</i>)-4-Methylcyclohexanol	$CH_3C_6H_{10}OH$	114.19	6, 14	0.9122^{20}_4	1.4614^{20}		171	70	misc alc, eth
m203	(<i>E</i>)-4-Methylcyclohexanol	$CH_3C_6H_{10}OH$	114.19	6, 14	0.9118^{21}_4	1.4559^{20}		173-175	70	misc alc; s eth
m204	2-Methylcyclohexanone	$CH_3C_6H_9(=O)$	112.17	7, 14	0.925^{20}_4	1.4478^{20}		162-163	46	i aq; s alc, eth
m205	3-Methylcyclohexanone	$CH_3C_6H_9(=O)$	112.17	7, 15	0.9155^{20}_4	1.4460^{20}		168-169	51	i aq; s alc, eth
m206	4-Methylcyclohexanone	$CH_3C_6H_9(=O)$	112.17	7, 18	0.916^{20}_4	1.4455^{20}		169-171	40	i aq; s alc, eth
m207	1-Methyl-1-cyclohexene		96.17	5, 66	0.809^{20}_4	1.4502^{20}	-121	111	-3	i aq; s alc, eth
m208	4-Methyl-1-cyclohexene		96.17	5, 67	0.799	1.4412^{20}	-115.5	102	-1	i aq; s alc, eth
m209	<i>N</i> -Methylcyclohexylamine	$C_6H_{11}NHCH_3$	113.20	12, 6	0.868	1.4560^{20}		149	29	

Methyl chloroform, t226

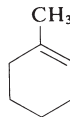
(*E*)-2-Methylcrotonic acid, m161



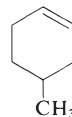
m191



m196



m207



m208

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

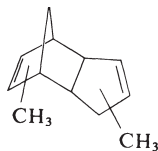
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m210	3-Methylcyclohexylamine	$C_6H_{10}(CH_3)NH_2$	113.20	12, 10	0.855	1.4525 ²⁰		150 ^{730mm}	22	
m211	4-Methylcyclohexylamine	$C_6H_{10}(CH_3)NH_2$	113.20	12, 12	0.855	1.4531 ²⁰		151–154	26	
m212	Methylcyclopentadiene dimer		160.26		0.941	1.4976 ²⁰	–51	200	26	
m213	Methylcyclopentane	$C_5H_9CH_3$	84.16	5, 27	0.7487 ²⁰	1.4097 ²⁰	–142.4	71.8	–27	0.013 aq
m214	3-Methyl-1,2-cyclopentanedione		112.13	7 ¹ , 310			105–107			
m215	2-Methylcyclopentanone		98.15	7 ² , 13	0.9200 ²⁰	1.4347 ²⁰	–76	139–140		s aq; v s alc, eth
m216	3-Methyl-2-cyclopenten-1-one		96.13	7 ¹ , 46	0.971	1.4780 ²⁰		74 ^{15mm}	65	
m217	2-Methylcyclopropanecarboxylic acid		100.12	9, 6	1.027	1.4395 ²⁰		191 ^{745mm}	87	
m218	Methyl decanoate	$CH_3(CH_2)_8COOCH_3$	186.30	2, 356			–18	223–224		i aq; misc alc, eth
m219	Methyl dichloroacetate	$Cl_2CHCOOCH_3$	142.97	2, 203	1.3808 ¹⁹	1.4421 ²⁰	–52	143	80	i aq; s alc
m220	Methyl 2,2-dichloro-1-methylcyclopropanecarboxylate		183.03		1.245	1.4639 ²⁰		74 ^{8mm}	74	
m221	Methyl 2,3-dichloropropionate	$ClCH_2CH(Cl)COOCH_3$	157.00	2 ¹ , 111	1.3282 ²⁰	1.4447 ²⁰		92 ^{50mm}	42	s alc
m222	Methyldichlorosilane	CH_3SiHCl_2	115.0		1.1047 ²⁰	1.4222 ²⁰	–93	41	–25	
m223	<i>N</i> -Methyldiethanolamine	$CH_3N(CH_2CH_2OH)_2$	119.16	4, 284	1.0377 ²⁰	1.4685 ²⁰		246–248	126	misc aq, alc

m224	<i>O</i> -Methyl- <i>N,N'</i> -diisopropylurea	$(\text{CH}_3)_2\text{CHNHC}(\text{OCH}_3)=\text{NCH}(\text{CH}_3)_2$	158.25		0.871	1.4358 ²⁰		50–52 ^{0.1mm}	35	
m225	Methyl 3,4-dimethoxybenzoate	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{COOCH}_3$	196.20	10, 396			57–60	283		
m226	Methyl 4,5-dimethoxy-2-nitrobenzoate	$(\text{CH}_3\text{O})_2\text{C}_6\text{H}_2(\text{NO}_2)\text{COOCH}_3$	241.20	10, 403			141–144			
m227	Methyl 2,2-dimethylpropionate	$(\text{CH}_3)_3\text{CCOOCH}_3$	116.16	2 ¹ , 139	0.873	1.3880 ²⁰		101–103	–1	misc alc, eth; sl s aq
m228	2-Methyl-3,5-dinitrobenzoic acid	$\text{CH}_3\text{C}_6\text{H}_2(\text{NO}_2)_2\text{COOH}$	226.15	9, 474			205–207			
m229	<i>N</i> -Methyldioctylamine	$(\text{C}_8\text{H}_{17})_2\text{NCH}_3$	255.49	4 ³ , 381		1.4424 ²⁰	–30.1	165 ^{15mm}		
m230	<i>N</i> -Methyldiphenylamine	$(\text{C}_6\text{H}_5)_2\text{NCH}_3$	183.26	12, 180	1.048 ²⁰ ₄	1.6193 ²⁰	–7.6	135 ^{6mm}		i aq; s alc, eth
m231	Methyldiphenylsilane	$(\text{C}_6\text{H}_5)_2\text{Si}(\text{H})\text{CH}_3$	198.3		0.997 ²⁰ ₄	1.569 ²⁰				
m232	<i>N,N'</i> -Methylenebisacrylamide	$\text{H}_2\text{C}=\text{CHCONHCH}_2\text{NHCOCH}=\text{CH}_2$	154.17				> 300			
m233	2,2'-Methylenebis(4-chlorophenol)	$\text{CH}_2[\text{C}_6\text{H}_3(\text{Cl})\text{OH}]_2$	269.13				177–178			100 EtOH; 100 eth; s PE

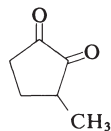
Methyl 4,6-dimethyl-2-oxo-2*H*-pyran-5-carboxylate, m288

Methyldinitrophenols, d631, d633a
Methyl enanthate, m261

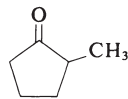
Methylene bromide, d88



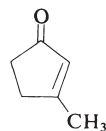
m212



m214



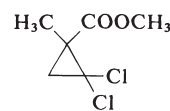
m215



m216



m217



m220

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m234	4,4'-Methylenebis-(<i>N,N</i> -dimethylaniline)	$\text{CH}_2[\text{C}_6\text{H}_4\text{N}(\text{CH}_3)_2]_2$	254.38	13, 239			90			
m235	4,4'-Methylenebis-(3-hydroxy-2-naphthoic acid)	$\text{CH}_2[\text{C}_{10}\text{H}_5(\text{OH})\text{COOH}]_2$	388.38	10, 575			$d > 280$			i aq, alc, eth, bz; sl s chl; s pyr
m236	1,1'-Methylenebis(3-methylpiperidine)	$\text{CH}_2(\text{CH}_3\text{C}_5\text{H}_9\text{N})_2$	210.37		0.887	1.4734 ²⁰		160 ^{50mm}	110	
m237	Methylene blue		373.90	27, 393			190 d			4 aq; 1.3 alc; s chl
m238	4,4'-Methylenedianiline	$\text{CH}_2(\text{C}_6\text{H}_4\text{NH}_2)_2$	198.26	13, 238			92		221	
m239	3,4-Methylenedioxybenzaldehyde		150.13	19, 115			37	264		0.2 aq; v s alc, eth
m240	1,2-Methylenedioxybenzene		122.12	19, 20	1.064	1.5398		173	55	
m241	3,4-Methylenedioxybenzoic acid		166.13	19, 269			229	subl 210		sl s aq, chl, alc, eth
m242	3,4-Methylenedioxybenzyl alcohol		152.14	19, 67			53–55			
m243	3,4-Methylenedioxy-6-propylbenzyl diethyleneglycol butyl ether		338.45		1.05	1.50 ²⁰		180 ^{1mm}	171	misc alc, bz, freons
m244	5-Methylene-2-norbornene		106.17		0.981	1.4819 ²⁰			4	
m245	Methylenesuccinic acid	$\text{H}_2\text{C}=\text{C}(\text{COOH})\text{CH}_2\text{COOH}$	130.10	2, 760	1.573		162 d			8.2 aq; 20 alc; v s bz, chl, eth, PE
m246	<i>N</i> -Methylethylamine	$\text{CH}_3\text{CH}_2\text{NHCH}_3$	59.11	4 ² , 589	0.690	1.3760		35	–12	v s aq, alc

m247	<i>N</i> -Methylethylenediamine	CH ₃ NHCH ₂ CH ₂ NH ₂	74.13	4 ¹ , 415	0.841	1.4395 ²⁰		114–116	41	
m248	<i>N</i> -Methylformamide	HCONHCH ₃	59.07	4, 58	0.9988 ²⁵	1.4300 ²⁵	–3.8	180–185	98	misc aq
m249	<i>N</i> -Methylformanilide	C ₆ H ₅ N(CH ₃)CHO	135.17	12, 234	1.095	1.5593 ²⁰	8–13	244	126	
m250	Methyl formate	HCOOCH ₃	60.05	2, 18	0.9815 ¹⁵	1.3465 ¹⁵	–99.0	31.5	–32	23 aq; misc alc
m251	5-Methylfuraldehyde		110.11	17, 289	1.1072 ¹⁸	1.5263 ²⁰		187	72	s aq; v s alc; misc eth
m252	2-Methylfuran		82.10	17, 36	0.915 ²⁰ ₄	1.4332 ²⁰	–88	63–66	–26	0.3 aq
m253	Methyl furoate		126.11	18, 274	1.179 ²⁰	1.4862 ²⁰		181	73	s alc, eth; sl s aq
m254	Methylgermanium tribromide	CH ₃ GeBr ₃	327.35		2.6337 ²⁰ ₄	1.5770 ²⁰		168		

Methylene bromochloride, b256

Methylene chloride, d190

4,4'-Methylenedianiline, d35

Methylene dimethyl ether, d441

Methylene iodide, d404

1,1'-Methylenedipiperidine, d695

β-Methylene-β-propiolactone, d422

(*E*)-3,6-*endo*-Methylene-1,2,3,6-tetrahydronaphthaloyl dichloride, n109

Methyl ethyl ketone, b393

Methyl fluoroform, t291

Methyl 2-furancarboxylate, m253

5-Methylfurfural, m251

α-Methyl-D-glucopyranoside, m256

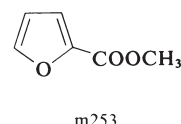
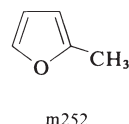
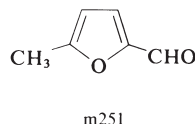
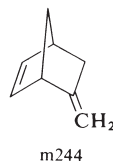
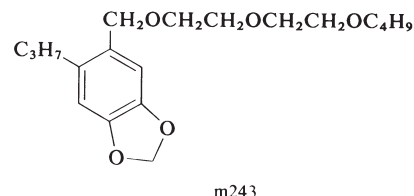
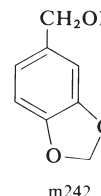
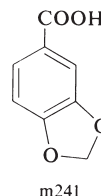
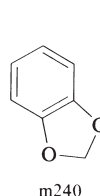
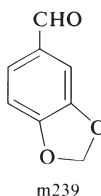
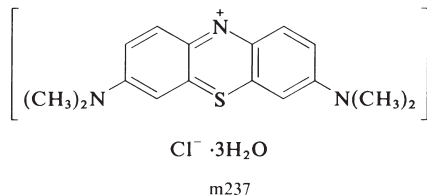


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

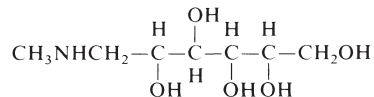
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m255	<i>N</i> -Methyl-D-glucamine		195.22				128–129			100 aq; 1.2 alc
m256	α -Methylglucoside		194.19	31, 179	1.46 ₄ ³⁰		168	200 ^{0.2mm}		63 aq; i alc, eth
m257	DL-2-Methyl-glutaronitrile	NCCH ₂ CH ₂ CH(CH ₃)CN	108.14	2, 656	0.950			125 ^{10mm}	126	
m258	<i>N</i> -Methylglycine	CH ₃ NHCH ₂ COOH	89.09	4, 345			d 212			42 aq; sl s alc
m259	Methyl glycolate	HOCH ₂ COOCH ₃	90.08	3, 236	1.168 ₄ ¹⁸		74	151		s aq; misc alc, eth
m260	2-Methylheptane	CH ₃ (CH ₂) ₄ CH(CH ₃) ₂	114.23	1, 161	0.6978 ₄ ²⁰	1.3974 ²⁰	−109.0	117.7	4	s eth; sl s alc
m261	Methyl heptanoate	CH ₃ (CH ₂) ₅ COOCH ₃	144.22	2, 339	0.8815 ₄ ²⁰	1.4115 ²⁰	−55.8	173.8	52	s alc, eth; sl s aq
m262	6-Methyl-5-hepten-2-one	(CH ₃) ₂ C=CHCH ₂ CH ₂ -COCH ₃	126.20	1 ² , 797	0.855 ₄ ¹⁶	1.4392 ²⁰	−67	73 ^{18mm}	50	misc alc, eth
m263	Methyl hexadecanoate	CH ₃ (CH ₂) ₁₄ COOCH ₃	270.46	2, 372			28	196 ^{15mm}		s alc, chl, eth
m264	2-Methylhexane	CH ₃ (CH ₂) ₃ CH(CH ₃) ₂	100.21	1, 156	0.6786 ²⁰	1.3849 ²⁰	−118.3	90.1	−3	s alc; misc eth
m265	Methyl hexanoate	CH ₃ (CH ₂) ₄ COOCH ₃	130.19	2, 323	0.9038 ₄ ⁰	1.4038 ²³	−71	151	54	v s alc, eth
m266	5-Methyl-2-hexanol	(CH ₃) ₂ CHCH ₂ CH ₂ -CH(OH)CH ₃	116.20	1, 416	0.814 ₄ ²⁰	1.4176 ²⁰		150	46	s alc, eth; i aq
m267	5-Methyl-2-hexanone	(CH ₃) ₂ CHCH ₂ CH ₂ -COCH ₃	114.19	1 ² , 756	0.888 ₄ ²⁰	1.4062 ²⁰		141	41	0.5 aq; misc alc, eth
m268	5-Methyl-3-hexen-2-one	(CH ₃) ₂ CHCH=CHCOCH ₃	112.17			1.4400 ²⁰				
m268a	1-Methylhexylamine	H(CH ₂) ₅ CH(NH ₂)CH ₃	115.22	4, 194	0.7665 ¹⁸	1.4175 ²⁰		144	54	sl s aq; s alc, eth
m269	1-Methylhydantoin		114.10	24, 244			157	subl		s aq, alc; 3 eth
m270	Methylhydrazine	CH ₃ NHNH ₂	46.07	4 ² , 957	0.866	1.4235 ²⁰	−52.4	87.5	21	misc aq, alc; s PE
m271	Methyl hydrazinocarboxylate	H ₂ NNHCOOCH ₃	90.08	3 ¹ , 46			70–73	108 ^{12mm}		
m272	Methyl hydrogen glutarate	HOOCCH ₂ CH ₂ CH ₂ COOCH ₃	146.14	2 ² , 565	1.169	1.4381 ²⁰		151 ^{10mm}	>112	

m273	Methyl hydrogen hexanedioate	$\text{HOOC}(\text{CH}_2)_4\text{COOCH}_3$	160.17	2, 652	1.081	1.4401 ²⁰	8–9	162 ^{10mm}	>112	s alc
m274	Methyl hydrogen succinate	$\text{HOOCCH}_2\text{CH}_2\text{COOCH}_3$	132.12	2, 608			56–59	151 ^{20mm}		v s aq, alc, eth
m275	Methyl hydroperoxide	CH_3OOH	48.04	1 ² , 270	1.997 ¹⁵ ₄	1.3642 ¹⁵		38 ^{65mm}		misc aq, alc, eth; s bz
m276	Methylhydroquinone		124.14	6, 874			125–128			
m277	Methyl 4-hydroxybenzoate	$\text{HOC}_6\text{H}_4\text{COOCH}_3$	152.15	10, 158			126–128	270 d		v s alc, eth, acet
m278	Methyl 2-hydroxyisobutyrate	$(\text{CH}_3)_2\text{C}(\text{OH})\text{COOCH}_3$	118.13	3 ² , 223	1.023	1.4112 ²⁰		137	42	v s aq, alc
m279	Methyl 4-hydroxyphenylacetate	$\text{HOC}_6\text{H}_4\text{CH}_2\text{COOCH}_3$	166.18	10, 191			57–60	162–163 ^{5mm}		
m280	1-Methylimidazole		82.11	23, 46	1.030	1.4970 ²⁰	–60	198	92	misc aq
m281	2-Methylimidazole		82.11	23, 65			143	268		
m282	4-Methylimidazole		82.11	23, 69			46–48	263	>112	

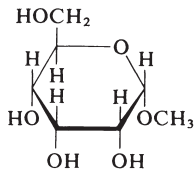
N-Methylguanidine acetic acid, c277
 4-Methylhexahydrophthalic anhydride, m196
 Methyl hydroxyacetate, m259

Methyl 4-hydroxy-3-methoxybenzoate, m445
 Methyl 2-hydroxypropionate, m291
 2,2'-Methyliminodiethanol, m223

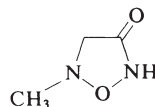
2,2'-Methyliminobis(acetaldehyde diethyl acetal), b169



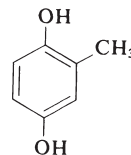
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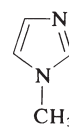
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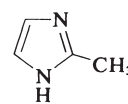
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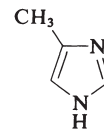
m276



m280



m281



m282

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m283	2-Methyl-1 <i>H</i> -indole		131.18	20, 311	1.07 ₄ ²⁰		58–60	273		v s alc, eth; s hot aq
m284	3-Methyl-1 <i>H</i> -indole		131.18	20, 315			95	266		s hot aq, alc, bz
m285	<i>N</i> -Methylisatoic anhydride		177.16	27, 265			165 d			
m286	Methyl isobutyrate	(CH ₃) ₂ CHCOOCH ₃	102.13	2, 290	0.891 ²⁰	1.3840 ²⁰	–84	93	<1	misc alc, eth; sl s aq
m287	Methyl isocyanate	CH ₃ NCO	57.05	4, 77	0.967	1.3695 ²⁰	–17	37–39	–18	s aq
m288	Methyl isodehyd- acetate		182.18	18, 410			60–63	167 ^{14mm}		
m289	Methyl isothio- cyanate	CH ₃ NCS	73.12	4, 77	1.069	1.5258 ³⁷	35–36	119	32	v s alc, eth; sl s aq
m290	5-Methylisoxazole		83.09	27, 16	1.018	1.4386 ²⁰		122	30	
m291	Methyl lactate	CH ₃ CH(OH)COOCH ₃	104.10	3, 280	1.088 ₄ ²⁰	1.4131 ²⁰	~66	144.8	52	misc aq(d), alc, eth
m292	Methyl mandelate	C ₆ H ₅ CH(OH)COOCH ₃	166.18	10, 202	1.1756 ²⁰		51–54	135 ^{12mm}		s aq, alc, bz, chl
m293	Methyl mercapto- acetate	HSCH ₂ COOCH ₃	106.14		1.187	1.4657 ²⁰		43 ^{10mm}	30	s alc, eth
m294	Methyl 3-mercapto- propionate	HSCH ₂ CH ₂ COOCH ₃	120.17	3 ² , 214	1.085	1.4640 ²⁰		55 ^{14mm}	60	
m295	Methylmercury chloride	CH ₃ HgCl	251.10		4.06 ²⁵		170			
m296	Methyl methacrylate	H ₂ C=C(CH ₃)COOCH ₃	100.12	2 ² , 398	0.9433 ²⁰	1.4146 ²⁰	–48.2	100.3	10	1.6 aq; s ketones, esters, CCl ₄
m297	Methyl methane- sulfonate	CH ₃ SO ₂ OCH ₃	110.13	4, 4	1.2943 ₄ ²⁰	1.4138 ²⁰		202–203	104	20 aq; 100 DMF
m298	Methyl methoxy- acetate	CH ₃ OCH ₂ COOCH ₃	104.11	3, 236	1.0511 ₄ ²⁰	1.3964 ²⁰		130	35	v s alc, eth; sl s aq

m299	Methyl 1-methoxybicyclo[2.2.2]oct-5-ene-2-carboxylate		196.25		1.086	1.4886 ²⁰		105 ^{17mm}	103	
m300	Methyl 4-methoxyphenylacetate	$\text{CH}_3\text{OC}_6\text{H}_4\text{CH}_2\text{COOCH}_3$	180.20	10, 191	1.135	1.5165 ²⁰		158 ^{19mm}	36	
m301	1-Methyl-4-(methylamino)piperidine		128.22		0.882	1.4672 ²⁰			55	
m302	Methyl 3-methylbutyrate	$(\text{CH}_3)_2\text{CHCH}_2\text{COOCH}_3$	116.16	2 ² , 274	0.881 ²⁰ ₄	1.3800 ²⁵		116–117		sl s aq; misc alc, eth
m303	2-Methyl-6-methylen-2-octanol	$\text{C}_2\text{H}_5\text{C}(\text{=CH}_2)(\text{CH}_2)_3\text{C}(\text{CH}_3)_2\text{OH}$	156.27		0.784	1.4431 ²⁰		84 ^{10mm}	76	

Methyl iodide, i40

Methyl isoamyl ketone, m267

Methyl isobutenyl ketone, m350

Methyl isobutyl ketone, m346

Methyl isonicotinate, m402

Methyl isopentyl ketone, m267

Methyl isovalerate, m302

2-Methylactic acid, h127

Methyl linoleate, m325

Methyl mercaptan, m33

Methylmercaptoanilines, m422, m423

4-Methylmercaptobenzaldehyde, m424

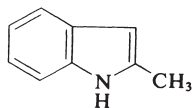
Methylmercaptophenols, m431a, m429

7-Methyl-3-methylene-1,6-octadiene, m453

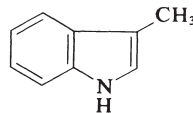
1-Methyl-4-(1-methylethenyl)cyclohexane, d649

5-Methyl-2-(1-methylethyl)cyclohexanol, m12

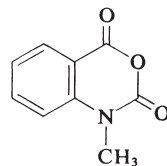
5-Methyl-2-(1-methylethyl)cyclohexanone, m13



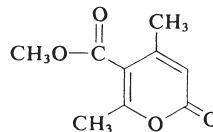
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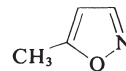
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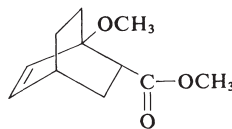
m285



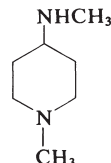
m288



m290



m299



m301

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m304	Methyl 2-methyl-3-furancarboxylate		140.14		1.116	1.4730 ²⁰		75 ^{20mm}	63	
m305	Methyl S-methylthiomethyl sulfoxide	CH ₃ S(=O)CH ₂ SCH ₃	124.22		1.191	1.5487 ²⁰		95 ^{2.5mm}	>112	
m306	Methyl 3-(methylthio)propionate	CH ₃ SCH ₂ CH ₂ COOCH ₃	134.20		1.077	1.4650 ²⁰		75 ^{13mm}	72	
m307	N-Methylmorpholine		101.15	27, 6	0.920	1.4349 ²⁰	−66	116	23	s aq, alc, eth
m308	1-Methylnaphthalene	C ₁₀ H ₇ CH ₃	142.20	5, 566	1.025 ₄ ¹⁴	1.6159 ²⁰	−30.5	244.7	82	v s alc, eth
m309	2-Methylnaphthalene	C ₁₀ H ₇ CH ₃	142.20	5, 567	1.029 ₄ ²⁰	1.6026 ⁴⁰	34.6	241.4		v s alc, eth
m310	2-Methyl-1,4-naphthoquinone		172.18	7 ² , 656			105–107			1.4 alc; 10 bz; s chl
m311	Methyl 1-naphthyl ketone	C ₁₀ H ₇ COCH ₃	170.21	7, 401	1.1336 ₄ ⁰	1.6284 ²⁰	12	296–298		s alc, eth; i aq
m312	Methyl 2-naphthyl ketone	C ₁₀ H ₇ COCH ₃	170.21	7, 402			53–55	300–301		sl s alc; s CS ₂
m313	Methyl nitrate	CH ₃ ONO ₂	77.04	1, 284	1.2075 ₄ ²⁰	1.3748 ²⁰	−83.0	64 explodes		sl s aq; s alc, eth
m314	Methyl nitrate	CH ₃ ONO	61.04	1, 284	0.991 (liquid)			−17.35		s alc, eth
m315	2-Methyl-4-nitroaniline	CH ₃ C ₆ H ₃ (NO ₂)NH ₂	152.15	12, 846	1.586 ₄ ¹⁴⁰		131–133			v s alc; s bz
m316	2-Methyl-5-nitroaniline	CH ₃ C ₆ H ₃ (NO ₂)NH ₂	152.15	12, 844			104–107			s alc, acet, eth
m317	4-Methyl-2-nitroaniline	CH ₃ C ₆ H ₃ (NO ₂)NH ₂	152.15	12, 100			115–116			v s alc; s eth
m318	Methyl 2-nitrobenzoate	O ₂ NC ₆ H ₄ COOCH ₃	181.15	9, 372	1.280	1.5350 ²⁰	−13	106 ^{0.1mm}	>112	s alc, eth

m319	2-Methyl-3-nitro-benzoic acid	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)\text{COOH}$	181.15	9, 471			182–184		
m320	4-Methyl-3-nitro-benzoic acid	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)\text{COOH}$	181.15	9, 502			187–190		
m321	5-Methyl-2-nitro-benzoic acid	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)_2\text{-COOH}$	181.15	9, 482			134–136		
m322	2-Methyl-5-nitro-imidazole		127.10	23 ¹ , 23			252–254		
m323	3-Methyl-2-nitro-phenol	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)\text{OH}$	153.14	6, 385			35–39		
m324	4-Methyl-2-nitro-phenol	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)\text{OH}$	153.14	6, 412	1.240 ₄ ²⁰	1.574 ⁴⁰	32–35	125 ^{22mm}	v s alc, eth
m325	Methyl 9,12-octa-decadienoate	$\text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CHCH}_2\text{-CH}=\text{CH}(\text{CH}_2)_7\text{COOCH}_3$	294.46		0.8886 ₄ ¹⁸	1.4593 ²⁵	–35	212 ^{16mm}	misc DMF
m326	Methyl octa-decanoate	$\text{CH}_3(\text{CH}_2)_{16}\text{COOCH}_3$	298.51	2, 379			38–39	215 ^{15mm}	> 112 s alc, eth
m327	Methyl cis-9-octa-decenoate	$\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH-}(\text{CH}_2)_7\text{COOCH}_3$	296.50	2, 467	0.879 ₄ ¹⁸	1.4521 ²⁰	19.9	168 ^{2mm}	misc abs alc, eth
m328	Methyloctadecyldi-chlorosilane	$\text{C}_{18}\text{H}_{37}\text{Si}(\text{CH}_3)\text{Cl}_2$	367.5		0.930 ₄ ²⁰			185 ^{2.5mm}	

Methyl 2-methylactate, m278
Methyl methyl-2-propenoate, m296
Methyl methylsulfynlmethyl sulfide, m305

Methyl myristate, m413
Methyl nicotinate, m404
4-Methyl-3-nitroanisole, m85

Methyl 6-nitrovertrate, m226
Methyl nonyl ketone, u5
Methyl oleate, m327

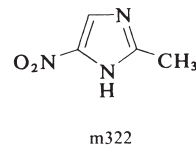
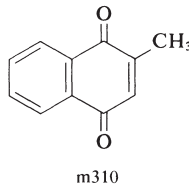
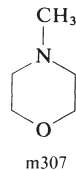
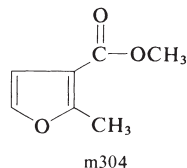


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m329	Methyl octanoate	$\text{CH}_3(\text{CH}_2)_6\text{COOCH}_3$	158.24	2, 348	0.8775_4^{20}	1.4160^{25}	−40	192.9		v s alc, eth; i aq
m330	Methyloctyldichlorosilane	$\text{C}_8\text{H}_{17}\text{Si}(\text{CH}_3)\text{Cl}_2$	227.3		0.976_4^{20}	1.444^{20}		$94^{6\text{mm}}$		
m331	3-Methyl-2-oxazolidinone		101.11		1.170	1.4541^{20}	15	87– $90^{1\text{mm}}$	> 112	
m332	2-Methyl-2-oxazoline		85.11	27, 11	1.005	1.4340^{20}		110	20	
m333	Methyl 2-oxocyclopentanecarboxylate		142.15	10, 597	1.145	1.4560^{20}		$105^{19\text{mm}}$	> 112	
m334	Methyl 2-oxopropionate	$\text{CH}_3\text{C}(=\text{O})\text{COOCH}_3$	102.09	3, 616	1.130	1.4065^{20}		134–137	39	misc alc, eth; sl s aq
m335	Methyl 2-oxo-1-pyrrolidineacetate		157.17		1.131	1.4719^{20}			110	
m336	2-Methylpentane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$	86.18	1, 148	0.6532^{20}	1.3725^{20}	−153.7	60.3	−23	
m337	3-Methylpentane	$(\text{CH}_3\text{CH}_2)_2\text{CHCH}_3$	86.18	1, 149	0.6643^{20}	1.3765^{20}	< −50 glass	63.3	−6	
m338	2-Methyl-2,4-pentanediol	$(\text{CH}_3)_2\text{C}(\text{OH})\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$	118.18	1, 486	0.9216_4^{20}	1.4270^{20}	< −50 glass	198.3	101	misc aq
m339	4-Methylpentanenitrile	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CN}$	97.16	2 ² , 290	0.8035_4^{20}	1.4061^{20}	−51.1	153.5		s alc; misc eth
m340	Methyl pentanoate	$\text{CH}_3(\text{CH}_2)_3\text{COOCH}_3$	116.16	2, 301	0.875	1.3962^{20}		128	22	sl s aq; misc alc, eth
m341	2-Methylpentanoic acid	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{COOH}$	116.16	2 ² , 288	0.9242_{20}^{20}	1.4135^{20}	−85 glass	196.4	107	1.3 aq
m342	3-Methylpentanoic acid	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{COOH}$	116.16	2, 331	0.9262^{20}	1.4159^{20}	−42	196–198	85	s alc, eth
m343	2-Methyl-1-pentanol	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{OH}$	102.18	1, 409	0.8242^{20}	1.4190^{20}		148.0	50	s alc, eth

m344	3-Methyl-3-pentanol	$(\text{CH}_3\text{CH}_2)_2\text{C}(\text{CH}_3)\text{OH}$	102.18	1, 411	0.8281 ²⁰	1.4186 ²⁰	< -38	122.4	46	misc alc, eth; sl s aq
m345	4-Methyl-2-pentanol	$(\text{CH}_3)_2\text{CHCH}_2\text{-CH}(\text{OH})\text{CH}_3$	102.18	1, 410	0.8080 ²⁰	1.4112 ²⁰	-90	131.7	41	1.6 aq
m346	4-Methyl-2-pentanone	$(\text{CH}_3)_2\text{CHCH}_2\text{COCH}_3$	100.16	1, 691	0.8006 ²⁰	1.3958 ²⁰	-83.5	115.7	13	1.7 aq; misc alc, bz, eth
m347	2-Methyl-1-pentene	$\text{CH}_3\text{CH}_2\text{CH}_2\text{-C}(\text{CH}_3)=\text{CH}_2$	84.16	1 ¹ , 90	0.6799 ²⁰	1.3920 ²⁰	-135.7	62.1	-26	s alc
m348	2-Methyl-2-pentene	$\text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2$	84.16	1, 217	0.6865 ²⁰	1.4003 ²⁰	-135.1	67.3	-23	s alc
m349	4-Methyl-2-pentenoic acid	$(\text{CH}_3)_2\text{CHCH}=\text{CHCHCOOH}$	114.14	2 ² , 406	0.9529	1.4489	35	115 ^{20mm}	46	i aq; v s alc
m350	4-Methyl-3-penten-2-one	$(\text{CH}_3)_2\text{C}=\text{CHCOCH}_3$	98.15	1, 736	0.854 ²⁰	1.4458 ²⁰	-42	129.5	30	3.1 aq
m350a	1-Methylpentylamine	$\text{CH}_3(\text{CH}_2)_4\text{-CH}(\text{NH}_2)\text{CH}_3$	101.19	4, 190	0.767 ²⁰		-19	116-118	13	s aq, alc, PE
m351	4-Methyl-1-pentyne	$(\text{CH}_3)_2\text{CHCH}_2\text{C}\equiv\text{CH}$	82.15		0.7041 ²⁰	1.3930 ²⁰	-104.8	61.2		
m352	3-Methyl-1-pentyn-3-ol	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)(\text{OH})\text{-C}\equiv\text{CH}$	98.15	1 ² , 506	0.8688 ²⁰	1.4318 ²⁰	-30.6	121-122	38	13 aq; misc bz, acet, PE, EtAc; s eth
m353	Methyl-(2-phenethyl)dichlorosilane	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{Si}(\text{CH}_3)\text{Cl}_2$	219.2		1.111 ²⁰	1.510 ²⁰		99 ^{6mm}		

o-Methylolphenol, h105
2-Methyloxacyclopropane, p227

Methyl oxirane, p227
Methyl palmitate, m263

Methyl pentyl ketone, h15

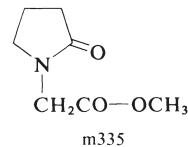
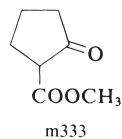
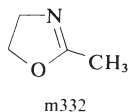
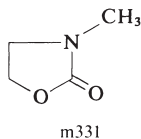


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m354	(1-Methylphenethyl)-trichlorosilane	$C_6H_5CH(CH_3)CH_2SiCl_3$	253.6		1.226 ₄ ²⁰	1.515 ²⁰		116 ^{10mm}		
m355	<i>N</i> -(4-Methylphenyl)-acetamide	$CH_3C_6H_4NHCOCH_3$	149.19	12 ² , 501	1.212 ¹⁵		153	307		s alc, EtAc, HOAc
m356	Methyl phenylacetate	$C_6H_5CH_2COOCH_3$	150.18	9, 434	1.044	1.5075 ²⁰		215	90	i aq; misc alc, eth
m357	Methylphenylchlorosilane	$C_6H_5(CH_3)Si(H)Cl$	156.7		1.1054 ₄ ²⁰	1.571 ²⁰		113 ^{100mm}		
m358	Methylphenyldichlorosilane	$C_6H_5Si(CH_3)Cl_2$	191.1		1.187 ₄ ²⁰			205–206		
m359	<i>p</i> -(1-Methyl-2-phenylethyl)phenol	$C_6H_5CH_2CH(CH_3)-C_6H_4OH$	212.29				73	335		
m360	1-Methyl-1-phenylhydrazine	$C_6H_5N(CH_3)NH_2$	122.17	15, 117	1.038 ₄ ²²	1.5834 ²⁰		118 ^{21mm}	96	misc alc, bz, chl, eth
m361	1-Methyl-3-phenylpropyl acetate	$C_6H_5CH_2CH_2CH(CH_3)-OOCCH_3$	192.26	6 ¹ , 258	0.991			74 ^{0.05mm}	>112	
m362	3-Methyl-1-phenyl-2-pyrazolin-5-one		174.20	24, 20			130	287 ^{265mm}		
m363	Methylphenylsilane	$C_6H_5Si(CH_3)H_2$	122.1		0.889 ₄ ²⁰	1.506 ²⁰		139–240		
m364	Methyl phenyl sulfide	$C_6H_5SCH_3$	124.21	6, 297	1.058	1.5852 ²⁰	–15	188		i aq; s alc
m365	<i>N</i> -Methylpiperazine		100.17		0.903	1.4655 ²⁰		138	42	v s aq, alc, eth
m366	2-Methylpiperazine		100.17	23, 17			65–67	155.6	22	78 aq; 37 acet; 32 bz
m367	4-Methyl-1-piperazinepropanol		158.25	23 ³ , 123		1.4835 ²⁰	28–30	120–121 ^{9mm}		
m368	<i>N</i> -Methylpiperidine	$C_5H_{10}N-CH_3$	99.19	20, 19	0.816	1.4378 ²⁰		106–107	<1	v s aq; misc alc, eth
m369	2-Methylpiperidine	$CH_3C_5H_9NH$	99.19	20, 95	0.844	1.4459 ²⁰	–5	119	8	v s aq; misc alc, eth

m370	3-Methylpiperidine	$\text{CH}_3\text{C}_5\text{H}_9\text{NH}$	99.19	20, 100	0.845	1.4470 ²⁰		126	<1	v s aq
m371	4-Methylpiperidine	$\text{CH}_3\text{C}_5\text{H}_9\text{NH}$	99.19	20, 101	0.838	1.4458 ²⁰		124	7	v s aq
m372	1-Methyl-3-piperidinemethanol		129.20	21 ² , 8	1.013	1.4772 ²⁰		140–145	94	
m373	1-Methyl-4-piperidone		113.16	21 ² , 215	0.920	1.4614 ²⁰			60	
m374	2-Methylpropanal	$(\text{CH}_3)_2\text{CHCHO}$	72.11	1, 671	0.7891 ²⁰	1.3727 ²⁰	–65	64.1		9 aq; misc alc, bz, chl, eth
m375	2-Methylpropane	$(\text{CH}_3)_3\text{CH}$	58.12	1, 124	0.557 ²⁰		–159.6	–11.7		13 mL aq; 1320 mL alc; 2890 mL eth
m376	<i>N</i> -Methyl-1,3-propanediamine	$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{NHCH}_3$	88.15	4 ¹ , 419	0.844	1.4468 ²⁰		139–141	35	
m377	2-Methyl-1,2-propanediamine	$(\text{CH}_3)_2\text{C}(\text{NH}_2)\text{CH}_2\text{NH}_2$	88.15	4, 266	0.841	1.4410 ²⁰			23	
m378	1-Methyl-1-propanethiol	$\text{CH}_3\text{CH}_2\text{CH}(\text{SH})\text{CH}_3$	90.19	1, 373	0.8246 ²⁵	1.4338 ²⁵	–165	84–85	21	sl s aq; v s alc, eth

Methylphenols, c279, c280, c281

Methyl-*m*-phenylene diisocyanate, t172

Methyl phenyl ether, m48

Methyl phenyl ketone, a31

2-Methyl-2-phenylpropane, b425

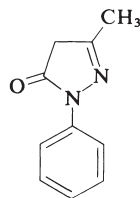
Methyl γ -picolinate, m402

Methylpiperidinol, h144

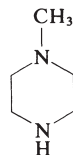
Methyl pivalate, m227

1-Methyl-1-propanethiol, b389

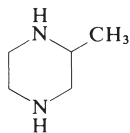
Methyl propargyl ether, m396



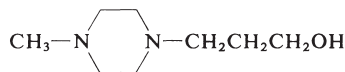
m362



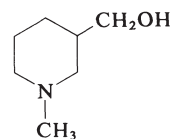
m365



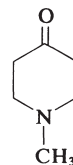
m366



m367



m372



m373

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

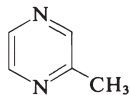
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m379	2-Methyl-1-propanethiol	$(\text{CH}_3)_2\text{CHCH}_2\text{SH}$	90.19	1, 378	0.8357 ₄ ²⁰	1.4396 ²⁰	−79	88.5	−9	v s alc, eth
m380	2-Methyl-2-propanethiol	$(\text{CH}_3)_3\text{CSH}$	90.19	1, 383	0.7943 ₄ ²⁵	1.4198 ²⁵	1.1	64.2	−26	i aq
m381	2-Methyl-1-propanol	$(\text{CH}_3)_2\text{CHCH}_2\text{OH}$	74.12	1, 373	0.8016 ²⁰	1.3958 ²⁰	−108	107.9	27	10 aq; misc alc, eth
m382	2-Methyl-2-propanol	$(\text{CH}_3)_3\text{COH}$	74.12	1, 379	0.7858 ₄ ²⁰	1.3877 ²⁰	25.8	82.4	15	misc aq, alc, eth
m383	2-Methylpropene	$(\text{CH}_3)_2\text{C}=\text{CH}_2$	56.10	1, 207	0.6266 ₄ ^{−140}		−140.4	−6.9		v s alc, eth
m384	2-Methyl-2-propene-1-sulfonic acid, Na salt	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{CH}_2\text{SO}_3^-\text{Na}^+$	158.15				>300			
m385	2-Methyl-2-propen-1-ol	$\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{CH}_2\text{OH}$	72.11	1, 443	0.857	1.4250 ²⁰		113–115	33	
m386	4-Methyl-2-(2-propenyl)phenol	$\text{CH}_3\text{C}_6\text{H}_3-(\text{CH}_2\text{CH}=\text{CH}_2)\text{OH}$	148.21	6 ¹ , 287	0.980	1.5385 ²⁰		238	101	
m387	6-Methyl-2-(2-propenyl)phenol	$\text{CH}_3\text{C}_6\text{H}_3-(\text{CH}_2\text{CH}=\text{CH}_2)\text{OH}$	148.21	6 ¹ , 287	0.992	1.5381 ²⁰		231–233	94	
m388	N-Methylpropionamide	$\text{CH}_3\text{CH}_2\text{CONHCH}_3$	87.12		0.9305 ²⁵	1.4345 ²⁵	−30.9	148		
m389	Methyl propionate	$\text{CH}_3\text{CH}_2\text{COOCH}_3$	88.11	2, 239	0.915 ₄ ²⁰	1.3770 ²⁰	−88	79.7	−2	6 aq; misc alc, eth
m390	2-Methylpropionic acid	$(\text{CH}_3)_2\text{CHCOOH}$	88.11	2, 288	0.950 ₄ ²⁰	1.3930 ²⁰	−46.1	154.7	55	23 aq; misc alc, chl, eth
m391	4'-Methylpropio-phenone	$\text{CH}_3\text{C}_6\text{H}_4\text{COCH}_2\text{CH}_3$	148.21	7, 317	0.993	1.5280 ²⁰	7.2	239	96	
m392	Methylpropyldichlorosilane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{Si}(\text{CH}_3)\text{Cl}_2$	157.1		1.04 ₄ ²⁵	1.425 ²⁵		125		
m393	Methyl propyl ether	$\text{CH}_3\text{CH}_2\text{CH}_2\text{OCH}_3$	74.12	1, 354	0.738 ²⁰			39.1		sl s aq; misc alc, eth

m394	2-Methyl-2-propyl-1,3-propanediol	$\text{C}_3\text{H}_7\text{C}(\text{CH}_3)(\text{CH}_2\text{OH})_2$	132.20	1 ¹ , 254			53–55	230		
m395	Methyl propyl sulfide	$\text{CH}_3\text{SCH}_2\text{CH}_2\text{CH}_3$	90.18	1 ³ , 1432	0.8424 ²⁰	1.4442 ²⁰	–113.0	95.5		s aq
m396	Methyl 2-propynyl ether	$\text{CH}_3\text{OCH}_2\text{C}\equiv\text{CH}$	70.09	1, 454	0.830	1.3961 ²⁰		61–62	< 1	
m397	2-Methylpyrazine		94.12	23, 94	1.030	1.5042 ²⁰	–29	135	50	v s aq, alc, eth
m398	2-Methylpyridine	$\text{CH}_3\text{C}_5\text{H}_4\text{N}$	93.13	20, 234	0.950 ¹⁵ ₄	1.5010 ²⁰	–67	128–129	26	v s aq; s alc, eth
m399	3-Methylpyridine	$\text{CH}_3\text{C}_5\text{H}_4\text{N}$	93.13	20, 239	0.961 ¹⁵ ₄	1.5068 ²⁰	–18.3	143.5	36	s aq, alc, eth
m400	4-Methylpyridine	$\text{CH}_3\text{C}_5\text{H}_4\text{N}$	93.13	20, 240	0.957 ¹⁵ ₄	1.5058	3.8	143–145	56	s aq, alc, eth
m401	Methyl 3-pyridine-carboxylate	$(\text{C}_5\text{H}_4\text{N})\text{COOCH}_3$	137.14	22, 39			39	209		s aq, alc, bz
m402	Methyl 4-pyridine-carboxylate	$(\text{C}_5\text{H}_4\text{N})\text{COOCH}_3$	137.14	22, 46	1.001	1.5122 ²⁰	8.5	207–209	82	
m403	1-Methyl-2-pyridone		109.13	21, 268	1.112	1.5690 ²⁰	7	250 ^{740mm}		
m404	N-Methylpyrrole		81.2	20, 163	0.914	1.4875 ²⁰	–57	113	15	i aq; misc alc, eth

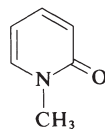
2-Methylpropenenitrile, m27
 2-Methylpropenoic acid, m26
 2-Methylpropionaldehyde, i73
 2-Methylpropionamide, i74
 2-Methylpropionic acid, i75
 2-Methylpropionitrile, i76

1-Methylpropyl acetate, b413
 2-Methylpropyl acetate, i62
 2-Methyl-2-propylamine, b418
 2-Methylpropylamine, i63
 (1-Methylpropyl)benzene, b424
 (2-Methylpropyl)benzene, i64

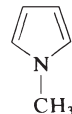
2-Methylpropyl formate, i66
 2-Methylpropyl lactate, i68
 Methyl propyl ketone, p41
 2-Methylpropyl 2-methylpropanoate, i67
 Methyl pyruvate, m334
 Methyl pyridyl ketones, a53, a54, a55



m397



m403



m404

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

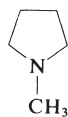
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m405	<i>N</i> -Methylpyrrolidine		85.15	20, 4	0.819 ₄ ²⁰	1.4247 ²⁰		80–81	–21	misc aq, eth
m406	<i>N</i> -Methyl-2-pyrrolidinone		99.13	21 ¹ , 213	1.0279 ²⁵	1.4680 ²⁵	–24.4	202	95	misc aq, alc, bz, eth
m407	2-Methylquinoline		143.19	20, 387	1.058	1.6108 ²⁰	–2	248	79	i aq; s chl, eth
m408	4-Methylquinoline		143.19	20, 395	1.0826 ₄ ²⁰	1.6200 ²⁰	9–10	261–263	>112	misc alc, bz, eth
m409	2-Methylquinoxaline		144.18	23 ¹ , 44	1.118	1.6156 ²⁰	180–181	245–247	107	misc aq
m410	Methyl salicylate	HOC ₆ H ₄ COOCH ₃	152.15	10, 70	1.1831 ²⁰	1.5240 ²⁰	–8.6	223.0	110	0.7 aq; s chl, eth; misc alc, HOAc
m411	α -Methylstyrene	C ₆ H ₅ C(CH ₃)=CH ₂	118.18	5, 484	0.909	1.5375 ²⁰	–23.2	165.5	45	
m412	Methylsuccinic acid	HOOCCH ₂ CH(CH ₃)COOH	132.12	2, 636	1.411	1.4303	110–112	d		66 aq; v s alc, eth
m413	Methyl tetradecanoate	CH ₃ (CH ₂) ₁₂ COOCH ₃	242.40	2 ² , 326	0.855	1.4362 ²⁰	18.4	323	>112	misc alc, bz, eth
m414	2-Methyl-3,3,4,4-tetrafluoro-2-butanol	HCF ₂ CF ₂ C(CH ₃) ₂ OH	160.11		1.282	1.3524 ²⁰		117	73	
m415	2-Methyltetrahydrofuran		86.13	17, 12	0.860	1.4056 ²⁰		78–80	–11	
m416	1-Methyl-1,2,3,6-tetrahydropyridine		97.16		0.837	1.4570 ²⁰		113–114	8	
m417	3-Methyltetrahydrothiophene-1,1-dioxide		134.20		1.191	1.4772 ²⁰		276	>112	
m418	4-Methyl-5-thiazole-ethanol		143.21		1.196	1.5508 ²⁰		135 ^{7mm}		
m419	2-Methyl-2-thiazoline		101.17	27, 13	1.067	1.5200 ²⁰	–101	145	37	
m420	Methyl thioacetate	CH ₃ COSCH ₃	90.14			1.4628		98	10	s alc, eth
m421	(Methylthio)acetonitrile	CH ₃ SCH ₂ CN	87.14		1.039	1.4826 ²⁰		63 ^{15mm}	67	

m422	2-(Methylthio)-aniline	$\text{CH}_3\text{SC}_6\text{H}_4\text{NH}_2$	139.22	13, 399	1.111	1.6239 ²⁰	234	>112	
m423	3-(Methylthio)-aniline	$\text{CH}_3\text{SC}_6\text{H}_4\text{NH}_2$	139.22	13 ¹ , 141	1.130	1.6423 ²⁰	165 ^{16mm}	>112	
m424	4-(Methylthio)-benzaldehyde	$\text{CH}_3\text{SC}_6\text{H}_4\text{CHO}$	152.22	8 ¹ , 533	1.144	1.6452 ²⁰	90 ^{1mm}		
m425	3-(Methylthio)-2-butanone	$\text{CH}_3\text{CH}(\text{SCH}_3)\text{COCH}_3$	118.20	1 ⁴ , 3993	0.975	1.4710 ²⁰	50–54 ^{20mm}	44	
m426	Methyl thiocyanate	CH_3SCN	73.12	3, 175	1.068 ²⁰	1.4697 ²⁰	–51	130–133	38
m427	3-Methylthiophene		98.17	17, 38	1.016	1.5180 ²⁰	–69.0	115.4	11
m428	5-Methyl-2-thiophenecarbaldehyde		126.18	17 ¹ , 151	1.170	1.5825 ²⁰		114 ^{25mm}	87
m429	4-(S-Methylthio)-phenol	$\text{CH}_3\text{SC}_6\text{H}_4\text{OH}$	140.20	6 ¹ , 419			83–85	153–156 ^{20mm}	

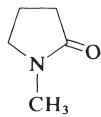
1-Methyl-2-(3-pyridyl)pyrrolidine, n20
Methylresorcinol, d390
Methylsalicylic acids, h137, h138
Methyl stearate, m326

Methylsuccinyl chloride, m188
methylsulfonic acid, m30
Methyl theobromine, c1
3-Methyl-2-thiabutane, i104

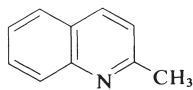
Methyl thienyl ketone, a57
Methyl thioglycolate, m293



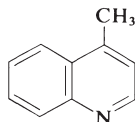
m405



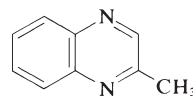
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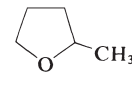
m407



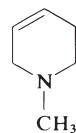
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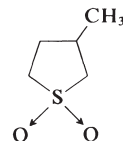
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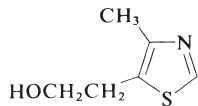
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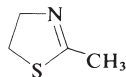
m416



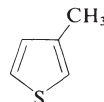
m417



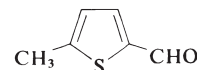
m418



m419



m427



m428

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

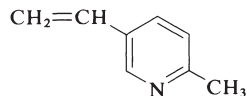
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m430	3-Methylthio-1,2-propanediol	$\text{CH}_3\text{SCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$	122.19		1.164	1.5160 ²⁰			>112	v s aq, alc
m431	<i>N</i> -Methylthiourea	$\text{CH}_3\text{NHC}(=\text{S})\text{NH}_2$	90.15	4, 70			119–121			
m432	<i>N</i> -Methyl- <i>o</i> -toluamide	$\text{CH}_3\text{C}_6\text{H}_4\text{CONHCH}_3$	149.19	9, 465	1.168 ¹⁵		69–71			
m433	<i>N</i> -Methyl- <i>p</i> -toluenesulfonamide	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{NHCH}_3$	185.25	11, 105			76–79			
m434	Methyl <i>p</i> -toluenesulfonate	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{OCH}_3$	186.23	11, 99			27.5			
m435	Methyltriacetoxysilane	$\text{CH}_3\text{Si}(\text{OOCCH}_3)_3$	220.3	4 ³ , 1896	1.175 ²⁰ ₄	1.408 ²⁰		88 ^{3mm}		
m436	Methyl 2,2,2-trichloroacetimidate	$\text{Cl}_3\text{CC}(=\text{NH})\text{OCH}_3$	176.43	2, 212	1.425	1.4780 ²⁰		149	none	
m437	Methyltrichlorogermane	CH_3GeCl_3	193.98		1.730			111		
m438	Methyl trifluoromethanesulfonate	$\text{CF}_3\text{SO}_2\text{OCH}_3$	164.10		1.450	1.3244 ²⁰		94–99	38	
m439	<i>N</i> -Methyl- <i>N</i> -trimethylsilylacetamide	$\text{CH}_3\text{CON}(\text{CH}_3)\text{-Si}(\text{CH}_3)_3$	145.3	4 ⁴ , 4011	1.439 ²⁰ ₄	0.901 ²⁰		154		
m440	<i>N</i> -Methyl- <i>N</i> -(trimethylsilyl)-trifluoroacetamide	$\text{CF}_3\text{CON}(\text{CH}_3)\text{-Si}(\text{CH}_3)_3$	199.25		1.075	1.3802 ²⁰		132	25	
m441	Methyltripropoxysilane	$\text{CH}_3\text{Si}(\text{OC}_3\text{H}_7)_3$	220.4		0.88 ²⁰ ₄	1.4085 ²⁰		83 ^{13mm}		
m442	(Methyl)triphenylphosphonium bromide	$[\text{CH}_3\text{P}(\text{C}_6\text{H}_5)_3]^+\text{Br}^-$	357.24				230–233			

m443	2-Methylundecanal	$\text{CH}_3(\text{CH}_2)_8\text{CH}(\text{CH}_3)\text{-CHO}$	184.32		0.830 ₄ ¹⁵	1.4321 ²⁰		271	93	s alc, eth
m444	Methyl urea	$\text{CH}_3\text{NHCONH}_2$	74.08	4, 64	1.204		101–102	d		v s aq, alc; i eth
m445	Methyl vanillate	$\text{CH}_3\text{OC}_6\text{H}_3(\text{OH})\text{COOCH}_3$	182.18	10, 396			64–65	285–287		s hot alc, hot PE
m446	Methyl vinyl ether	$\text{CH}_3\text{OCH=CH}_2$	58.08	1 ³ , 1857	0.7511 ₄ ²⁰	1.3947	–112	5.5	–56	0.8 aq; v s alc
m447	2-Methyl-5-vinylpyridine		119.17		0.898	1.5437 ²⁰		100 ^{50mm}	65	
m448	Morpholine		87.12	27, 5	1.007 ₄ ²⁰	1.4542 ²⁰	–4.9	128.9	35	misc aq, alc, bz, eth
m449	4-Morpholine-carbonitrile		112.12		1.109	1.4730 ²⁰		73 ^{0.6mm}	104	
m450	N-Morpholino-1-cyclohexene		167.25		0.995	1.5128 ²⁰		117–122	68	
m451	2-(N-Morpholino)-ethanesulfonic acid		195.24				> 300			

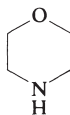
4-Methyl-2-thiouracil, h120
Methyltrichlorosilane, t238
Methyltriethoxysilane, t266a
Methyl trimethylacetate, m227
Methyltris(2-methoxyethoxy)silane, t429
β-Methylumbelliferone, h140
Methyluracil, d391

Methyl urethane, m181
Methyl valerate, m340
3-Methylvaleric acid, m342
4-Methylvaleronitrile, m339
Methyl veratrate, m225
Michler's ketone, b171
Monoethyl adipate, e149

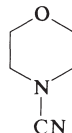
Monoglyme, d439
Monomethyl adipate, m273
Monomethyl glutarate, m272
Monomethyl succinate, m274
Mordent violet 5, a60
4-Morpholinoethanol, h122
1-Morpholinocyclopentene, c361



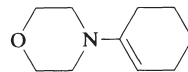
m447



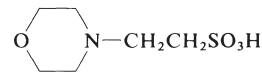
m448



m449



m450



m451

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
m452	3-(<i>N</i> -Morpholino)-1,2-propanediol		161.20		1.157		37–38	191 ^{30mm}	>112	
m453	β -Myrcene	$(\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_2-\text{C}(=\text{CH}_2)\text{CH}=\text{CH}_2$	136.24	1, 264	0.794 ₄ ²⁰	1.4709 ²⁰		166–168	39	s alc, chl, eth, HOAc
n1	1-Naphthaldehyde	$\text{C}_{10}\text{H}_7\text{CHO}$	156.18	7, 400	1.150 ₄ ²⁰	1.6520 ²⁰	1–2	161 ^{15mm}	>112	s alc, eth
n2	Naphthalene	C_{10}H_8	128.17	5, 531	1.162 ₄ ²⁰	1.5821 ¹⁰⁰	80.2 subl above mp	217.7	78	0.3 aq; 7 alc; 33 bz; 50 chl
n3	1-Naphthalenecarboxylic acid	$\text{C}_{10}\text{H}_7\text{COOH}$	172.18	9, 647			160–162	300		v s hot alc, eth
n4	1,5-Naphthalenediamine	$\text{C}_{10}\text{H}_6(\text{NH}_2)_2$	158.20	13, 203			185–187			s hot aq, hot alc
n5	1,8-Naphthalenediamine	$\text{C}_{10}\text{H}_6(\text{NH}_2)_2$	158.20	13, 204	1.1265 ₄ ⁹⁹	1.6828 ⁹⁹	66.5	205 ^{12mm}		sl s aq; s alc, eth
n6	1-Naphthalenemethylamine	$\text{C}_{10}\text{H}_7\text{CH}_2\text{NH}_2$	157.22	12, 1316	1.073	1.6429 ²⁰		290–293	>112	
n7	1,8-Naphthalic anhydride		198.18	17, 521			267–269			sl s HOAc
n8	1,8-Naphthalimide		197.19	21, 527			300			sl s alc; i bz, eth, aq
n9	1-Naphthol	$\text{C}_{10}\text{H}_7\text{OH}$	144.17	6, 596	1.0954 ₄ ⁹⁹	1.6206 ⁹⁹	96	288		v s alc, bz, chl, eth
n10	2-Naphthol	$\text{C}_{10}\text{H}_7\text{OH}$	144.17	6, 627	1.217 ⁴		121–123	285–286	161	0.1 aq; 125 alc; 6 chl; 77 eth; s alk
n11	1,4-Naphthoquinone		158.16	7, 724	1.422		128	subl < 100		s bz, chl, eth, alk
n12	(2-Naphthoxy)acetic acid	$\text{C}_{10}\text{H}_7\text{OCH}_2\text{COOH}$	202.21	6, 645			155–157			
n13	2-(1-Naphthyl)-acetamide	$\text{C}_{10}\text{H}_7\text{CH}_2\text{CONH}_2$	185.23	9, 666			181–183			i aq; s bz, CS_2

n14	1-Naphthyl acetate	$C_{10}H_7OOCCH_3$	186.21	6, 608			43–46			s alc, eth
n15	1-Naphthylacetic acid	$C_{10}H_7CH_2COOH$	186.21	9, 666			135	d		3.3 alc; v s chl, eth
n16	1-Naphthylacetonitrile	$C_{10}H_7CH_2CN$	167.21	9, 667		1.6192 ²⁰	33–35	194 ^{18mm}	>112	s alc
n17	1-Naphthylamine	$C_{10}H_7NH_2$	143.18	12, 1212	1.123 ²⁵ ₂₅	1.6703	50	301	157	0.2 aq; v s alc, eth
n18	2-Naphthylsulfonic acid	$C_{10}H_7SO_3H$	208.23	11, 171	1.441 ²⁵		91	d		77 aq; s alc, eth
n19	1-(1-Naphthyl)-2-thiourea	$C_{10}H_7NHC(=S)NH_2$	202.28	12, 1241			198			0.6 aq; 2.4 acet; s alc
n20	Nicotine		162.24	23, 117	1.0097 ²⁰ ₄	1.5282 ²⁰	–79	123 ^{17mm}		misc aq; v s alc, eth, PE

MSTFA, m440

Mucic acid, t84

Mucochloric acid, d208

Myristoyl chloride, t41

Myristic acid, t39

Myristic acid, t40

Myristyl bromide b352

Naphthacene, b7

1-Naphthaleneacetamide, n13

1-Naphthaleneacetonitrile, n16

Naphthalenediols, d392, d393, d394, d395

1-Naphthol-2-carboxylic acid, h148

3-Naphthol-2-carboxylic acid, h149

1-Naphthol-3,6-disulfonic acid, h151

2-Naphthol-3,6-disulfonic acid, h150

1-Naphthonitrile, c293

(2-Naphthoxy)acetic acid, n12

N-1-Naphthylaniline, p130

Natural orange 6, h152

NBA, b218

NBS, b351

Neohexane, d489

Neohexene, d499

Neopentane, d592

Neopentyl alcohol, d595

Neopentyl glycol, d594

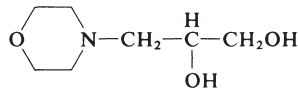
Neral, d563

Nerolidol, h184

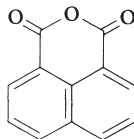
Nicotinaldehyde, p256

Nicotinic acid, p256

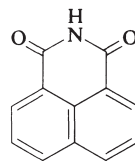
Nicotinonitrile, c296



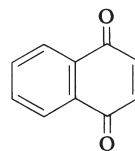
m452



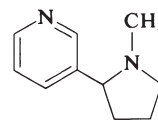
n7



n8



n11



n20

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

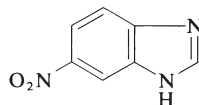
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
n21	Nitrilotriacetic acid	$\text{N}(\text{CH}_2\text{COOH})_3$	191.14	4, 369			246 d			0.1 aq; s hot alc
n22	<i>m</i> -Nitroacetophenone	$\text{O}_2\text{NC}_6\text{H}_4\text{COCH}_3$	165.15	7, 288			76–78	202		s alc, eth
n23	<i>p</i> -Nitroacetophenone	$\text{O}_2\text{NC}_6\text{H}_4\text{COCH}_3$	165.15	7, 288			78–80	202		s alc
n24	<i>o</i> -Nitroaniline	$\text{O}_2\text{NC}_6\text{H}_4\text{NH}_2$	138.13	12, 687	1.442 ¹⁵		69–70	284		s hot aq, alc, chl
n25	<i>m</i> -Nitroaniline	$\text{O}_2\text{NC}_6\text{H}_4\text{NH}_2$	138.13	12, 698	1.43		114	306		0.1 aq; 5 alc; 6 eth
n26	<i>p</i> -Nitroaniline	$\text{O}_2\text{NC}_6\text{H}_4\text{NH}_2$	138.13	12, 711	1.437 ¹⁴		146	260 ^{100mm}	165	4 alc; 3.3 eth; s bz
n27	3-Nitrobenzaldehyde	$\text{O}_2\text{NC}_6\text{H}_4\text{CHO}$	151.12	7, 250	1.2792 ²⁰		58	164 ^{23mm}		s alc, chl, eth
n28	4-Nitrobenzaldehyde	$\text{O}_2\text{NC}_6\text{H}_4\text{CHO}$	151.12	7, 256	1.496		106–107			s alc, bz, HOAc
n29	2-Nitrobenzamide	$\text{O}_2\text{NC}_6\text{H}_4\text{CONH}_2$	166.12	9, 373	1.462 ³²		174–178	317		s hot aq, hot alc, eth
n30	Nitrobenzene	$\text{C}_6\text{H}_5\text{NO}_2$	123.11	5, 233	1.205 ¹⁵	1.5546 ¹⁵	5.8	210.8	87	v s alc, bz, eth
n31	2-Nitrobenzene-1,4-dicarboxylic acid	$\text{O}_2\text{NC}_6\text{H}_3(\text{COOH})_2$	211.13	9, 851			270–272			
n32	3-Nitrobenzene-1,2-dicarboxylic acid	$\text{O}_2\text{NC}_6\text{H}_3(\text{COOH})_2$	211.13	9, 823			216 d			2 aq; v s hot alc
n33	4-Nitrobenzene-1,2-dicarboxylic acid	$\text{O}_2\text{NC}_6\text{H}_3(\text{COOH})_2$	211.13	9, 828			163–166			v s aq, alc; s eth
n34	5-Nitrobenzene-1,3-dicarboxylic acid	$\text{O}_2\text{NC}_6\text{H}_3(\text{COOH})_2$	211.13	9, 840			260–261			0.15 aq; v s alc, eth
n35	2-Nitrobenzene-sulfonyl chloride	$\text{O}_2\text{NC}_6\text{H}_4\text{SO}_2\text{Cl}$	221.62	11, 67			65–67			s eth; d hot aq, alc
n36	6-Nitrobenzimidazole		163.14	23, 135			207–209			s alc, acid
n37	2-Nitrobenzoic acid	$\text{O}_2\text{NC}_6\text{H}_4\text{COOH}$	167.12	9, 370	1.58		146–148			0.7 aq; 33 alc; 22 eth
n38	3-Nitrobenzoic acid	$\text{O}_2\text{NC}_6\text{H}_4\text{COOH}$	167.12	9, 376	1.494		142			0.3 aq; 33 alc; 40 acet
n39	4-Nitrobenzoic acid	$\text{O}_2\text{NC}_6\text{H}_4\text{COOH}$	167.12	9, 389	1.58		242.8			9 alc; 2 eth; 5 acet

n40	4-Nitrobenzonitrile	O ₂ NC ₆ H ₄ CN	148.12	9, 397			146–149			s HOAc; sl s aq, alc
n41	3-Nitrobenzoyl chloride	O ₂ NC ₆ H ₄ COCl	185.57	9, 381			32–35	275–278		d aq, alc; v s eth
n42	4-Nitrobenzoyl chloride	O ₂ NC ₆ H ₄ COCl	185.57	9, 394			75	205 ^{105mm}		d aq, alc; s eth
n43	<i>N</i> -(<i>p</i> -Nitrobenzoyl)-glycine	O ₂ NC ₆ H ₄ CONHCH ₂ COOH	224.17	9, 395			131–133			
n44	3-Nitrobenzyl alcohol	O ₂ NC ₆ H ₄ CH ₂ OH	153.14	6, 449			30–32	180 ^{3mm}		s aq, alc, eth
n45	4-Nitrobenzyl alcohol	O ₂ NC ₆ H ₄ CH ₂ OH	153.14	6, 450			92–94	185 ^{12mm}		v s alc, eth; sl s aq
n46	4-Nitrobenzyl bromide	O ₂ NC ₆ H ₄ CH ₂ Br	216.04	5, 334			98–100			2 alc; v s eth
n47	4-Nitrobenzyl chloride	O ₂ NC ₆ H ₄ CH ₂ Cl	171.58	5, 329			70–73			8 alc; s eth
n48	2-Nitrobiphenyl	O ₂ NC ₆ H ₄ C ₆ H ₅	199.21	5, 582	1.44 ₄ ²⁵	1.613 ²⁵	36.7	325	179	s alc, acet, CCl ₄
n49	4-Nitrobiphenyl	O ₂ NC ₆ H ₄ C ₆ H ₅	199.21	5, 583			112–114	340		sl s alc; v s eth
n50	1-Nitrobutane	CH ₃ CH ₂ CH ₂ CH ₂ NO ₂	103.18	1, 123	0.975 ₂₀ ²⁰	1.4112	–81.3	152.8		sl s aq; misc alc, eth
n51	3-Nitro-2-butanol	CH ₃ CH(NO ₂)CH(OH)CH ₃	119.12	1, 373	1.1296 ₄ ²⁵	1.4414 ²⁰		92 ^{10mm}	91	
n52	2-Nitrodiphenylamine	O ₂ NC ₆ H ₄ NHC ₆ H ₅	214.22	12, 690			76–78			i aq; s alc

Ninhydrin, i16
Nioxime, c323
2,2',2''-Nitrilotriethanol, t264

1,1',1''-Nitrilotris(2-propanol), t309
2-Nitro-*p*-anisidine, m79
5-Nitro-*o*-anisidine, m78

Nitroanisoles, m81, m82
4-Nitrobenzyl cyanide, n65
Nitrocresols, m323, m324



n36

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
n53	Nitroethane	$\text{CH}_3\text{CH}_2\text{NO}_2$	75.07	1, 99	1.0528 ₂₀ ²⁰	1.3920 ²⁰	−90	114.1	30	4.5 aq; misc alc, eth; s alk, chl
n54	1-Nitroguanidine	$\text{O}_2\text{NNHC}(=\text{NH})\text{NH}_2$	104.07	3, 126			d 225			0.4 aq; sl s MeOH
n55	5-Nitro-1 <i>H</i> -indazole		163.14	23, 129			207–209			s alc, bz, eth, acet
n56	Nitromethane	CH_3NO_2	61.04	1, 74	1.1322 ₄ ²⁵	1.3795 ²⁵	−28.4	101.2	35	11 aq; s alc, eth
n57	1-Nitronaphthalene	$\text{C}_{10}\text{H}_7\text{NO}_2$	173.17	5, 553	1.223		59–60	304		s alc; v s chl, eth
n58	3-Nitro-2-pentanol	$\text{CH}_3\text{CH}_2\text{CH}(\text{NO}_2)\text{CH}(\text{OH})\text{CH}_3$	133.15	1, 385	1.0818 ₄ ²⁵	1.4430 ²⁰		100 ^{10mm}	90	
n59	2-Nitrophenethyl alcohol	$\text{O}_2\text{NC}_6\text{H}_4\text{CH}_2\text{CH}_2\text{OH}$	167.16	6, 218	1.190	1.5637 ²⁰	2	267	> 112	
n60	2-Nitrophenol	$\text{O}_2\text{NC}_6\text{H}_4\text{OH}$	139.11	6, 213	1.495		44–45	214–216		s alc, bz, eth, alk
n61	4-Nitrophenol	$\text{O}_2\text{NC}_6\text{H}_4\text{OH}$	139.11	6, 226	1.495		112–114	279		s aq; v s alc, chl, eth
n62	4-Nitrophenyl acetate	$\text{O}_2\text{NC}_6\text{H}_4\text{OOCCH}_3$	181.15	6, 233			77–79			s aq; v s alc, bz, eth
n63	2-Nitrophenylacetic acid	$\text{O}_2\text{NC}_6\text{H}_4\text{CH}_2\text{COOH}$	181.15	9, 454			139–142			s hot aq, alc
n64	4-Nitrophenylacetic acid	$\text{O}_2\text{NC}_6\text{H}_4\text{CH}_2\text{COOH}$	181.15	9, 455			153			s alc, bz, eth
n65	4-Nitrophenylacetonitrile	$\text{O}_2\text{NC}_6\text{H}_4\text{CH}_2\text{CN}$	162.15	9, 456			117			s alc, eth
n66	4-Nitrophenyl chloroformate	$\text{O}_2\text{NC}_6\text{H}_4\text{OOCCL}$	201.57	6 ¹ , 120			77–79	162 ^{19mm}		
n67	2-Nitro- <i>p</i> -phenylenediamine	$\text{O}_2\text{NC}_6\text{H}_3(\text{NH}_2)_2$	153.14	13, 120			137–140			
n68	4-Nitro- <i>o</i> -phenylenediamine	$\text{O}_2\text{NC}_6\text{H}_3(\text{NH}_2)_2$	153.14	13, 29			199–201			s acid
n69	4-Nitrophenylhydrazine	$\text{O}_2\text{NC}_6\text{H}_4\text{NHNH}_2$	153.14	15, 468			156 d			s alc, chl, eth, hot bz

n70	2-Nitrophenyl phenyl ether	$O_2NC_6H_4OC_6H_5$	215.21	6 ² , 222	1.2539 ²²	1.575 ²⁰	< -20	184 ^{8mm}		s alc, eth
n71	4-Nitrophenyl phenyl ether	$O_2NC_6H_4OC_6H_5$	215.21	6, 232			53-56	320		s bz, eth
n72	3-Nitrophthalic anhydride		193.11	17, 486			163-165			sl s aq, bz
n73	1-Nitropropane	$CH_3CH_2CH_2NO_2$	89.09	1, 115	1.0009 ²⁰	1.4016 ²⁰	-104.0	131.2	33	1.4 aq; misc alc, eth
n74	2-Nitropropane	$(CH_3)_2CHNO_2$	89.09	1, 116	0.9876 ²⁰	1.3949 ²⁰	-91.3	120.3	37	1.7 aq; misc alc, eth
n75	2-Nitro-1-propanol	$CH_3CH(NO_2)CH_2OH$	105.09	1, 358	1.1841 ²⁵ ₄	1.4379 ²⁰		99 ^{10mm}	100	s aq, alc, eth
n76	4-Nitropyridine- <i>N</i> -oxide	$O_2NC_5H_4N(O)$	140.10				159-162			
n77	8-Nitroquinoline		174.16	20, 373			89-91			s alc, bz, eth; i aq
n78	Nitrosobenzene	C_6H_5NO	107.11	5, 230			67-69	59 ^{18mm}		i aq; s alc
n79	<i>N</i> -Nitrosodi- methylamine	$(CH_3)_2NNO$	74.08	8, 84	1.0048 ²⁰ ₄	1.4368 ²⁰		151-153	61	v s aq, alc, eth
n80	<i>p</i> -Nitrosodi- phenylamine	$C_6H_5NHC_6H_4NO$	198.22				144-145			v s alc, bz, chl, eth
n81	1-Nitroso-2-naphthol	$C_{10}H_6(NO)OH$	173.16	7, 712			109-110			3 alc; s bz, eth, alk

Nitroglycerin, g21

5-Nitroisophthalic acid, n34

3-Nitrophenyl disulfide, b194

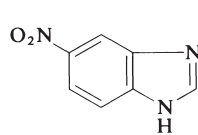
4-Nitrophenyl disulfide, b195

4-(*p*-Nitrophenylthio)aniline, a243

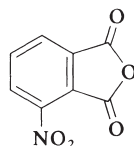
3-Nitro-*o*-phthalic acid, n32

4-Nitro-*o*-phthalic acid, n33

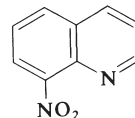
N-Nitrosophenylhydroxylamine, c284



n55



n72



n77

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
n82	1-Nitroso-2-naphthol-3,6-di-sulfonic acid, di-Na salt hydrate		377.26	11 ² , 190			>300			2.5 aq; sl s alc
n83	4-Nitrosophenol	ONC ₆ H ₄ OH	123.11	7, 622			d 126			s aq; v s alc, eth; explodes on contact with conc acid, alk, or fire
n84	β -Nitrostyrene	C ₆ H ₅ CH=CHNO ₂	149.15	5, 478			58	250		s alc; v s eth
n85	2-Nitrotoluene	CH ₃ C ₆ H ₄ NO ₂	137.14	5, 318	1.1622 ¹⁹ ₁₅	1.5472 ²⁰	−10	222	106	s alc, bz
n86	3-Nitrotoluene	CH ₃ C ₆ H ₄ NO ₂	137.14	5, 321	1.1581 ²⁰ ₄	1.5459 ²⁰	15.5	231.9	101	misc alc, eth; s bz
n87	4-Nitrotoluene	CH ₃ C ₆ H ₄ NO ₂	137.14	5, 323	1.392		53–54	238	106	s alc, bz, chl, eth
n88	2-Nitro- α,α,α -trifluorotoluene	CF ₃ C ₆ H ₄ NO ₂	191.11	5 ² , 251			31–32	105 ^{20mm}		v s alc, bz
n89	3-Nitro- α,α,α -trifluorotoluene	CF ₃ C ₆ H ₄ NO ₂	191.11	5, 327	1.436 ¹⁶ ₄	1.4715 ²⁰	−2.4	200–205	87	s alc, eth
n90	Nonadecane	CH ₃ (CH ₂) ₁₇ CH ₃	268.51	1, 174	0.7776 ³² ₄	1.4335 ³⁸	31.9	330.6	168	s eth; sl s alc
n91	1,8-Nonadiyne	HC≡C(CH ₂) ₅ C≡CH	120.20	1 ² , 248	0.8159 ²¹ ₄	1.4492 ²⁰	−21	55 ^{13mm}	41	
n92	Nonane	CH ₃ (CH ₂) ₇ CH ₃	128.26	1, 165	0.7176 ²⁰ ₄	1.4054 ²⁰	−53.5	150.8	31	s abs alc, eth
n93	1,9-Nonanediamine	H ₂ N(CH ₂) ₉ NH ₂	158.29	4, 272			37–38	258		
n94	Nonanedinitrile	NC(CH ₂) ₇ CN	150.23	2, 709	0.929	1.4460 ²⁰		176 ^{11mm}	>112	v s alc, bz, eth
n95	1,9-Nonanedioic acid	HOOC(CH ₂) ₇ COOH	188.22	2, 707	1.029 ²⁰ ₄		106.5	286 ^{100mm}		0.24 aq; v s alc; 3 eth
n96	1,9-Nonanediol	HO(CH ₂) ₉ OH	160.26	1, 493			45–47	177 ^{15mm}		
n97	Nonanenitrile	CH ₃ (CH ₂) ₇ CN	139.24	2, 354	0.821 ¹⁵ ₄	1.4260 ²⁰	−34.2	224.0	81	s alc, eth
n98	Nonanoic acid	CH ₃ (CH ₂) ₇ COOH	158.24	2, 352	0.906 ²⁰ ₄	1.4330 ²⁰	12.5	254	100	s alc, chl, eth
n99	1-Nonanol	CH ₃ (CH ₂) ₈ OH	144.26	1, 423	0.8274 ²⁰ ₄	1.4338 ²⁰	−5.5	213.1	75	0.6 aq; misc alc, eth
n100	5-Nonanone	(C ₄ H ₉) ₂ CO	142.24	1, 710	0.806 ²⁰ ₄	1.4190 ²⁰	−50	187	60	misc alc, eth

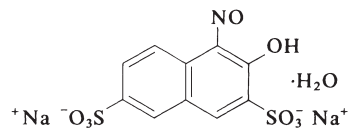
n101	Nonanoyl chloride	$\text{CH}_3(\text{CH}_2)_7\text{COCl}$	176.69	2, 353	0.946_{15}^{15}	1.4377^{20}	-60.5	215.4	81	d aq, alc: s eth
n102	1-Nonene	$\text{H}(\text{CH}_2)_7\text{CH}=\text{CH}_2$	126.24	1 ² , 202	0.7292^{20}	1.4157^{20}	-81.4	146.9	46	
n103	Nonyl aldehyde	$\text{CH}_3(\text{CH}_2)_7\text{CHO}$	142.24	1, 708	0.827_{19}^{19}	1.4240^{20}		185	63	
n104	Nonylamine	$\text{CH}_3(\text{CH}_2)_8\text{NH}_2$	143.27	4, 198	0.782	1.4330^{20}		201	62	sl s aq; s alc, eth
n105	Nopol		166.26		0.973	1.4930^{20}		230-240	98	
n106	Nopyl acetate		210.3		0.9805^{25}	1.4721^{20}				
n107	Norbornane		96.17	5 ² , 45			82-84			s alc
n108	2-Norbornanone		110.16	7, 57			88-91	168-172	33	
n109	<i>trans</i> -5-Norbornene-2,3-dicarbonyl dichloride		219.07		1.349	1.5165^{20}		$118^{11\text{mm}}$	110	

Nitroso-R-salt, n82

Nitroterephthalic acid, n31

2-Nitro-*p*-toluidine, m317

4-Nitro-*o*-toluidine, m315



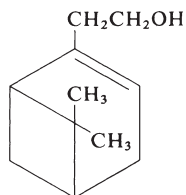
n82

5-Nitro-*o*-toluidine, m316

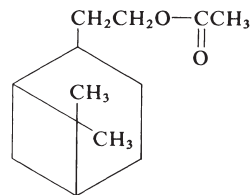
4-Nitroveratrole, d444

Nitroxyls, d556, d557, d558, d559

Nonyl alcohol, n99



n105



n106

2,5-Norbornadiene, b129

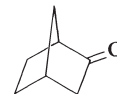
exo-2-Norbornanamine, a250

5-Norbornen-2-carbaldehyde, b131

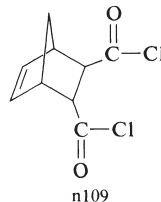
Norbornene, b130



n107



n108



n109

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
n110	5-Norbornen-2-yl acetate		152.19		1.044	1.4700 ²⁰		76 ¹⁴ mm	62	
n111	<i>exo</i> -2-Norbornyl formate		140.18		1.048	1.4622 ²⁰		67 ¹⁶ mm	53	
n112	(+)-Norephedrine HCl		187.67	13 ³ , 371			174–176			
o1	(<i>Z,Z</i>)-9,12-Octadecadienoic acid	CH ₃ (CH ₂) ₄ CH=CHCH ₂ -CH=CH(CH ₂) ₇ COOH	280.44	2, 496	0.9025 ₄ ²⁰	1.4699 ²⁰	−5	230 ¹⁶ mm		v s eth; misc PE; s abs alc
o2	Octadecanamide	CH ₃ (CH ₂) ₁₆ CONH ₂	283.50	2, 384			108–109	251 ¹² mm		s hot alc, hot eth
o3	Octadecane	CH ₃ (CH ₂) ₁₆ CH ₃	254.50	1, 173	0.7767 ₄ ²⁸	1.4367 ²⁸	28.2	316.7	165	s acet, eth; sl s alc
o4	1-Octadecanethiol	CH ₃ (CH ₂) ₁₇ SH	286.57			1.4648	29–31	360	185	s eth; sl s alc
o5	Octadecanoic acid	CH ₃ (CH ₂) ₁₆ COOH	284.48	2, 377	0.847 ⁷⁰	1.4299 ⁸⁰	70	383		4.9 alc; 20 bz; 50 chl; 3.9 acet
o6	1-Octadecanol	CH ₃ (CH ₂) ₁₇ OH	270.50	1, 431	0.8123 ₄ ⁵⁸	1.4388 ²⁰	57.9	203 ¹⁰ mm		s alc, eth
o7	9,12,15-Octadecatrienoic acid	CH ₃ (CH ₂ CH=CH) ₃ CH ₂ -(CH ₂) ₆ COOH	278.44	2, 499	0.791 ₄ ¹⁸	1.4800 ²⁰		230 ¹⁷ mm	>112	s alc, bz, eth
o8	1-Octadecene	CH ₃ (CH ₂) ₁₅ CH=CH ₂	252.49	1, 226	0.791 ₄ ¹⁸	1.4439 ²⁰	17.7	314.9	148	s hot acet
o9	9-Octadecen-1-amine	CH ₃ (CH ₂) ₇ CH=CH-(CH ₂) ₈ NH ₂	267.50		0.813	1.4578 ²⁰			154	
o10	(<i>Z</i>)-9-Octadecenoic acid	CH ₃ (CH ₂) ₇ CH=CH-(CH ₂) ₇ COOH	282.47	2, 463	0.8906 ₄ ²⁰	1.4571 ²⁰	4	286 ¹⁰⁰ mm		misc alc, eth; s bz, chl
o11	(<i>E</i>)-9-Octadecenoic acid	CH ₃ (CH ₂) ₇ CH=CH-(CH ₂) ₇ COOH	282.47	2 ² , 441	0.851 ⁷⁹	1.4308 ⁹⁹	44–45	288 ¹⁰⁰ mm		s bz, chl, eth
o12	(<i>Z</i>)-9-Octadecen-1-ol	CH ₃ (CH ₂) ₇ CH=CH-(CH ₂) ₈ OH	268.49	1, 453	0.849 ₄ ²⁰	1.4610 ²⁰	13–19	195 ⁸ mm	>112	s alc, eth
o13	Octadecylamine	CH ₃ (CH ₂) ₁₇ NH ₂	269.52	4, 196	0.777 ²⁷		50–52	232 ³² mm	148	s alc, bz, eth
o14	Octadecyl isocyanate	CH ₃ (CH ₂) ₁₇ NCO	295.51		0.847	1.4501 ²⁰		170 ² mm	185	

o15	Octadecyltri-chlorosilane	$\text{CH}_3(\text{CH}_2)_{17}\text{SiCl}_3$	387.94		0.984	1.4602 ²⁰		223 ^{10mm}	89	
o16	Octadecyl vinyl ether	$\text{CH}_3(\text{CH}_2)_{17}\text{OCH}=\text{CH}_2$	296.54		0.821 ³⁰ ₄	1.4440 ³⁰	28	187 ^{5mm}	177	
o17	1,7-Octadiene	$\text{H}_2\text{C}=\text{CH}(\text{CH}_2)_4\text{CH}=\text{CH}_2$	110.20		0.746	1.4221 ²⁰		114–121	9	
o18	1 <i>H</i> ,1 <i>H</i> ,5 <i>H</i> -Octa-fluoro-1-pentanol	$\text{HCF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}$	232.08		1.6647 ²⁰	1.3190 ²⁰		140–141	74	
o19	Octamethylcyclo-tetrasilazane	$[\text{—}(\text{CH}_3)_2\text{SiNH—}]_4$	292.7		0.95 ²²	1.458 ²⁵		224–225		
o20	Octamethylcyclo-tetrasiloxane	$[\text{—}(\text{CH}_3)_2\text{SiO—}]_4$	296.62		0.9558 ²⁰	1.3968 ²⁰	17.5	175	90	
o21	Octamethyltri-siloxane	$[(\text{CH}_3)_3\text{SiO}]_2\text{—Si}(\text{CH}_3)_2$	236.0		0.8200 ²⁰	1.3848 ²⁰	~–80	152–153	38	s bz, PE; sl s alc
o22	Octane	$\text{CH}_3(\text{CH}_2)_6\text{CH}_3$	114.23	1, 159	0.7025 ²⁰ ₄	1.3974 ²⁰	–56.8	125.7	15	s eth; sl s alc
o23	1,8-Octanediamine	$\text{H}_2\text{N}(\text{CH}_2)_8\text{NH}_2$	144.26	4, 271			50–52	225	165	
o24	1,8-Octanedioic acid	$\text{HOOC}(\text{CH}_2)_6\text{COOH}$	174.20	2, 691			140–144	230 ^{15mm}		0.16 aq; 0.6 eth; s alc
o25	1,2-Octanediol	$\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{OH})\text{—CH}_2\text{OH}$	146.23	1 ³ , 2217			36–38	132 ^{10mm}	>112	

Norbornylene, b130

Norcamphor, n107

Norleucine, a183

Norvaline, a253

NTA, n21

Octadecyl bromide, b319

Octadecyl mercaptan, o4

2,3,4,6,7,8,9,10-Octahydropyrimido

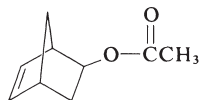
[1,2-*a*]azepine, d46

Octaldehyde, o40

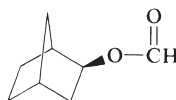
Octamethylene glycol, o26

Octanal, o40

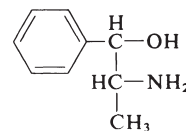
1,8-Octanedicarboxylic acid, d9



n110



n111



n112

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
o26	1,8-Octanediol	$\text{HO}(\text{CH}_2)_8\text{OH}$	146.23	1, 490			59–61	172 ^{20mm}		v s alc; sl s aq, eth
o27	Octanenitrile	$\text{CH}_3(\text{CH}_2)_6\text{CN}$	125.22	2, 349	0.8135 ²⁰	1.4202 ²⁰	–45.6	205.2	73	s eth; sl s alc
o28	1-Octanethiol	$\text{CH}_3(\text{CH}_2)_7\text{SH}$	146.30	1 ³ , 1710	0.843	1.4525 ²⁰	–49.2	199.0	68	s alc
o29	Octanoic acid	$\text{CH}_3(\text{CH}_2)_6\text{COOH}$	144.21	2, 347	0.9088 ²⁰	1.4279 ²⁰	16.6	239.3	110	0.07 aq; v s alc, chl, eth, PE
o30	1-Octanol	$\text{CH}_3(\text{CH}_2)_7\text{OH}$	130.23	1, 418	0.8258 ²⁰	1.4296 ²⁰	–15.0	195.2	81	0.06 aq; misc alc, chl, eth
o31	DL-2-Octanol	$\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{OH})\text{CH}_3$	130.23	1, 419	0.8207 ²⁰	1.4202 ²⁰	–38.6	179–180	71	0.08 aq; misc alc, eth
o32	DL-3-Octanol	$\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$	130.23	1 ¹ , 208	0.8216 ²⁰	1.4262 ²⁰		174–176	65	
o33	4-Octanol	$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_2\text{CH}_3$	130.23		0.8192 ²⁰	1.425 ²⁰		176.6	71	
o34	2-Octanone	$\text{CH}_3(\text{CH}_2)_5\text{COCH}_3$	128.22	1, 704	0.819 ²⁰	1.4150 ²⁰	–16	173	62	i aq; misc alc, eth
o35	3-Octanone	$\text{CH}_3(\text{CH}_2)_4\text{COCH}_2\text{CH}_3$	128.22	1, 706	0.8220 ²⁰	1.4150 ²⁰		167–168	46	i aq; misc alc, eth
o36	4-Octanone	$\text{CH}_3(\text{CH}_2)_3\text{COCH}_2\text{CH}_2\text{CH}_3$	128.22	1, 706	0.809	1.4139 ²⁰		164	45	
o37	Octanoyl chloride	$\text{CH}_3(\text{CH}_2)_6\text{COCl}$	162.66	2, 348	0.955 ¹⁵	1.4350 ²⁰	< –70	195	75	d aq, alc; s eth
o38	Octaphenylcyclotetrasiloxane	$[\text{—}(\text{C}_6\text{H}_5)_2\text{SiO—}]_4$	793.2		1.185			340 ^{1mm}		s alc, bz, HOAc
o39	1-Octene	$\text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}_2$	112.22	1, 221	0.7149 ²⁰	1.4087 ²⁰	–101.7	121.3	21	i aq; misc alc, eth
o40	Octyl aldehyde	$\text{CH}_3(\text{CH}_2)_6\text{CHO}$	128.22	1, 704	0.821 ²⁰	1.4183 ²⁰	12–15	163.4	51	sl s aq; misc alc
o41	Octylamine	$\text{CH}_3(\text{CH}_2)_7\text{NH}_2$	129.25	4, 196	0.782	1.4290 ²⁰	–5 to –1	175–177	62	i aq; s alc, eth
o42	4-Octylaniline	$\text{CH}_3(\text{CH}_2)_5\text{C}_6\text{H}_4\text{NH}_2$	205.35	12, 1185				175 ^{13mm}		
o43	Octyltrichlorosilane	$\text{CH}_3(\text{CH}_2)_7\text{SiCl}_3$	247.7		1.07 ²⁰	1.447 ²⁰		226 ^{730mm}		
o44	1-Octyne	$\text{CH}_3(\text{CH}_2)_5\text{C}\equiv\text{CH}$	110.19	1, 258	0.7457 ²⁰	1.4159 ²⁰	–79.3	126.2		i aq; s alc, eth
o45	1-Octyn-3-ol	$\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{OH})\text{C}\equiv\text{CH}$	126.20		0.864	1.4410 ²⁰			63	

o46	L-(+)-Ornithine	$\text{H}_2\text{N}(\text{CH}_2)_3\text{CH}(\text{NH}_2)\text{COOH}$	132.16	4,420			142			v s aq, alc; sl s eth
o47	Oxacycloheptane		100.16		0.890	1.440 ²⁰		122	10	
o48	Oxalic acid	HOOCCOOH	90.04	2,502	1.90 ₄ ¹⁷		189 d			9.5 aq; 24 alc; 1.3 eth
o49	Oxalic acid dihydrate	$\text{HOOC}\text{COOH}\cdot 2\text{H}_2\text{O}$	126.07	2,502	1.653 ₄ ¹⁹		-2H ₂ O, 102			14 aq; 40 alc; 1 eth
o50	Oxalyl bromide	BrCOCOBr	215.84			1.5220		103 ^{720mm}	none	
o51	Oxalyl chloride	ClCOCOCl	126.93	2,542	1.488 ₄ ¹³	1.4340 ¹³	-12	64	none	s eth; violent d aq, alc
o52	Oxalyl dihydrazide	$\text{H}_2\text{NNHCO}\text{CONHNH}_2$	118.10	2,559			240 d			s hot aq; sl s alc, eth
o53	Oxamic hydrazide	$\text{H}_2\text{NCO}\text{CONHNH}_2$	103.08	2,559			218 d			s alk; sl s aq; i eth
o54	Oxamide	$\text{H}_2\text{NCO}\text{CONH}_2$	88.07	2,545	1.667 ₄ ²⁰		d 350			sl s hot aq, alc
o55	2-Oxazolidone		87.08	27,135			86-89	220 ^{48mm}		
o56	2-Oxobutyric acid	$\text{CH}_3\text{CH}_2\text{C}(=\text{O})\text{COOH}$	102.09	3,629	1.200 ₄ ¹⁷	1.3972 ²⁰	32-34	82 ^{16mm}		v s aq, alc; v sl s eth

tert-Octylamine, t102

Octyl bromide, b320

Octyl cyanide, n97

Octyl chloride, c190

Octyl iodide, i46

Oleic acid, o11

Oleyl alcohol, o12

Oleylamine, o9

Orthanolic acid, a118

7-Oxabicyclo[2.2.1]heptane, e6

7-Oxabicyclo[4.1.0]heptane, e5

6-Oxabicyclo[3.1.0]hexane, e9

2-Oxabicyclo[6.1.0]nonane, e7a

Oxacyclobutane, t345

Oxacyclopentane, t66

Oxalylurea, i6

1,4-Oxathiane, t164

Oxepane, o47

Oxetane, t345

Oxirane, e129

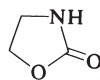
2-Oxo-10-bornanesulfonic acid, c7

3-Oxobutanoic acid, a24

3-Oxobutyraldehyde dimethyl acetal, d435



o47



o55

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

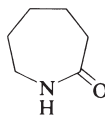
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
o57	2-Oxohexamethyl-eneimine		113.16	21 ² , 216	1.02 ₄ ⁷⁵	1.4935	69.2	180 ⁵⁰ mm		84 aq
o58	4-Oxopentanoic acid	CH ₃ COCH ₂ CH ₂ COOH	116.12	3, 671	1.1447 ₄ ²⁵	1.4396 ²⁰	33–35	245.8	137	v s aq, alc, bz, eth
o59	2-Oxopropionaldehyde	CH ₃ COCHO	72.06	1, 762	1.0455 ²⁴	1.4209 ²⁰		72	none	s aq, alc
o60	2-Oxopropionic acid	CH ₃ COCOOH	88.06	3, 608	1.267 ₄ ¹⁵	1.4315 ²⁰	11.8	165 d	82	misc aq, alc, eth
o61	2,2'-Oxydiacetic acid	HOOCCH ₂ OCH ₂ COOH	134.09	3, 234			142–145	d		v s aq, alc; sl s eth
o62	4,4'-Oxydianiline	H ₂ NC ₆ H ₄ OC ₆ H ₄ NH ₂	200.24	13, 441			190 d			
o63	3,3'-Oxydipropionitrile	NCCH ₂ CH ₂ OCH ₂ CH ₂ CN	124.14		1.043	1.4405 ²⁰		112 ^{0.5} mm	> 112	
p1	Paraformaldehyde	(CH ₂ O) _x		1, 566			156 d		71	slowly s aq; s alk; i alc, eth
p2	Paraldehyde	[—CH(CH ₃)O—] ₃	132.16	19, 385	0.9984 ¹⁵	1.4049 ²⁰	12.5	124		11 aq; misc alc, chl
p3	Parathion	(C ₂ H ₅ O) ₂ P(=S)(O)-C ₆ H ₄ NO ₂	291.27		1.26 ₄ ²⁵	1.5370 ²⁵	6	375		v s alc, bz, eth
p4	DL-Patchenol		166.26	6 ² , 64	0.987	1.5045 ²⁰		234–238	107	
p5	Pentabromoethylbenzene	CH ₃ CH ₂ C ₆ Br ₅	500.67	5, 357			137–139			
p6	Pentabromophenol	C ₆ Br ₅ OH	488.62	6, 206			223–226	subl		sl s alc, eth
p7	Pentachloroacetone	Cl ₂ CHCOCCl ₃	230.31	1, 656	1.690	1.4967 ²⁰	21 anhyd	192	none	i aq; v s acet
p8	Pentachlorobenzene	C ₆ HCl ₅	250.34	5, 205	1.8342 ¹⁶		82–85	275–277		v s bz, chl, eth
p9	Pentachloroethane	Cl ₂ CHCCl ₃	202.30	1, 87	1.6712 ₄ ²⁵	1.5030 ²⁰	–29.0	160.5	none	0.05 aq; misc alc, eth
p10	Pentachloronitrobenzene	C ₆ Cl ₅ NO ₂	295.34	5, 247	1.718 ₄ ²⁵		140–143			s bz, chl
p11	Pentachlorophenol	C ₆ Cl ₅ OH	266.34	6, 194	1.978 ₄ ²²		190–191	310 d		v s alc; s bz; 148 eth
p12	Pentachloropyridine	C ₅ Cl ₅ N	251.33	20, 232			124–126			

p13	Pentadecane	$\text{CH}_3(\text{CH}_2)_{13}\text{CH}_3$	212.42	1, 172	0.7684^{20}_4	1.4319^{20}	9.9	270.6	132	v s alc, eth
p14	8-Pentadecanone	$[\text{CH}_3(\text{CH}_2)_6]_2\text{CO}$	226.40	1, 717			41–43	178		s alc
p15	3-Pentadecylphenol	$\text{C}_{15}\text{H}_{31}\text{C}_6\text{H}_4\text{OH}$	304.52				45–48	$195^{1\text{mm}}$		
p16	1,2-Pentadiene	$\text{CH}_3\text{CH}_2\text{CH}=\text{C}=\text{CH}_2$	68.12	1, 251	0.6926^{20}_4	1.4209^{20}	–137.3	44.9		
p17	(<i>E</i>)-1,3-Pentadiene	$\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$	68.12	1, 251	0.6760^{20}	1.4301^{20}	–87.5	42.0	–28	
p18	(<i>Z</i>)-1,3-Pentadiene	$\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$	68.12	1, 251	0.6910^{20}	1.4363^{20}	–140.8	44.1	–28	
p19	1,4-Pentadiene	$\text{H}_2\text{C}=\text{CHCH}_2\text{CH}=\text{CH}_2$	68.12	1, 251	0.6608^{22}_4	1.3888^{20}	–148.3	26.0	4	
p20	Pentaerythritol	$\text{C}(\text{CH}_2\text{OH})_4$	136.15	1, 528	1.38^{25}_4	1.548	260	subl		6 aq; v sl s alc; i eth
p21	Pentaerythrityl tetrabromide	$\text{C}(\text{CH}_2\text{Br})_4$	387.76	1, 142			158–160	305–306		
p22	Pentaerythrityl tetranitrate	$\text{C}(\text{CH}_2\text{ONO}_2)_4$	316.15	1 ² , 602	1.773^{20}_4		140		sensi- tive to shock; ex- plodes on percu- ssion	acet; sl s eth, alc

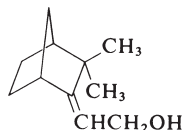
3-Oxo-*N*-phenylbutanamide, a32
 2,2'-Oxybis(chloroethane), b158
 1,1'-Oxybis(2-methylpropane), d407
 1,1'-Oxybis(pentane), d651
 3,3'-Oxybis(1-propene), d26
 2,2'-Oxydiethanethiol, b186

2,2'-Oxydiethanol, b181
 Palmitic acid, h35
 Pamoic acid, m235
 Parabanic acid, i6
 Pelargonaldehyde, n103
 Pelargonic acid, n98

Pelargonoyl chloride, n101
 Pelargononitrile, n97
 Pentabromophenyl ether, b197
 Pentaerythritol diformal, t126



o57



p4

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p23	Pentafluorobenzonitrile	C_6F_5CN	193.07		1.532	1.4425 ²⁰		185–190	29	
p24	Pentamethylbenzene	$C_6H(CH_3)_5$	148.25	5, 443	0.917 ₄ ²⁰	1.527 ²⁰	54.4	231		v s alc, bz
p25	1,2,3,4,5-Pentamethylcyclopentadiene		136.24		0.870	1.4733 ²⁰		58 ^{13mm}	44	
p26	1,5-Pentamethylene-tetrazole		138.17	26 ² , 213			59–61	194 ^{12mm}		
p27	Pentanal	$CH_3CH_2CH_2CH_2CHO$	86.13	1, 676	0.8095 ₄ ²⁰	1.3942 ²⁰	−92	102–103	12	1.4 aq; misc alc, eth
p28	Pentane	$CH_3CH_2CH_2CH_2CH_3$	72.15	1, 130	0.6262 ₄ ²⁰	1.3575 ²⁰	−129.7	36.1	−49	misc alc, eth
p29	1,5-Pentanediamine	$H_2N(CH_2)_5NH_2$	102.18	4, 266	0.873 ₄ ²⁵	1.4591 ²⁰	−129.7	178–180	62	s aq, alc; sl s eth
p30	1,5-Pentanediol	$HO(CH_2)_5OH$	104.15	1, 481	0.9941 ²⁰	1.4494 ²⁰	−15.6	242.5	125	s aq, alc; sl s eth
p31	2,3-Pentanedione	$CH_3CH_2COCOCH_3$	100.11	1, 776	0.957	1.4068 ²⁰	−52	110–112	19	
p32	2,4-Pentanedione	$CH_3COCH_2COCH_3$	100.11	1, 777	0.9721 ²⁵	1.4510 ²⁰	−23.1	140.6	40	17 aq; misc alc, eth
p33	Pentanenitrile	$CH_3CH_2CH_2CH_2CN$	83.13	2, 301	0.8035 ₄ ¹⁵	1.3991 ¹⁵	−96.8	141.3	40	i aq; s alc, eth
p34	1-Pentanesulfonic acid, Na salt	$CH_3(CH_2)_4SO_3^-Na^+$	174.19	4 ³ , 23			>300			4 aq
p35	1-Pentaneithiol	$CH_3(CH_2)_4SH$	104.22	1, 384	0.840	1.4460 ²⁰	−75.7	126.6	18	i aq; misc alc, eth
p36	Pentanoic acid	$CH_3(CH_2)_3COOH$	102.13	2, 299	0.9390 ₄ ²⁰	1.4080 ²⁰	−33.7	185.5	88	2.4 aq; v s alc, eth
p37	1-Pentanol	$CH_3(CH_2)_4OH$	88.15	1, 383	0.8148 ₄ ²⁰	1.4100 ²⁰	−78.9	137.8	32	2.7 aq; misc alc, eth
p38	2-Pentanol	$CH_3CH_2CH_2CH(OH)CH_3$	88.15	1, 384	0.8393 ₄ ²⁰	1.4064 ²⁰	glass	119.0	40	16.6 aq; misc alc, eth
p39	3-Pentanol	$CH_3CH_2CH(OH)CH_2CH_3$	88.15	1,385	0.8150 ₄ ²⁵	1.4079 ²⁵	−69	115.6	40	5.2 aq; s alc, eth
p40	γ-Pentanolactone		100.12	17, 235	1.057	1.4330	−31	207–208	81	
p40a	δ-Pentanolactone		100.12	17, 235	1.079	1.4575 ²⁰		60 ^{0.5mm}	100	

p41	2-Pentanone	$\text{CH}_3\text{CH}_2\text{CH}_2\text{COCH}_3$	86.13	1, 676	0.8095 ²⁰	1.3903	−77.8	101.7	7	misc acet, bz, eth, PE
p42	3-Pentanone	$\text{CH}_3\text{CH}_2\text{COCH}_2\text{CH}_3$	86.13	1, 679	0.8143 ²⁰	1.3923 ²⁰	−39.0	102.0	12	3.4 aq
p43	Pentanophenone	$\text{C}_6\text{H}_5\text{CO}(\text{CH}_2)_3\text{CH}_3$	162.23	7, 327	0.988	1.5143 ²⁰		107 ^{5mm}	102	s alc, eth
p44	Pentanoyl chloride	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{COCl}$	120.58	2, 301	1.016	1.4216 ²⁰		125–127	23	
p45	1,4,7,10,13-Pentaoxacyclopentadecane	$[\text{—CH}_2\text{CH}_2\text{O—}]_5$	220.27			1.4615 ²⁰		135 ^{0.2mm}		
p46	3,6,9,12,15-Pentaoxahexadecanol	$\text{CH}_3\text{O}(\text{CH}_2\text{CH}_2\text{O})_4\text{CH}_2\text{—CH}_2\text{OH}$	252.31		0.933	1.4500 ²⁰		133 ^{0.005mm}	>112	
p47	1-Pentene	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$	70.14	1, 210	0.6410 ²⁰ ₄	1.3714 ²⁰	−165.2	30.0		misc alc, bz, eth
p48	(E)-2-Pentene	$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$	70.14	1,210	0.6482 ²⁰ ₄	1.3793 ²⁰	−140.2	36.3	−45	misc alc, eth
p49	(Z)-2-Pentene	$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$	70.14	1, 210	0.6503 ²⁰ ₄	1.3830 ²⁰	−151.4	36.9		misc alc, eth
p50	4-Pentenoic acid	$\text{H}_2\text{C}=\text{CHCH}_2\text{CH}_2\text{COOH}$	100.11	2, 425	0.9843 ¹⁸ ₄	1.4341 ¹⁸	<−18	187–189		sl s aq; s alc, eth
p51	3-Penten-2-one	$\text{CH}_3\text{CH}=\text{CHCOCH}_3$	84.12	1, 732	0.8624 ²⁰ ₄	1.4405 ²⁰		121–124	21	s aq
p52	Pentyl acetate	$\text{CH}_3(\text{CH}_2)_4\text{OOCCH}_3$	130.19	2, 131	0.8753 ²⁰	1.4028 ²⁰	<−100	149.2	23	0.17 aq
p53	Pentylamine	$\text{CH}_3(\text{CH}_2)_4\text{NH}_2$	87.17	4, 175	0.752	1.4110 ²⁰	−55	104	4	v s aq; misc alc, eth
p54	Pentylbenzene	$\text{CH}_3(\text{CH}_2)_4\text{C}_6\text{H}_5$	148.25	5, 434	0.8594 ²⁰ ₄	1.4885 ²⁰	−78.3	202.2	65	s alc; misc bz, eth

Pentalin, p9
pentamethylene glycol, p30
Pentamethylene oxide, t76
Pentamethylethyl alcohol, t338

1,5-Pentanedicarboxylic acid, h8
Pentanedinitrile, g14
Pentanedioic acid, g11
2,5,8,11,14-Pentaoxapentadecane, b190

Penetetic acid, d299
sec-Pentylamine, a251
tert-Pentylamine, d601

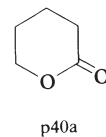
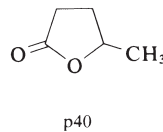
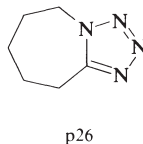
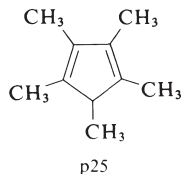


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p55	4- <i>tert</i> -Pentylcyclohexanone		168.28	7 ³ , 173	0.920	1.4677 ²⁰		125 ^{16mm}	104	
p56	4- <i>tert</i> -Pentylphenol	CH ₃ CH ₂ C(CH ₃) ₂ -C ₆ H ₄ OH	164.25	6, 548	0.962 ₄ ²⁰		93	262.2		s alc, eth
p57	1-Pentyne	CH ₃ CH ₂ CH ₂ C≡CH	68.11	1, 250	0.6901 ₄ ²⁰	1.3852 ²⁰	-105.7	40.2		v s alc; misc eth
p58	L-Perillaldehyde		150.22	7, 158	0.9645 ₄ ²⁰	1.5072 ²⁰		105 ^{10mm}	95	
p59	Peroxyacetic acid	CH ₃ C(=O)OOH	76.05		1.226 ₄ ¹⁵		0.1	105 explodes 110		v s aq, alc, eth
p60	Petroleum ether	principally pentanes and hexanes			0.640			35-80	-40	misc bz, chl, eth, CCl ₄
p61	Phenanthrene		178.23	5, 667	1.179 ²⁵		100	340		1.6 alc; 50 bz; 30 eth
p62	9,10-Phenanthrene-dione		208.22	7, 796	1.405 ⁴		209-211			s bz, eth, hot alc
p63	1,10-Phenanthroline		180.21	23, 227			117			1.4 bz; s alc, acet
p64	Phenol	C ₆ H ₅ OH	94.11	6, 110	1.0576 ₄ ⁴¹	1.5418 ⁴¹	40.9	181.8	79	6.7 aq; 8.2 bz; v s alc, chl, eth, alk
p65	Phenolphthalein		318.33	18, 143	1.299 ₄ ²⁵		258-262			8.2 alc; 1 eth
p66	Phenothiazine		199.28	27, 63			185.1	371		v s bz; s eth; sl s alc
p67	Phenothiazine-10-carbonyl chloride		261.73	27, 66			168-171			
p68	Phenoxyacetic acid	C ₆ H ₅ OCH ₂ COOH	152.15	6, 161			98	285 sl d		1.3 aq; v s alc, bz, HOAc, CS ₂ , eth
p69	Phenoxyacetyl chloride	C ₆ H ₅ OCH ₂ COCl	170.60	6, 162	1.235	1.5340 ²⁰		225-256		d aq, alc; s eth
p70	<i>p</i> -Phenoxyaniline	C ₆ H ₅ OC ₆ H ₄ NH ₂	185.23	13, 438			82-84	189 ^{14mm}		s hot aq; v s alc, eth

p71	2-Phenoxybutyric acid	$\text{CH}_3\text{CH}_2\text{CH}(\text{OC}_6\text{H}_5)\text{-COOH}$	180.20	6, 163			79–83	258		sl s aq
p72	2-Phenoxyethanol	$\text{C}_6\text{H}_5\text{OCH}_2\text{CH}_2\text{OH}$	138.17	6, 146	1.102 ²² ₄	1.5370 ²⁰	14	245.2	110	s aq; v s alc, eth
p73	1-Phenoxy-2-propanol	$\text{C}_6\text{H}_5\text{OCH}_2\text{CH}(\text{OH})\text{CH}_3$	152.19	6 ¹ , 85	1.063 ²⁵ ₄	1.523 ²⁰	13–18	240	135	
p74	Phenoxy-2-propanone	$\text{C}_6\text{H}_5\text{OCH}_2\text{COCH}_3$	150.18	6, 151	1.097	1.5210 ²⁰		230	85	
p75	DL-2-Phenoxy-propionic	$\text{CH}_3\text{CH}(\text{OC}_6\text{H}_5)\text{COOH}$	166.18	6, 163			116–119	265		s alc; sl s aq

Peracetic acid, p59

Perdeuterocyclohexane, c313

Perylene, d49

Phenacetin, e45

Phenacyl bromide, b221

Phenacyl chloride, c28

9,10-Phenanthraquinone, p62

Phenazone, a309

1,2,4-Phenyl triacetate, t193

Phenethyl alcohol, p113

sec-Phenethyl alcohol, m138

Phenethylamine, p114

Phenethyl bromide, b283

Phenethyl chloride, c108

p-Phenetidine, e24

Phenetole, e28

Phenoxyacetone, p74

4-Phenoxybutyl bromide, b243

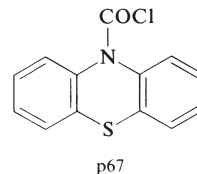
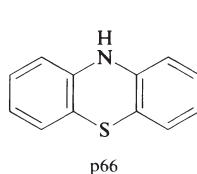
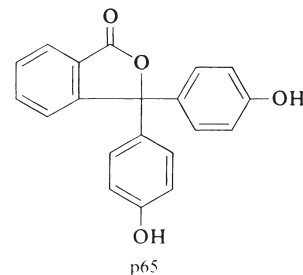
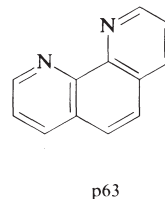
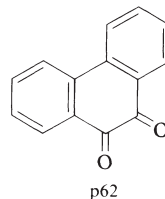
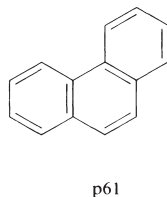
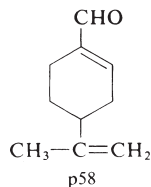
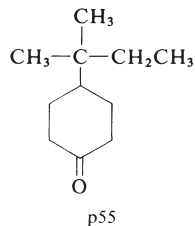


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p76	3-Phenoxytoluene	$C_6H_5OC_6H_4CH_3$	184.24	6, 377	1.051	1.5727 ²⁰		271–273	>112	
p76a	Phenylacetaldehyde	$C_6H_5CH_2CHO$	120.15	7, 292	1.027 ²⁵ ₂₅	1.5273 ²⁰	33–34	195	86	sl s aq; s alc, eth
p77	2-(2-Phenyl- acetamido)- acetaldoxime	$C_6H_5CH_2CONHCH_2-$ $CH=NOH$	192.22				147–151			
p78	Phenyl acetate	$C_6H_5OOCCH_3$	136.15	6, 152	1.073 ²⁰ ₄	1.5030 ²⁰		196	76	misc alc, eth, chl
p79	Phenylacetic acid	$C_6H_5CH_2COOH$	136.15	9, 431	1.091 ⁷⁷ ₄		76.5	265.5		s hot aq, alc, eth
p80	Phenylacetonitrile	$C_6H_5CH_2CN$	117.15	9, 441	1.0214 ¹⁵ ₁₅	1.5233 ²⁰	–23.8	233.5	101	i aq; misc alc, eth
p81	Phenylacetyl chloride	$C_6H_5CH_2COCl$	154.60	9, 436	1.169	1.5325 ²⁰		95 ^{12mm}		d aq, alc
p82	Phenylacetylene	$C_6H_5C\equiv CH$	102.14	5, 511	0.9300 ²⁰ ₄	1.5470 ²⁰	–44.9	142.4	31	misc alc, eth
p83	Phenylacetylurea	$C_6H_5CH_2CONHCONH_2$	178.19				212–216			sl s alc, bz, chl, eth
p84	L-3-Phenyl- α - alanine	$C_6H_5CH_2CH(NH_2)COOH$	165.19	14, 495			d 283			3 aq; s hot alc; i eth
p85	2-(Phenylamino)- benzoic acid	$C_6H_5NHC_6H_4COOH$	213.24	14, 327			185 d			s hot alc
p86	Phenyl 4-amino- salicylate	$H_2NC_6H_3(OH)COOC_6H_5$	229.24				153			0.7 mg aq
p87	<i>p</i> -Phenylazoaniline	$C_6H_5N=NC_6H_4NH_2$	197.24	16 ¹ , 310			128	>360		v s alc, bz, chl, eth
p88	Phenylazoformic acid 2-phenylhydrazide	$C_6H_5N=NC(=O)NHNHC_6H_5$	240.27	16, 24			156– 159 d			
p89	<i>p</i> -Phenylazophenol	$C_6H_5N=NC_6H_4OH$	198.23	16, 96			155–157	230 ^{20mm}		v s alc, eth
p90	2-Phenylbenzimi- dazole		194.24	23, 230			291			s abs alc; sl s bz, chl
p91	Phenyl benzoate	$C_6H_5COOC_6H_5$	198.22	9, 116	1.235		70	314		v s hot alc; sl s eth
p92	<i>N</i> -Phenylbenzylamine	$C_6H_5CH_2NHC_6H_5$	183.25	12, 1023	1.061		27–38	306–307		s alc, chl, eth
p93	1-Phenylbiguanide	$C_6H_5NHC(=NH)NH-$ $C(=NH)NH_2$	177.21				144–146			v s aq, alc

p94	1-Phenyl-2-butanone	$\text{CH}_3\text{CH}_2\text{COCH}_2\text{C}_6\text{H}_5$	148.21	7, 314	0.998	1.5122 ²⁰		112 ^{15mm}	90	s alc; misc eth; i aq
p95	4-Phenyl-2-butanone	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{COCH}_3$	148.21	7, 314	0.989	1.5122 ²⁰		235	98	s alc, eth
p96	(<i>E</i>)-4-Phenyl-3-buten-2-one	$\text{C}_6\text{H}_5\text{CH}=\text{CHCOCH}_3$	146.19	7, 364	1.0097 ⁴⁵	1.5836 ⁴⁵	41.5	261	65	v s alc, bz, chl, eth
p97	4-Phenylbutylamine	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{CH}_2\text{-CH}_2\text{NH}_2$	149.24	12, 1165	0.944	1.5196 ²⁰		124 ^{17mm}	101	
p98	2-Phenyl-3-butyne-2-ol	$\text{CH}_3\text{C}(\text{OH})(\text{C}_6\text{H}_5)\text{C}\equiv\text{CH}$	146.19	6 ² , 559			51–52	217–218		0.8 aq; s alc, bz, acet
p99	2-Phenylbutyric acid	$\text{CH}_3\text{CH}_2\text{CH}(\text{C}_6\text{H}_5)\text{COOH}$	164.20	9 ² , 356			42–44	270–272		s bz, eth
p100	4-Phenylbutyric acid	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH}$	164.20	9, 539			50–52	165 ^{10mm}		s alc, eth
p101	DL-2-Phenylbutyronitrile	$\text{CH}_3\text{CH}_2\text{CH}(\text{C}_6\text{H}_5)\text{CN}$	145.21	9, 541	0.974	1.5086 ²⁰		114– 115 ^{15mm} 71 ^{9mm}	>112	
p102	Phenyl chloroformate	$\text{C}_6\text{H}_5\text{OOCCL}$	156.57							
p103	<i>S</i> -Phenyl chlorothioformate	$\text{C}_6\text{H}_5\text{SCOCL}$	172.6		1.269 ³⁰	1.5786 ³⁰	–14	101 ^{10mm}	116	

Phenylacetaldehyde dimethyl acetal, d450

N-Phenylacetamide, a18

Phenylacetone, p144

2-Phenylacetoacetone nitrile, a51

α -Phenylacetophenone, d22

β -Phenylacrylic acid, c267

γ -Phenylallyl alcohol, c270

o-Phenylanisole, m56

N-Phenylantranilic acid, p85

Phenylarsonic acid, b11

Phenylazoformic acid 2-phenylhydrazide, d660

N-Phenylbenzamide, b5

Phenylbenzene, b134

Phenylbenzoic acid, b135

p-Phenylbenzyl alcohol, b138

Phenylboric acid, b12

1-Phenylbutane, b423

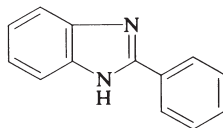
2-Phenylbutane, b424

1-Phenyl-1,3-butanedione, b64

4-Phenyl-*sec*-butyl acetate, m361

Phenyl Cellosolve, p72

Phenyl chloride, c41



p90

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p104	Phenylcyclohexane	$C_6H_5C_6H_{11}$	160.26	5, 503	0.9427 ²⁰	1.5263 ²⁰	7.0	240.1	98	v s alc, eth
p105	Phenyl dichloro-phosphate	$C_6H_5OP(O)Cl_2$	210.98	6, 179	1.412	1.5230 ²⁰		241–243	>112	
p106	<i>N</i> -Phenyldiethanol-amine	$C_6H_5N(CH_2CH_2OH)_2$	181.24	12, 183	1.120 ⁶⁰ ₂₀		56–58	350 sl d		5 aq; v s alc; 29 eth; 25 bz
p107	<i>o</i> -Phenylenediamine	$C_6H_4(NH_2)_2$	108.14	13, 6			103–104	256–258		v s alc, chl, eth
p108	<i>m</i> -Phenylethanol	$C_6H_4(NH_2)_2$	108.14	13 ¹ , 10	1.139 ¹⁵ ₁₅		62–63	234–237		s aq, alc, acet, chl
p109	<i>p</i> -Phenylenediamine	$H_2NC_6H_4NH_2$	108.14	13, 61			145–147	267	68	1 aq; s alc, chl, eth
p110	<i>o</i> -Phenylene phosphorochloridite		174.52	27, 809	1.466	1.5712 ²⁰		80 ^{20mm}	>112	
p111	1-Phenyl-1,2-ethanediol	$C_6H_5CH(OH)CH_2OH$	138.17	6, 907			66–68	272–274		v s aq, alc, bz, eth, chl, HOAc
p112	1-Phenylethanol	$CH_3CH(C_6H_5)OH$	122.17	6, 475	1.0150 ²⁰ ₂₀	1.5211 ²⁰	21.4	203.9		2.3 aq
p113	2-Phenylethanol	$C_6H_5CH_2CH_2OH$	122.17	6, 478	1.018 ²⁵ ₂₅	1.5317 ²⁰	–27	221	102	2 aq; misc alc, eth
p114	2-Phenylethylamine	$C_6H_5CH_2CH_2NH_2$	212.28	12, 1096	0.9640 ²⁵ ₄	1.5332 ²⁰		195	90	s aq; v s alc, eth
p115	D-(–)- α -Phenyl-glycine	$C_6H_5CH(NH_2)COOH$	151.17	14, 460			305–310			
p116	1-Phenylheptane	$C_6H_5(CH_2)_6CH_3$	176.30	5, 451	0.860	1.4842 ²⁰		233	95	
p117	1-Phenylhexane	$C_6H_5(CH_2)_5CH_3$	162.28	5 ² , 337	0.861	1.4865 ²⁰	–61	226	83	misc eth
p118	Phenylhydrazine	$C_6H_5NHNH_2$	108.14	15 ² , 44	1.0978 ²⁰ ₄	1.6070 ²⁰	19.5	243.5 d	88	misc alc, bz, chl, eth
p119	Phenyl 3-hydroxy-2-naphthoate	$C_{10}H_6(OH)COOC_6H_5$	264.28	10, 335			129–132	261 ^{160mm}		
p119a	2-Phenyl-2-imidazoline		146.19	23, 154			94–99			
p120	2-Phenylindole		193.25	20, 467			17	250 ^{10mm}		
p121	Phenyl isocyanate	C_6H_5NCO	119.12	12, 437	1.0956 ²⁰ ₄	1.5350 ²⁰	–30	162–163	55	d aq, alc; s eth
p122	Phenyl isothiocyanate	C_6H_5NCS	135.19	12, 453	1.1288 ²⁵ ₄	1.6497 ²⁰	–21	221	87	i aq; s alc, eth

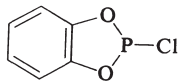
p123	<i>N</i> -Phenylmaleimide		173.17	21, 400			89–90	163 ^{12mm}		s alc, chl, eth
p124	Phenylmalonic acid	$C_6H_5CH(COOH)_2$	180.16				155 d			
p125	Phenylmercury(II) acetate	$C_6H_5HgOOCCH_3$	336.74				149			0.17 aq; s alc, bz, acet
p126	Phenylmercury(II) chloride	C_6H_5HgCl	313.15				250–252			s bz, eth, pyr
p127	Phenylmercury(II) hydroxide	C_6H_5HgOH	294.70	16, 952			190 d			
p128	Phenylmethanethiol	$C_6H_5CH_2SH$	124.21	6, 453	1.058 ²⁰			194–195	70	
p129	<i>N</i> -Phenylmorpholine		163.22	27, 6			57	268		1.0 aq; v s hot alc
p130	<i>N</i> -Phenyl-1-naphthylamine	$C_{10}H_7NHC_6H_5$	219.29	12, 1224			60–62	226 ^{15mm}		s alc, bz, chl, eth
p130a	1-Phenyloctane	$C_6H_5(CH_2)_7CH_3$	190.33	5, 453	0.8572 ²⁰ ₄	1.4840 ²⁰	–36	261–263	107	misc eth
p131	2-Phenylphenol	$C_6H_5C_6H_4OH$	170.21	6 ² , 623	1.213		57	282	123	s alc, chl, eth, alk
p132	4-Phenylphenol	$C_6H_5C_6H_4OH$	170.21	6, 674			164–165	305	165	s alc, chl, eth, alk

2-Phenylcinchoninic acid, p149
 α -Phenyl-*o*-cresol, h113
Phenylethane, e68
Phenylethanenitrile, p80
1-Phenylethanol, m138
Phenylethanolamine, a262

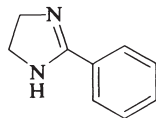
N-Phenylethanolamine, a300
Phenylethene, s11
N-Phenylformamide, f31
Phenylglyoxylic acid, b70
Phenylglyoxylonitrile, b68

1-Phenyl-1-hydroxy-2-methylaminopropanes, e1, e2
2,2'-(Phenylimino)diethanol, p106

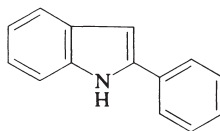
p-(2-Phenylisopropyl)phenol, m359
Phenyl- α -methylstyryl ketone, d658
1-Phenylpentane, p54



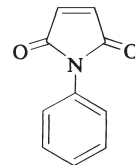
p110



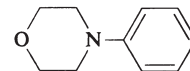
p119a



p120



p123



p129

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p133	<i>N</i> -phenyl- <i>p</i> -phenylenediamine	$C_6H_5NHC_6H_4NH_2$	184.24	13, 76			73–75			
p134	Phenyl <i>N</i> -phenylphosphoramido-chloridate	$C_6H_5NHP(=O)(Cl)OC_6H_5$	267.66	12, 588			132–134			
p135	Phenylphosphinic acid	$C_6H_5PH(O)OH$	142.09	16, 791			83–85			
p136	Phenylphosphonic acid	$C_6H_5P(O)(OH)_2$	158.09	16, 803			163–166			
p137	Phenylphosphonic dichloride	$C_6H_5P(O)Cl_2$	194.99	16, 804	1.375	1.5600 ²⁰	3	258	>112	
p138	Phenylphosphono-thioic dichloride	$C_6H_5P(S)Cl_2$	211.05	16, 807	1.360	1.6244 ²⁰		205 ^{130mm}		
p139	<i>N</i> -Phenylpiperazine		162.24		1.0621 ²⁰ ₄	1.5875 ²⁰		286	>112	i aq; misc alc
p140	2-Phenyl-1,2-propanediol	$CH_3C(C_6H_5)(OH)CH_2OH$	152.19	6, 930			44–45	160–162 ^{26mm}	>112	
p141	3-Phenyl-1-propanol propanethiol	$C_6H_5CH_2CH_2CH_2SH$	152.26	6 ¹ , 253	1.010	1.5494 ²⁰		109 ^{10mm}	90	
p142	1-Phenyl-1-propanol	$C_6H_5CH(OH)CH_2CH_3$	136.19	6, 502	0.9915 ²⁵ ₄	1.5169 ²³		219		misc alc, bz
p143	3-Phenyl-1-propanol	$C_6H_5CH_2CH_2CH_2OH$	136.19	6, 503	1.008	1.5257 ²⁰	–18	235	109	s aq; misc alc, eth
p144	1-Phenyl-2-propanone	$C_6H_5CH_2COCH_3$	134.18	7 ² , 233	1.0157 ²⁰ ₄	1.5160 ²⁰	27	100 ^{13mm}	84	v s alc, eth; misc bz
p145	2-Phenylpropionaldehyde	$CH_3CH(C_6H_5)CHO$	134.18	7 ² , 237	1.009 ²⁰ ₄	1.5175 ²⁰		202–205	69	i aq; s alc
p146	3-Phenylpropionic acid	$C_6H_5CH_2CH_2COOH$	150.18	9, 508	1.047 ¹⁰⁰ ₄		47–48	280		0.6 aq; s bz, alc, chl, eth, HOAc, PE
p147	1-Phenyl-3-pyrazolidinone		162.19	24, 2			121			10 hot aq; hot alc; s alk, acid

p148	2-Phenylpyridine	$C_6H_5C_5H_4N$	155.20	20, 424		1.6242 ²⁰		268–270	>112	s alc, eth
p149	2-Phenyl-4-quinolinecarboxylic acid		249.27	22, 103			214–215			0.8 alc; 1 eth; 0.3 chl
p150	Phenyl salicylate	$C_6H_4(OH)COOC_6H_5$	214.22	10, 76	1.25		41–43	173 ^{12mm}		17 alc; 66 bz; s acet, chl, eth; 0.015 aq
p151	Phenylselenenyl chloride	C_6H_5SeCl	191.52	6 ³ , 1110			63–65	120 ^{20mm}		
p152	Phenylsuccinic acid	$HOOCCH_2-CH(C_6H_5)COOH$	194.19	9, 865			167–169	$-H_2O$, >168		s hot aq, alc, eth
p153	S-Phenyl thioacetate	$C_6H_5SCOCH_3$	152.22			1.5720 ²⁰		100 ^{6mm}	79	
p154	1-Phenyl-2-thiourea	$C_6H_5NHC(S)NH_2$	152.22	12, 388	1.3		154			0.25 aq; s alc, alk
p155	Phenyltrichlorosilane	$C_6H_5SiCl_3$	211.56	16, 911	1.329 ²⁰	1.5230 ²⁰		201	91	

2-Phenylpropane, i91

3-Phenyl-2-propenoic acid, c267

3-Phenyl-2-propen-1-ol, c270

3-Phenyl-2-propenoyl chloride, c268

3-Phenylpropyl alcohol, p143

Phenyl propyl ketone, b500

3-Phenylpropyl mercaptan, p141

Phenyl sulfide, d688

Phenyl sulfone, d689

Phenylsulfonic acid, b22

Phenyl sulfoxide, d690

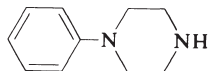
(Phenylthio)acetic acid, t160

Phenyl thiocarbamide, p154

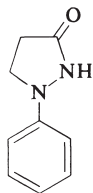
α -Phenyl-*o*-toluic acid, b84

Phenyl *m*-tolyl ether, p76

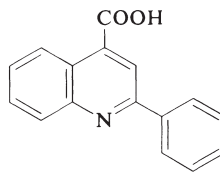
Phenyl trifluoromethyl ketone, t289



p139



p147



p149

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p156	1-Phenyltridecane	$C_6H_5(CH_2)_{12}CH_3$	260.47		0.8555 ₄ ²⁰	1.4814 ²⁰	10	346	> 112	
p157	Phenyltriethoxy-silane	$C_6H_5Si(OC_2H_5)_3$	240.38	16, 911	0.996	1.4604 ²⁰		113 ^{1.0mm}	42	
p158	Phenyltrimethoxy-silane	$C_6H_5Si(OCH_3)_3$	198.3		1.064 ₄ ²⁰	1.4734 ²⁰		211		
p159	Phenyltrimethyl-ammonium bromide	$[C_6H_5N(CH_3)_3]^+Br^-$	216.13	12 ² , 88			210 d			v s aq; s hot alc
p160	Phenyltrimethyl-ammonium chloride	$[C_6H_5N(CH_3)_3]^+Cl^-$	171.67	12, 158			237 subl			s aq; v s alc; sl s chl
p161	Phenyltrimethyl-ammonium iodide	$[C_6H_5N(CH_3)_3]^+I^-$	263.12	12 ² , 88			175			s aq, alc; sl s acet
p162	Phenyltrimethyl-ammonium tribromide	$C_6H_5N(CH_3)_3^+Br_3^-$	375.95				114–116			
p163	Phenyltrimethylsilane	$C_6H_5Si(CH_3)_3$	150.30	16 ¹ , 525	0.873	1.4907 ²⁰		168–170	44	
p164	Phenyltris(trimethylsiloxy)silane	$[(CH_3)_3SiO]_3SiC_6H_5$	372.8		0.970 ₄ ²⁵	1.459 ²⁵		264–266	121	
p165	Phenylurea	$C_6H_5NHCONH_2$	136.15	12, 346	1.302		145–147	238		s hot aq, hot alc, eth
p166	Phenylvinyl-dichlorosilane	$H_2C=CH(C_6H_5)SiCl_2$	203.2		1.196 ₄ ²⁵	1.534 ²⁵		87 ^{1.5mm}		
p167	<i>o</i> -Phthalic acid	$C_6H_4(COOH)_2$	166.13	9, 791	1.593 ₄ ²⁰		206–208			0.6 aq; 10 alc; 0.5 eth; v sl s chl
p168	Phthalic anhydride		148.12	17, 469	1.53		130.8	285 subl		0.6 aq(d); s alc
p169	Phthalide		134.13	17, 310	1.164 ₄ ⁹⁹		72–74	290		s alc
p170	Phthalimide		147.13	21, 458			238	subl		v s alk; v sl s bz, PE
p171	<i>o</i> -Phthaloyl dichloride	$C_6H_4(COCl)_2$	203.02	9, 805	1.409 ²⁰	1.5684 ²⁰	15–16	280–282	> 112	d aq, alc; s eth

p172	Phthalylsulfa- thioazole		403.44				272 d		s alk; sl s alc; i chl
p173	Picric acid	(O ₂ N) ₃ C ₆ H ₂ OH	229.11	6, 265	1.763 ₄ ²⁰		122–123	explodes > 300	1.3 aq; 8.2 alc; 10 bz; 2.9 chl; 1.6 eth
p174	Pinane		138.3	5, 93	0.839 ₄ ²⁰	1.4616 ²⁰	–50	167–168	
p175	(+)- α -Pinene		136.24	5, 146	0.8591 ₄ ²⁰	1.4660 ²⁰	–55	155–156	32
p176	(–)- β -Pinene		136.24	5, 154	0.8590 ²⁰	1.4666 ²⁰	–61.5	166	32
p177	α -Pinene oxide		152.24	5, 152	0.964	1.4690 ²⁰		103 ^{50mm}	65
p178	β -Pinene oxide		152.24	17 ² , 44	0.976	1.4765 ²⁰		100 ^{27mm}	66

Phloroglucinol, t305

Phorone, d529

Phthalaldehydic acid, f33

m-Phthalic acid, b16

p-Phthalic acid, b17

Phthalonitrile, d236

Picolinaldehyde, p251

Picolines, m398, m399, m400

Picolinic acids, p255, p257

Picolinonitrile, c295

Picolylamines, a223, a224

Picramide, t381

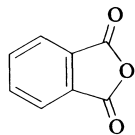
Pimelic acid, h8

Pinacol, d491

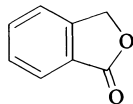
Pinacolone, d497

Pinacolyl alcohol, d496

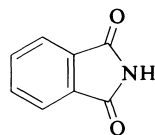
3-Pinanol, i83



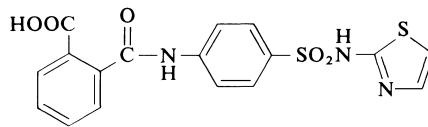
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p169



p170



p172



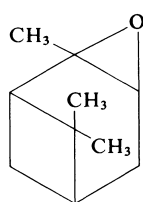
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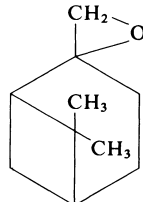
p175



p176



p177



p178

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

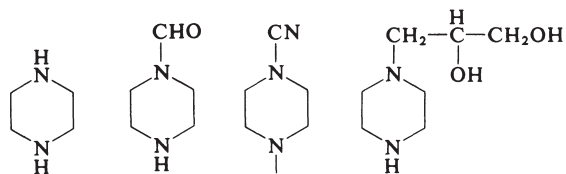
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p179	Piperazine		86.14	23, 4		1.446 ¹¹³	108–110	145–146	109	v s aq; 50 alc; i eth
p180	1-Piperazinecarb- aldehyde		114.15		1.107	1.5094 ²⁰		97 ^{0.5mm}	101	
p181	1,4-Piperazinedi- carbonitrile		136.16	23 ¹ , 5			167–170			
p182	3-(1-Piperazinyl)- 1,2-propanediol		160.22				73–77	133 ^{0.1mm}		
p183	Piperidine		85.15	20, 6	0.8659 ¹⁵	1.4525 ²⁰	–10.5	106.4	4	misc aq; s alc, bz, chl
p184	1-Piperidine- carbonitrile		110.16	20, 56	0.951	1.4705 ²⁰		102 ^{10mm}	97	
p185	<i>N</i> -Piperidineethanol		129.20	20, 25	0.9732 ²⁵ ₂₅	1.4804 ²⁰		200–202	68	misc aq; s alc
p186	2-Piperidineethanol		129.20	21, 2	1.010 ¹⁷		38–40	234	102	v s aq, alc, eth
p187	3-Piperidinemethanol		115.18	21 ² , 8	1.026			107 ^{3.5mm}	> 112	
p188	1-Piperidinepropio- nitrile		138.21		0.933	1.4695 ²⁰		111 ^{16mm}		
p189	3-Piperidino-1,2- propanediol		159.23	20, 34			77–80			
p190	trans-Piperitol		154.3		0.9178 ²⁵	1.4729 ²⁰				
p191	Propane	CH ₃ CH ₂ CH ₃	44.10	1, 104	0.5842 ^{–42}	1.3397 ^{–42}	–187.7	–42.1		6.5 mL aq; 790 mL alc; 926 mL eth; 1300 mL chl; 1450 mL bz
p192	1,2-Propanediamine	CH ₃ CH(NH ₂)CH ₂ NH ₂	74.13	4, 257	0.878 ¹⁵	1.4460 ²⁰		119.7	33	misc aq, bz; s alc, eth
p193	1,3-Propanediamine	H ₂ NCH ₂ CH ₂ CH ₂ NH ₂	74.13	4, 261	0.884 ²⁵ ₄	1.4575 ²⁰	–12	140	48	misc alc, eth; s aq
p194	1,2-Propanediol	CH ₃ CH(OH)CH ₂ OH	76.10	1, 472	1.0364 ²⁰ ₄	1.4331 ²⁰	–60	188	107	misc aq, acet, chl; s alc, eth
p195	1,3-Propanediol	HOCH ₂ CH ₂ CH ₂ OH	76.10	1, 475	1.0597 ²⁰ ₄	1.4396 ²⁰	–26.7	214.4	79	misc aq, alc

p196	1,3-Propanedithiol	$\text{HSCH}_2\text{CH}_2\text{CH}_2\text{SH}$	108.23	1, 476	1.0772 ₄ ²⁰	1.5405 ²⁰	-79	169	40	misc alc, bz, eth,
p197	1-Propanesulfonyl chloride	$\text{CH}_2\text{CH}_2\text{CH}_2\text{SO}_2\text{Cl}$	142.60	4, 8	1.2864 ₄ ¹⁵			66 ^{8mm}		chl d hot aq, hot alc
p198	1,3-Propane sultone		122.14		1.392		30-33	180 ^{30mm}		

Pipecolines, m369, m370, m371
 1-Piperazineethanol, h123
 1-Piperidinecarboxyaldehyde, f35
 Piperonal, m239
 Piperonyl alcohol, m242
 Piperonyl butoxide, m243
 Piperonylic acid, m241
 Pivalaldehyde, d596

Pivalamide, d597
 Pivalic acid, d598
 Pivalic anhydride, d599
 Pivaloyl chloride, d600
 Pivaloyloxymethyl chloride, c151
 POPOP, b198
 PPO, d679
 Prehnitene, t97

Procaine, d271
 Proline, p273
 Propadiene, a78
 1-Propanal, p211
 1,3-Propanedicarboxylic acid, g11
 Propanedioic acid, m3
 1,2-Propanediol cyclic carbonate, p225

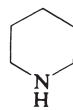


p179

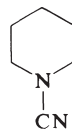
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p181

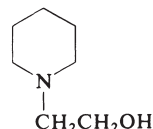
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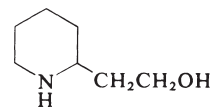
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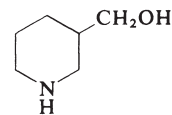
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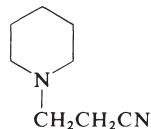
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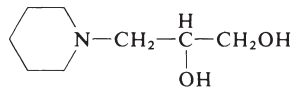
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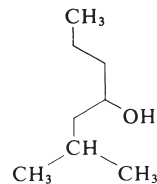
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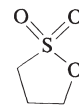
p188



p189



p190



p198

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p199	1-Propanethiol	$\text{CH}_3\text{CH}_2\text{CH}_2\text{SH}$	76.16	1, 359	0.836_4^{25}	1.4380^{20}	-113.1	67.7	-20	s alc, eth
p200	2-Propanethiol	$\text{CH}_3\text{CH}(\text{SH})\text{CH}_3$	76.16	1, 367	0.809_4^{25}	1.4255^{20}	-130.5	52.6	-34	misc alc, eth; sl s aq
p201	1,2,3-Propanetriol triacetate	$\text{H}_3\text{CCOO-CH}(\text{CH}_2\text{OOCCH}_3)_2$	218.21	2, 147	1.596_4^{20}	1.4302^{20}	-78	258-260	148	7.2 aq; misc alc, bz, chl, eth
p202	1-Propanol	$\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$	60.10	1, 350	0.8037_4^{20}	1.3856^{20}	-126.2	97.2	15	misc aq, alc, eth
p203	2-Propanol	$(\text{CH}_3)_2\text{CHOH}$	60.10	1, 360	0.7855_4^{20}	1.3772^{20}	-89.5	82.4	22	misc aq, alc, chl, eth
p204	2-Propenal	$\text{H}_2\text{C}=\text{CHCHO}$	56.07	1, 725	0.8389^{20}	1.4017^{20}	-87.0	52.7	-18	21 aq; s alc, eth
p205	Propene	$\text{H}_2\text{C}=\text{CHCH}_3$	42.08	1, 196	0.6104_4^{-48}	1.3567^{-40}	-185.2	-47.7		45 mL aq; 1200 mL alc; 500 mL acet
p206	2-Propene-1-thiol	$\text{H}_2\text{C}=\text{CHCH}_2\text{SH}$	74.15	1, 440	0.925_4^{23}			67-68	21	misc alc, eth
p207	(Z)-1,2,3-Propene-tricarboxylic acid		174.11	2, 849			d 200			50 aq; s alc; sl s eth
p208	1-Propen-2-yl acetate	$\text{H}_2\text{C}=\text{C}(\text{OOCCH}_3)\text{CH}_3$	100.12		0.909	1.4000^{20}		97	18	
p209	<i>o</i> -Propenylphenol	$\text{CH}_3\text{CH}=\text{CHC}_6\text{H}_4\text{OH}$	134.18	6 ¹ , 279	1.044	1.5754^{20}		230-231	90	
p210	β -Propiolactone		72.06		1.1460_4^{20}	1.4131^{20}	-33.4	162.3	70	37 aq(hyd); misc alc (reacts), bz, eth, acet
p211	Propionaldehyde	$\text{CH}_3\text{CH}_2\text{CHO}$	58.08	1, 629	0.8071_4^{20}	1.3646^{19}	-81	48-49	-9	30 aq; misc alc, eth
p212	Propionamide	$\text{CH}_3\text{CH}_2\text{CONH}_2$	73.10	2, 243	0.9597_4^{20}	1.4160^{110}	79	222.2		v s aq, alc, chl, eth
p213	Propionic acid	$\text{CH}_3\text{CH}_2\text{COOH}$	74.09	2, 234	0.9934_4^{20}	1.3865^{20}	-21	140.8	51	misc aq; s alc, chl, eth
p214	Propionic anhydride	$[\text{CH}_3\text{CH}_2\text{C}(=\text{O})]_2\text{O}$	130.14	2, 242	1.0125_4^{20}	1.4047^{20}	-45	167	73	d aq; s alc, chl, eth
p215	Propionitrile	$\text{CH}_3\text{CH}_2\text{CN}$	55.08	2, 245	0.7818_4^{20}	1.3658^{20}	-92.8	97.2	6	10 aq; misc alc, eth

p216	Propionyl chloride	$\text{CH}_3\text{CH}_2\text{COCl}$	92.53	2, 243	1.065^{20}_4	1.4051^{20}	-94	80	11	d aq, alc
p217	Propiophenone	$\text{C}_6\text{H}_5\text{COCH}_2\text{CH}_3$	134.18	7 ² , 231	1.0105^{20}_4	1.5258^{20}	18.6	218.0	87	misc bz, eth, abs alc
p218	Propoxytrimethyl- silane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{OSi}(\text{CH}_3)_3$	132.3		0.768^{20}_4	1.384^{20}		100 ^{735mm}		
p219	Propyl acetate	$\text{CH}_3\text{CH}_2\text{CH}_2\text{OOCCH}_3$	102.13	2, 129	0.836^{20}_4	1.3844^{20}	-92	101.6	12	2.3 aq; misc alc, eth
p220	Propylamine	$\text{CH}_3\text{CH}_2\text{CH}_2\text{NH}_2$	59.11	4, 136	0.7173^{20}	1.3882^{20}	-83.0	47.9	-37	misc aq, alc, eth
p221	2-(Propylamino)- ethanol	$\text{C}_3\text{H}_7\text{NHCH}_2\text{CH}_2\text{OH}$	103.17	4, 282	0.900	1.4415^{20}		182 ^{746mm}	78	
p222	Propylbenzene	$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}_6\text{H}_5$	120.20	5, 390	0.8621^{20}_4	1.4912^{20}	-99.6	159.2	47	s alc, eth
p223	Propyl benzoate	$\text{C}_6\text{H}_5\text{COOCH}_2\text{CH}_2\text{CH}_3$	164.20	9, 112	1.0232^{20}	1.5003^{20}	-51.6	231.2		i aq; s alc, eth
p224	Propylcyclohexane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}_6\text{H}_{11}$	126.24	5 ² , 23	0.7929^{20}_4	1.4370^{20}	-94.9	156.7		s bz, eth
p225	Propylene carbonate		102.09		1.2041^{20}_4	1.4210^{20}	-55	240	132	v s aq, alc, bz, eth
p226	Propyleneimine		57.09		0.8017^{25}	1.4084^{25}		66.0		misc aq, alc, PE

1,2,3-Propanetriol, g16
 Propanetriol diacetates, g17, g18
 2-Propanone, a26
 Propargyl alcohol, p242
 Propargyl chloride, c232
 Propenamide, a62
 2-Propenenitrile, a64
 2-Propenoic acid, a63

2-Propen-1-ol, a81
 2-Propenyl acetate, a80
 Propenylanisole, m97
 N-2-Propenyl-2-propen-1-amine, d25
 (2-Propenyl)thiourea, a101
 Propiolic acid, p241
 Propyl chloride, c210
 Propylene, p205

Propylene dibromide, d92
sec-Propylene chlorohydrin, c213
 Propylenediamine, p192
 Propylene glycol, p194
 Propylene glycol isopropyl ether, i86
 Propylene glycol monomethyl ether, m95
 Propylene glycol monophenyl ether, p73

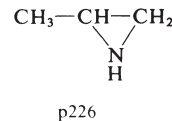
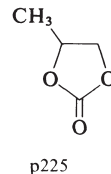
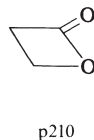
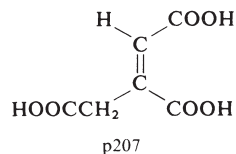


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

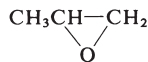
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p227	Propylene oxide	$\text{CH}_3\text{CH}-\text{CH}_2$ O	58.08	17, 6	0.8287 ²⁰	1.3660 ²⁰	-112.1	37-38	-37	41 aq; misc alc, eth
p228	Propylene sulfide	$\text{CH}_3\text{CH}-\text{CH}_2$ S	102.18	1, 354	0.736	1.3800 ²⁰	-123	88-90	4	
p229	Propyl formate	$\text{CH}_3\text{CH}_2\text{CH}_2\text{OOCH}$	88.10	2, 21	0.9006 ²⁰	1.3769 ²⁰	-92.9	80.9	-3	2 aq; misc alc, eth
p230	Propyl 4-hydroxybenzoate	$\text{HOC}_6\text{H}_4\text{COOCH}_2\text{CH}_2\text{CH}_3$	180.20	10, 160			86-87			0.05 aq; v s alc, eth
p231	Propyl isocyanate	$\text{CH}_3\text{CH}_2\text{CH}_2\text{NCO}$	85.11	4 ¹ , 366	0.908	1.3970 ²⁰		83-84	26	
p232	Propyl lactate	$\text{CH}_3\text{CH}(\text{OH})\text{COOC}_3\text{H}_7$	132.16	3, 265	0.996 ²⁰	1.4167 ²⁵		86 ^{40mm}		s aq, alc, eth
p233	Propyl nitrate	$\text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}_2$	105.09	1, 355	1.0538 ²⁰	1.3976 ²⁰	-100	110.1	23	s alc, eth
p234	2-Propylpentanoic acid	$(\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{CHCOOH}$	144.21	2, 350	0.921	1.4250 ²⁰	may explode on heating			
p235	<i>o</i> -Propylphenol	$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}_6\text{H}_4\text{OH}$	136.19	6, 499	1.015 ²⁰	1.5279 ²⁰			220	
p236	Propylphosphonic dichloride	$\text{CH}_3\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Cl}_2$	160.97	4, 596	1.290	1.4643 ²⁰			224-226	93
p237	Propyltrichlorosilane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{SiCl}_3$	177.53	4, 630	1.1851 ²⁰	1.429 ²⁰			88-90 ^{50mm}	>112
p238	Propyltriethoxysilane	$\text{C}_3\text{H}_7\text{Si}(\text{OC}_2\text{H}_5)_3$	206.4		0.892 ²⁰	1.396 ²⁰		123-124	2	
p239	Propyl 3,4,5-trihydroxybenzoate	$(\text{HO})_3\text{C}_6\text{H}_2\text{COOC}_3\text{H}_7$	212.20				150	179-180		
p240	Propyne	$\text{CH}_3\text{C}\equiv\text{CH}$	40.06	1, 246	0.691 ⁻²⁰	1.3725 ⁻²⁰	-102.8	-23.2		0.35 aq; 1 alc; 83 eth
p241	2-Propynoic acid	$\text{HC}\equiv\text{CCOOH}$	70.05	2, 477	1.138 ²⁰	1.4320 ²⁰	9	102 ^{200mm}	58	v s alc; 3000mL eth
p242	2-Propyn-1-ol	$\text{HC}\equiv\text{CCCH}_2\text{OH}$	56.06	1, 454	0.9715 ²⁰	1.4320 ²⁰	-51.8	113.6	33	s aq, alc, eth
p243	(+)-Pulegone		152.24	7, 81	0.9346 ¹⁵	1.4850 ²⁰		224	82	misc aq, alc, bz, chl

p244	Pyrazine		80.09	23, 91	1.031 ₄ ⁶¹	1.4953 ⁶¹	53	115–116		v s aq, alc, eth
p245	Pyrazole		68.08	23, 39		1.4203	70	186–188		s aq, alc, bz, eth
p246	Pyrene		202.26	5, 693			150–151			
p247	Pyridazine		80.09	23, 89	1.1035 ₄ ²⁵	1.5230 ²³	–8	208	85	misc aq, bz; v s alc, eth
p248	Pyridine	C ₅ H ₅ N	79.10	20, 181	0.9782 ₄ ²⁵	1.5067 ²⁵	–41.6	115.2	20	misc aq, alc, eth
p249	Pyridine- <i>d</i> ₅	C ₅ D ₅ N	84.14		1.05	1.5079 ²⁰		114.4	20	
p250	2-Pyridinealdoxime	(C ₅ H ₄ N)CH=NOH	122.13	21 ¹ , 288			110–112			
p251	2-Pyridinecarb- aldehyde	(C ₅ H ₄ N)CHO	107.11	21 ¹ , 287	1.126	1.5370 ²⁰		181	54	
p252	3-Pyridinecarb- aldehyde	(C ₅ H ₄ N)CHO	107.11	21 ¹ , 288	1.135	1.5493 ²⁰		97 ^{15mm}	60	
p253	4-Pyridinecarb- aldehyde	(C ₅ H ₄ N)CHO	107.11	21, 287	1.172	1.5440 ²⁰		78 ^{12mm}	54	s aq, eth
p254	3-Pyridinecarbamide	(C ₅ H ₄ N)CONH ₂	122.13	22, 40	1.400	1.466	130–133			100 aq; 66 alc
p255	Pyridine-2-car- boxylic acid	(C ₅ H ₄ N)COOH	123.11	22, 33			134–136	subl		s aq, alc, bz
p256	Pyridine-3-car- boxylic acid	(C ₅ H ₄ N)COOH	123.11	22, 38	1.473		236.6	subl		1.4 aq; s alk

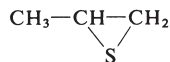
Propylene oxide, e10
 Propyl gallate, p239
 Propyl iodide, i48
 Propyl mercaptan, p199

6-Propyl-2-thiouracil, h129
 Protocatechualdehyde, d376
 Pseudocumene, t334
 Pyrene, b52

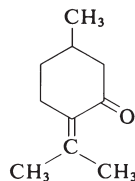
3,6-Pyridazinediol, d400
 2,3-Pyridinediol, d401



p227



p228



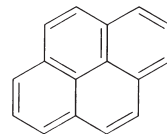
p243



p244



p245



p246



p247

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

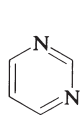
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
p257	Pyridine-4-carboxylic acid	$(C_5H_4N)COOH$	123.11	22, 45			319	260 ^{15mm}		0.52 aq; i alc, bz, eth
p258	4-Pyridinecarboxylic hydrazide	$(C_5H_4N)CONHNH_2$	137.14	22 ¹ , 504			171.4			14 aq; 2 alc; 0.1 chl
p259	2,3-Pyridinedicarboxylic acid	$(C_5H_3N)(COOH)_2$	167.12	22, 150			190 d			0.56 aq; s alk
p260	2,5-Pyridinedicarboxylic acid	$(C_5H_3N)(COOH)_2$	167.12	22, 153			236–237	subl d		s hot acid
p261	2,6-Pyridinedicarboxylic acid	$(C_5H_3N)(COOH)_2$	167.12	22, 154			250 d			sl s aq; v sl s alc
p262	Pyridine- <i>N</i> -oxide	$C_5H_5N(O)$	95.10	20 ² , 131			66	270		
p263	3-Pyridinesulfonic acid	$(C_5H_4N)SO_3H$	159.16	22, 387			>300			v s aq
p264	2-Pyridylmethanol	$(C_5H_4N)CH_2OH$	109.13	21 ¹ , 203	1.131	1.5420 ²⁰		113 ^{16mm}		v s aq, alc, eth
p265	3-Pyridylmethanol	$(C_5H_4N)CH_2OH$	109.13	21, 50	1.124	1.5445 ²⁰		154 ^{28mm}		v s aq, eth
p266	3-(3-Pyridyl)-1-propanol	$(C_5H_4N)CH_2CH_2CH_2OH$	137.18		1.045	1.5295 ²⁰				
p267	Pyrimidine		80.09	23, 89	1.016	1.5035 ²⁰	20–22	123–124	31	misc aq; s alc, eth
p268	2,4(1H,3H)-Pyrimidinedione		112.09	24, 312			335			0.3 aq; s alk
p269	Pyrrole		67.09	20, 159	0.9691 ²⁰ ₄	1.5102 ²⁰	–23.4	129.8	38	4.5 aq; v s alc, eth
p270	Pyrrolidine		71.12	20, 4	0.8520 ²² ₄	1.4431 ²⁰	–57.8	88–89	2	misc aq; s alc, chl, eth
p271	1-Pyrrolidinecarbo-dithioic acid, ammonium salt		164.29				153–155			
p272	1-Pyrrolidinecarbo-nitrile		96.13		0.954	1.4690 ²⁰		77 ^{1.8mm}	107	

p273	L-(−)-2-Pyrrolidinecarboxylic acid	115.13	22, 2			d 220		162 aq; 66 abs alc
p274	1-Pyrrolidino-1-cyclohexene	151.25		0.940	1.5225 ²⁰		115 ^{15mm}	39
p275	2-Pyrrolidinone	85.11	21, 236	1.116 ²⁵ ₄	1.486 ²⁵	25	245	145
p276	3-(N-Pyrrolidino)-1,2-propanediol	145.20	20 ¹ , 4			46–48	158 ^{30mm}	misc aq, alc, bz, chl, eth, EtAc
q1	Quinhydrone	218.20	7, 617	1.401 ²⁰ ₄		171		s hot aq, alc, eth

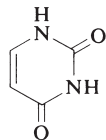
Pyridinols, h173, h174, h175
 3-Pyridinol *N*-oxide, h177
 2(1*H*)-Pyridone, h173
 2-(2-Pyridyl)pyridine, d705
 Pyrocatechol, d377

Pyrogallol, t304
 Pyromellitic acid, b26
 Pyromellitic dianhydride, b27
 Pyromucic acid, f42
 Pyromucic aldehyde, f39

Pyrrolidinedithiocarbamate, p271
 Pyruvic acid, o60
 Pyruvic aldehyde, o59
 Pyruvic aldehyde dimethyl acetal, d451
 Quinaldine,



p267



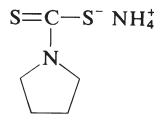
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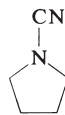
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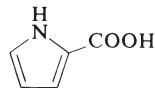
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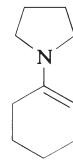
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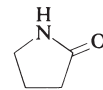
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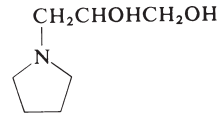
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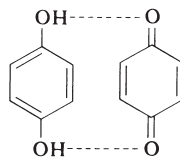
p274



p275



p276



q1

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
q2	Quinine		324.44			1.625	177 d			125 alc; 1.2 bz; 83 chl
q3	Quinoline		129.16	20, 339	1.095 ₄ ²⁰	1.6273 ²⁰	−14.9	237	101	0.6 aq; misc alc, eth
q4	Quinoxaline		130.15	23, 176	1.1334 ₄ ⁴⁸	1.6231 ⁴⁸	29–30	229.5		v s aq, alc, bz, eth
q5	Quinuclidine		111.19	20, 144			156 sealed tube			v s aq, alc, eth
r1	D-Raffinose pentahydrate		594.52	31, 462			80	d 118		14 aq; 10 MeOH
r2	Rhodamine B		479.02	19, 346			165			v s aq, alc
r3	Rhodanine		133.19	27, 242	0.868		170 may explode on rapid heating			v s hot aq, alc, eth
r4	Riboflavin		376.37				d 278			v s alk(d); i eth
r5	D-(−)-Ribose		150.13	1 ¹ , 434			87			s aq; sl s alc
s1	Saccharin		183.19	27, 168			229–230			0.34 aq; 3 alc; 8 acet
s2	Safrole		162.19	19, 39	1.095 ²⁰	1.5370 ²⁰	11.2	232–234	97	v s alc; misc chl eth
s3	Semicarbazide	H ₂ NNHCONH ₂	75.07	3, 98			96			v s aq, alc; i eth

Quinizarin, d372

Quinolinic acid, p259

8-Quinolinol, h178

p-Quinone, b59

Resacetophenone, d370

Resorcinol, d378

Resorcinol dimethyl ether, d432

Resorcinol monoacetate, d380

Resorcinol sulfide, t145

 α -Resorcylaldehyde, d375 α -Resorcyclic acid, d385 β -Resorcyclic acid, d383

Ribofuranose, r5

Rosaniline, b2

Rubeanic acid, d710

Slicyl alcohol, h105

Salicylaldehyde, h94

Salicylaldoxime, h97

Salicylamide, h98

Salicylanilide, h161

Salicylic acid, h99

Salol, p150

Sarcosine, m258

Sebacic acid, d9

Sebacoyl chloride, d11

Semioxamazide, 053

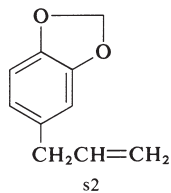
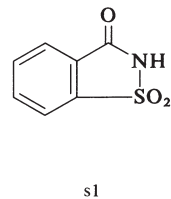
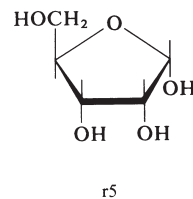
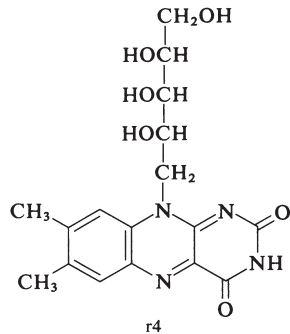
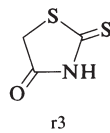
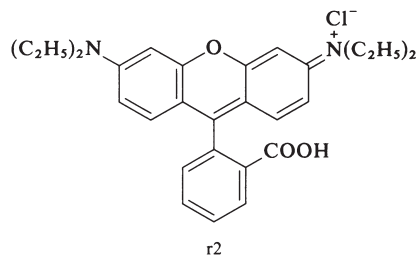
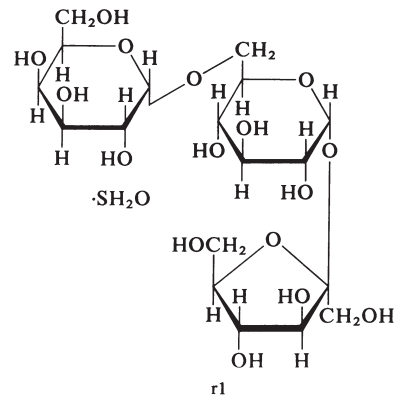
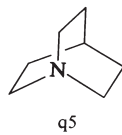
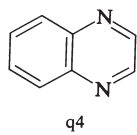
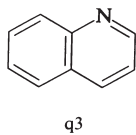
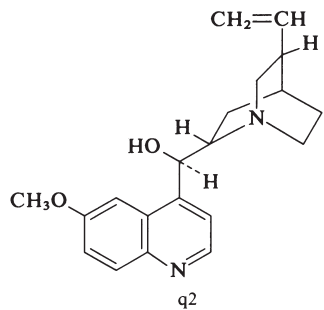


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
s4	L-Serine	$\text{HOCH}_2\text{CH}(\text{NH}_2)\text{COOH}$	105.09	4, 505			222 d			s aq; v sl s alc, eth
s5	D-Sorbitol		182.17	1, 533	1.472^{-5}		110–112			83 aq; s hot alc, acet
s6	L-(–)-Sorbitose		180.16	1, 927	1.65^{15}		165			55 aq; v sl s alc
s7	Squalane	$[(\text{CH}_3)_2\text{CH}(\text{CH}_2)_3-\text{CH}(\text{CH}_3)(\text{CH}_2)_3-\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2-]_2$	422.80	1 ¹ , 72	0.810	1.4530^{15}	–38	350	218	s bz, chl, eth, PE
s8	Squalene	$\{\text{CH}_2[\text{C}(\text{CH}_3)=\text{CHCH}_2-\text{CH}_2]_2\text{C}(\text{CH}_3)=\text{CHCH}_2-\}$	410.73	1 ¹ , 130	0.8584_4^{20}	1.4965^{20}	–75	$285^{25\text{mm}}$	200	v s eth, acet, PE
s9	<i>trans</i> -Stilbene	$\text{C}_6\text{H}_5\text{CH}=\text{CHC}_6\text{H}_5$	180.25	5, 630	0.970		124	206–207		v s bz, eth
s10	L-Strychnine		334.42	27 ² , 723	1.36_4^{20}		284–286	$270^{5\text{mm}}$		6.2 alc; 20 chl; 0.55 bz; 15 mg aq
s11	Styrene	$\text{C}_6\text{H}_5\text{CH}=\text{CH}_2$	104.15	5, 474	0.9060^{20}	1.5468^{20}	–30.6	145.1	31	s alc, acet, eth
s12	Succinamic acid	$\text{H}_2\text{NCOCH}_2\text{CH}_2\text{COOH}$	117.10	2, 614			153–156			s aq; sl s alc; i eth
s13	Succinamide	$\text{H}_2\text{NCOCH}_2\text{CH}_2\text{CONH}_2$	116.12	2, 614			260 d	125 subl		0.45 aq; i alc, eth
s14	Succinic acid	$\text{HOOCCH}_2\text{CH}_2\text{COOH}$	118.09	2, 601	1.552		187–190	235 d		7.7 aq; 5.4 alc; 2.8 acet; 0.88 eth; i bz
s15	Succinic acid 2,2-dimethylhydrazide	$\text{HOOCCH}_2\text{CH}_2\text{CONH}-\text{N}(\text{CH}_3)_2$	160.17				154–155			11 aq; 2.5 acet; 5 MeOH
s16	Succinic anhydride		100.07	17, 407			119.6	261		s alc, chl; v sl s eth
s17	Succinimide		99.09	21, 369	1.41		125–127	287		33 aq; 4 alc; i eth
s18	Succinonitrile	$\text{NCCH}_2\text{CH}_2\text{CN}$	80.09	2, 615	0.985		46–48	265–267	>112	
s19	Succinyl chloride	$\text{ClCOCH}_2\text{CH}_2\text{COCl}$	154.98	2, 613	1.395_4^{15}	1.473^{15}	17	192–193	76	d aq, alc; s bz
s20	Sucrose		342.30	31, 424	1.587_4^{25}		192 d			200 aq; 0.59 alc
s21	Sulfamethazine		278.34				198–201			0.15 aq; s alk
s22	Sulfanilamide	$\text{H}_2\text{NC}_6\text{H}_4\text{SO}_2\text{NH}_2$	172.21	14, 698			164–166			0.76 aq; 2.7 alc; 20 acet; s acid, alk

s23	Sulfoacetic acid	$\text{HO}_3\text{SCH}_2\text{COOH}$	140.11	4, 21		84–86	245 d		s aq, alc; i eth, chl
s24	<i>o</i> -Sulfobenzoic acid cyclic anhydride		184.17	19, 110			186 ^{18mm}		s bz, chl, eth; i aq
s25	4,4'-Sulfonylbis- (2,6-dibromo- phenol)	$[\text{HO}(\text{Br})_2\text{C}_6\text{H}_2]_2\text{SO}_2$	565.88	6, 865		289–292			

Senecioic acid, m163

Skatole, m284

Sodium tetraphenylborate, t128

Solketal, d515

Sorbic acid, h42

Sorbic aldehyde, h40

Stearamide, o2

Stearic acid, o5

Stearyl bromide, b319

Styrene dibromide, d79

Styrene glycol, p111

Styrene oxide, e9

Suberic acid, o24

Suberonitrile, d239

Succinic acid monoamide, s12

Succinonitrile, b380

Succinyl dihydrazide, s15

Sulfanilic acid, a120

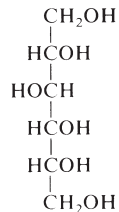
N-Sulfinylaniline, t152

3-Sulfoalanine, a288

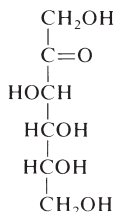
Sulfolane, t106

3-Solfolene, d368

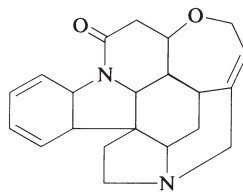
Sulfonyldianilines, d36, d37



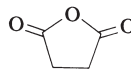
s5



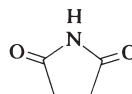
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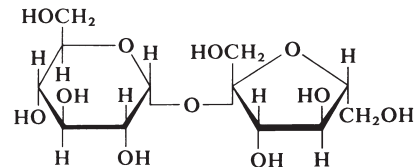
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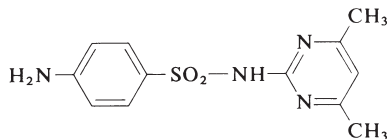
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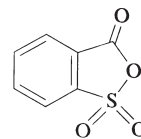
s17



s20



s21



s24

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
s26	4,4'-Sulfonylbis-(methyl benzoate)	$(\text{CH}_3\text{OOC}_6\text{H}_4)_2\text{SO}_2$	334.35	10 ² , 109			195–196			
s27	4,4'-Sulfonyldiphenol	$(\text{HOC}_6\text{H}_4)_2\text{SO}_2$	250.27	6, 861	1.3663 ¹⁵		245–247			s alc, eth, acet; i aq
s28	5-Sulfosalicylic acid	$\text{HO}_3\text{SC}_6\text{H}_3(\text{OH})\text{COOH}$	254.21	11, 411			120			v s aq, alc; s eth
t1	D-(–)-Tartaric acid		150.09	3, 520	1.7598 ²⁰ ₄		168–170			139 aq; 33 alc; 0.4 eth
t2	<i>meso</i> -Tartaric acid hydrate	$\text{HOOCCH}(\text{OH})\text{-CH}(\text{OH})\text{COOH} \cdot x\text{H}_2\text{O}$	150.09	3, 528	1.666 ²⁰ ₄		140			125 aq
t3	Tartrazine		534.37	25, 252						v s aq
t4	<i>p</i> -Terphenyl	$\text{C}_6\text{H}_5\text{C}_6\text{H}_4\text{C}_6\text{H}_5$	230.31	5, 695			212–213	383		
t5	α -Terpinene		136.24	5, 126	0.8375 ²⁰ ₄	1.4775 ²⁰		174	46	misc alc, eth
t6	γ -Terpinene		136.24	5, 128	0.853 ¹⁵ ₄	1.4754 ¹⁶		183	51	
t7	Terpinen-4-ol		154.25	6, 55	0.9338 ²⁰ ₄	1.4820 ²⁰	36.4	219	79	v s alc, eth
t8	Tetraallyloxysilane	$(\text{H}_2\text{C}=\text{CHCH}_2\text{O})_4\text{Si}$	256.4		0.9824 ²⁰ ₄	1.4336 ²⁰		114 ^{12mm}		
t9	1,1,2,2,-Tetrabromoethane	$\text{Br}_2\text{CHCHBr}_2$	345.67	1, 94	2.9529 ²⁵	1.6323 ²⁵	0.0	243.5	none	misc alc, eth; 0.07 aq
t10	Tetrabromophthalic anhydride		463.72	17, 485			274–276			sl s bz; i aq, alc
t11	$\alpha,\alpha,\alpha',\alpha'$ -Tetrabromo- <i>o</i> -xylene	$\text{C}_6\text{H}_4(\text{CHBr}_2)_2$	421.77	5, 367			114–116			v s chl
t12	$\alpha,\alpha,\alpha',\alpha'$ -Tetrabromo- <i>m</i> -xylene	$\text{C}_6\text{H}_4(\text{CHBr}_2)_2$	421.77	5, 375			105–108			v s bz, chl
t13	Tetrabutoxysilane	$(\text{C}_4\text{H}_9\text{O})_4\text{Si}$	320.5		0.899 ²⁰ ₄	1.413 ²⁰		115 ^{3mm}		
t14	Tetrabutylammonium bromide	$(\text{C}_4\text{H}_9)_4\text{N}^+\text{Br}^-$	322.38				103–104			
t15	Tetrabutylammonium chloride	$(\text{C}_4\text{H}_9)_4\text{N}^+\text{Cl}^-$	277.92	4 ³ , 292			83–86			

t16	Tetrabutylammonium fluoride trihydrate	$(C_4H_9)_4N^+F^- \cdot 3H_2O$	315.52	4 ³ , 292			62–63			
t17	Tetrabutylammonium hydrogen sulfate	$(C_4H_9)_4N^+HSO_4^-$	339.54				169–171			
t18	Tetrabutylammonium iodide	$(C_4H_9)_4N^+I^-$	369.38	4, 157			145–148			sl s aq; s alc, eth
t19	Tetrabutylammonium tetrafluoroborate	$(C_4H_9)_4N^+BF_4^-$	329.28	4 ³ , 293			160–162			
t20	Tetrabutyltin	$(C_4H_9)_4Sn$	347.15		1.057	1.4742 ²⁰	–97	145 ^{10mm}	107	
t21	1,1,3,3-Tetrachloroacetone	$Cl_2CHCOCHCl_2$	195.86	1, 656	1.624 ¹⁵	1.497 ¹⁸		182 ^{745mm}	none	v s acet, chl
t22	1,2,3,4-Tetrachlorobenzene	$C_6H_2Cl_4$	215.89	5, 204			46–47	254	>112	v s eth; sl s alc
t23	1,2,4,5-Tetrachlorobenzene	$C_6H_2Cl_4$	215.89	5, 205	1.858 ²²		138–140	240–246	>112	s bz, chl, eth

Sylvan, m252
Sylvic acid, a1
2,4,5-T, t242
TAPS, t427

Taurine, a161
Terephthaldehyde, b13
Terephthaldicarboxaldehyde, b13
Terephthalic acid, b17

Terephthaloyl chloride, b15
TES, t424
Tetracene, b7

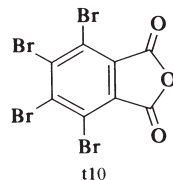
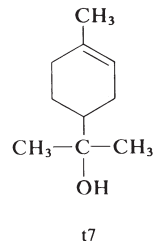
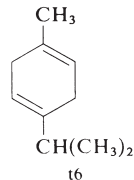
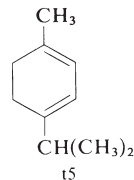
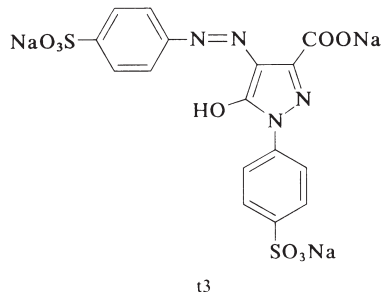
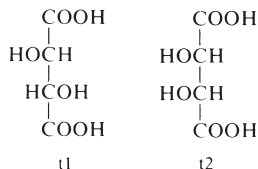


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t24	Tetrachloro- <i>o</i> -benzoquinone	$C_6Cl_4(=O)_2$	245.88	7, 602			127–129			
t25	Tetrachloro- <i>p</i> -benzoquinone	$C_6Cl_4(=O)_2$	245.88	7, 602			290	subl		s eth; sl s chl; i aq
t26	Tetrachloro-1,2-difluoroethane	Cl_2CFCl_2	203.83		1.6447 ²⁵	1.4130 ²⁵	26.0	92.8		0.012 aq
t27	1,1,1,2-Tetrachloroethane	$ClCH_2CCl_3$	167.85	1, 86	1.598	1.4819 ²⁰		130	none	0.02 aq; misc alc
t28	1,1,2,2-Tetrachloroethane	$Cl_2CHCHCl_2$	167.85	1, 86	1.5866 ²⁵ ₄	1.4910 ²⁵	–43.8	146.3	none	0.3 aq; misc alc, chl, eth, PE
t29	Tetrachloroethylene	$Cl_2C=CCl_2$	165.83	1, 187	1.6230 ²⁰ ₄	1.5057 ²⁰	–22.4	121.1	none	misc alc, chl, eth
t30	2,3,5-Tetrachloro-nitrobenzene	$HC_6Cl_4NO_2$	260.89	5, 247	1.744 ²⁵ ₄		98–101	304		s alc, bz, chl
t31	Tetrachlorophthalic anhydride		285.90	17, 484			254–258	371		d hot aq; sl s eth
t32	3,4,5,6-Tetrachlorophthalimide		284.91	21, 505			>300			
t33	1,1,2,3-Tetrachloro-2-propene	$ClCH=C(Cl)CHCl_2$	179.86	1 ¹ , 83	1.530	1.5163 ²⁰	165		none	
t34	2,3,5,6-Tetrachloro-thioanisole	$HC_6Cl_4SCH_3$	262.0				59–61			
t35	2,4,5,6-Tetrachloro- <i>m</i> -xylene	$C_6Cl_4(CH_3)_2$	243.95	5, 373			220–222			
t36	Tetracosane	$CH_3(CH_2)_{22}CH_3$	338.66	1, 175	0.7786 ⁵¹	1.4283 ⁷⁰	51.1	391		9.4 chl; s eth
t37	Tetracyanoethylene	$(NC)_2C=C(CN)_2$	128.09				200	subl 120		
t38	Tetradecane	$CH_3(CH_2)_{12}CH_3$	198.40	1, 171	0.7627 ²⁰ ₄	1.4290 ²⁰	5.9	253.5		v s alc, eth
t39	Tetradecanoic acid	$CH_3(CH_2)_{12}COOH$	228.38	2, 365	0.8528 ⁷⁰ ₄	1.4273 ⁷⁰	58.5	250 ^{100mm}		v s bz, chl, eth; s alc

t40	1-Tetradecanol	$\text{CH}_3(\text{CH}_2)_{13}\text{OH}$	214.39	1, 428	0.8151 ⁵⁰	1.4358 ⁵⁰	37.8	264		s eth; sl s alc
t41	Tetradecanoyl chloride	$\text{CH}_3(\text{CH}_2)_{12}\text{COCl}$	246.82	2, 368			−1	168 ^{15mm}		d aq, alc; s eth
t42	1-Tetradecene	$\text{CH}_3(\text{CH}_2)_{11}\text{CH}=\text{CH}_2$	196.38	1, 226	0.775 ¹⁵ ₄	1.4351 ²⁰	−12.9	251.2	115	v s alc; s eth
t43	7-Tetradecene	$\text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}-$ $(\text{CH}_2)_5\text{CH}_3$	196.38		0.764	1.4351 ²⁰		250	99	
t44	1-Tetradecylamine	$\text{CH}_3(\text{CH}_2)_{13}\text{NH}_2$	213.41	4, 201			40–42	162 ^{15mm}		
t45	4-Tetradecylaniline	$\text{CH}_3(\text{CH}_2)_{13}\text{C}_6\text{H}_4\text{NH}_2$	213.41	12 ³ , 2780			46–49			
t46	Tetradecyltrichloro-silane	$\text{CH}_3(\text{CH}_2)_{13}\text{SiCl}_3$	331.8			1.382		156 ^{3mm}		
t47	Tetraethoxysilane	$(\text{CH}_3\text{CH}_2\text{O})_4\text{Si}$	208.33		0.934 ²⁰ ₄	1.383 ²⁰	−77	165.8	46	d aq; s alc
t48	Tetraethylammonium bromide	$(\text{CH}_3\text{CH}_2)_4\text{N}^+\text{Br}^-$	210.16	4, 104	1.397 ²⁰ ₄		287 d			v s aq, alc, acet, chl
t49	Tetraethylammonium chloride	$(\text{CH}_3\text{CH}_2)_4\text{N}^+\text{Cl}^-$	165.71	4, 104	1.0801 ²¹ ₄		37.5			141 aq; s alc; 8.2 chl
t50	Tetraethylammonium hydroxide	$(\text{CH}_3\text{CH}_2)_4\text{N}^+\text{OH}^-$	147.26	4, 103						misc aq
t51	Tetraethylene glycol	$(\text{HOCH}_2\text{CH}_2\text{OCH}_2-\text{CH}_2)_2\text{O}$	194.23	1, 468	1.125 ²⁰ ₂₀	1.4590 ²⁰	−6	307.8	176	misc aq, alc, bz, eth
t52	Tetraethylene glycol dimethacrylate	$[\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COOCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2]_2\text{O}$	330.37		1.08			220 ^{1mm}	62	
t53	Tetraethylene glycol monomethyl ether	$\text{CH}_3\text{O}(\text{CH}_2\text{CH}_2\text{O})_3\text{CH}_2\text{CH}_2\text{OH}$	208.26		0.987	1.4453 ²⁰		166 ^{11mm}	>112	

Tetraethyl orthosilicate, t47

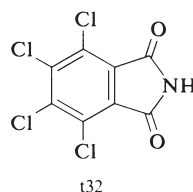
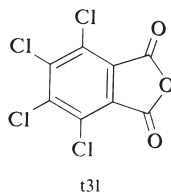


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t54	Tetraethylenepent-amine	$(\text{H}_2\text{NCH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2)_2\text{NH}$	189.31		0.999 ²⁰ ₂₀	1.5055 ²⁰	−40	340	185	misc aq, alc, eth
t55	<i>N,N,N',N'</i> -Tetraethylethylene-diamine	$(\text{C}_2\text{H}_5)_2\text{NCH}_2\text{CH}_2\text{N}(\text{C}_2\text{H}_5)_2$	172.32	4, 251	0.808	1.4343 ²⁰		189–192	58	
t56	Tetraethylgermanium	$(\text{C}_2\text{H}_5)_4\text{Ge}$	188.84	4, 631	1.1989		−90	165.5		s alc, eth; i aq
t57	Tetraethyllead	$(\text{C}_2\text{H}_5)_4\text{Pb}$	323.45	4, 639	1.653 ²⁰ ₄	1.5198 ²⁰	−136	152 ^{291mm}		s bz; misc eth
t58	Tetraethylpyrophosphate	$[(\text{C}_2\text{H}_5\text{O})_2\text{P}(\text{O})]_2\text{O}$	290.20		1.185 ²⁰ ₄	1.4196 ²⁰	d 170			d aq; misc alc, bz, chl
t59	Tetraethylpyrophosphate	$[(\text{C}_2\text{H}_5\text{O})_2\text{P}]_2\text{O}$	258.19		1.057	1.4341 ²⁰		81 ^{1mm}	>112	
t60	Tetraethylsilane	$(\text{C}_2\text{H}_5)_4\text{Si}$	144.34	4 ² , 1007	0.762 ²⁰ ₄	1.4246 ²⁰		153–155		i aq
t61	Tetraethylthiuram disulfide	$[(\text{C}_2\text{H}_5)_2\text{NC}(=\text{S})\text{S}—]_2$	296.54	4, 122	1.30		70			3.8 alc; 7.1 eth; s bz, acet, chl; 0.02 aq
t62	Tetraethyltin	$(\text{C}_2\text{H}_5)_4\text{Sn}$	234.94	4, 632	1.199 ²⁰ ₄		−112	181		i aq; s eth
t63	Tetrafluoroethylene	$\text{F}_2\text{C}=\text{CF}_2$	100.02	1 ³ , 638	1.1507 ^{−40}		−131.2	−75.6		i aq
t64	2,2,3,3-Tetrafluoro-1-propanol	$\text{HCF}_2\text{CF}_2\text{CH}_2\text{OH}$	132.06		1.4853 ²⁰ ₄	1.3197 ²⁰	−15	109–110	49	
t65	1,2,3,6-Tetrahydrobenzaldehyde	$\text{C}_6\text{H}_9\text{CHO}$	110.16	7 ¹ , 48	0.940	1.4745 ²⁰		163–164	57	
t66	Tetrahydrofuran		72.11	17, 10	0.8892 ²⁰ ₄	1.4072 ²⁰	−108.5	66	−17	misc aq, alc eth, PE
t67	2,5-Tetrahydrofuran-dimethanol		132.16		1.1542 ²⁵ ₄	1.4766 ²⁵	<−50	265		misc aq, alc, bz, chl; s eth
t68	Tetrahydro-2-furan-methanol		102.13	17 ² , 106	1.0524 ²⁰	1.4520 ²⁰	<−80	178	83	misc aq, alc, bz, chl, eth, acet
t69	Tetrahydro-2-furan-methylamine		101.15	18 ² , 415	0.980	1.4560 ²⁰		154 ^{744mm}	45	

t70	2-(Tetrahydrofuryl-oxy)tetrahydropyran		186.25		1.030	1.4606 ²⁰			97	
t71	1,2,3,4-Tetrahydroisoquinoline		133.19	20, 275	1.064	1.5668 ²⁰	-30	232-233	98	
t72	Tetrahydrolinalool	(CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ -C(CH ₃)(OH)CH ₂ CH ₃	158.28		0.925 ²⁵	1.433 ²⁰				
t73	1,2,3,4-Tetrahydronaphthalene	C ₁₀ H ₁₂	132.21	5, 491	0.9702 ²⁰	1.5414 ²⁰	-35.8	207.6	77	misc alc, bz, chl, eth, acet, PE
t74	cis-1,2,3,6-Tetrahydrophthalic anhydride		152.15	17, 462			101-102			
t75	cis-1,2,3,6-Tetrahydrophthalimide		151.17				134-138			
t76	Tetrahydropyran		86.14		0.8814 ²⁰	1.4211 ²⁰	-45	88	-20	misc aq, alc, eth
t77	Tetrahydropyran-2-methanol		116.16		1.0254 ²⁰	1.4580 ²⁰	-70 glass	187	93	misc aq, alc, bz, eth

Tetraglyme, b190

1,2,3,4-Tetrahydrobenzene, c330

Tetrahydrodicyclopentadiene, t253

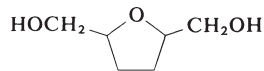
Tetrahydro-2,5-dimethoxyfuran, d457

Tetrahydrofurfurylamine, t69

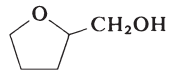
Tetrahydrofurfuryl alcohol, t68



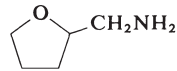
t66



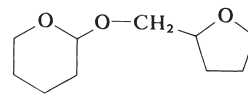
t67



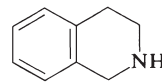
t68



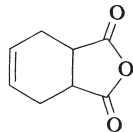
t69



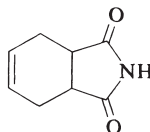
t70



t71



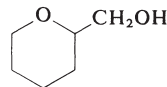
t74



t75



t76



t77

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

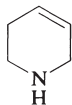
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t78	1,2,3,6-Tetrahydro-pyridine		83.13	20 ³ , 1912	0.911	1.4800 ²⁰	−48	108	16	
t79	3,4,5,6-Tetrahydro-pyrimidinethiol		116.19	24, 5			210–212			
t80	1,2,3,4-Tetrahydro-quinoline		133.19	20, 262	1.061	1.5924	15–16	249	100	s aq; misc alc, eth
t81	Tetrahydrothiophene		88.17	17 ¹ , 5	0.9987 ²⁰	1.5048 ²⁰	−96.2	120.9	12	misc alc, eth; i aq
t82	1,4,9,10-Tetra-hydroxyanthracene		242.23	8, 431			147–149			
t83	2,2',4,4'-Tetra-hydroxybenzo-phenone	$[(\text{HO})_2\text{C}_6\text{H}_3]_2\text{C}=\text{O}$	246.22	8, 496			200–203			
t84	Tetrahydroxyhexane-dioic acid	$\text{HOOC}[\text{CH}(\text{OH})]_4\text{COOH}$	210.14	3, 581			230 d			0.003 aq; s alk
t85	Tetrakis(2-ethyl-butoxy)silane	$[\text{CH}_3\text{CH}_2\text{CH}(\text{C}_2\text{H}_5)\text{-CH}_2\text{O}]_4\text{Si}$	432.8		0.892 ₄ ²⁰	1.430 ²⁰		171 ^{2mm}		
t86	Tetrakis(2-ethyl-hexoxy)silane	$[\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)\text{-CH}_2\text{O}]_4\text{Si}$	549.95		0.880 ₄ ²⁰	1.4388 ²⁰		194 ^{1mm}	190	
t87	<i>N,N,N',N'</i> -Tetrakis(p-hydroxy-propyl)ethylene diamine	$\{[\text{CH}_3\text{CH}(\text{OH})\text{CH}_2]_2\text{-NCH}_2\text{-}\}_2$	292.42	4 ⁴ , 1685	1.013	1.4812 ²⁰		175–181 ^{0.8mm}		
t88	Tetrakis(isopropoxy)silane	$[(\text{CH}_3)_2\text{CHO}]_4\text{Si}$	264.4		0.877 ₄ ²⁰	1.385 ²⁰		64 ^{5mm}		
t89	Tetrakis(2-methoxy-ethoxy)silane	$(\text{CH}_3\text{OCH}_2\text{CH}_2\text{O})_4\text{Si}$	328.4		1.079 ₄ ²⁰	1.422 ²⁰		182 ^{10mm}		
t90	Tetrakis(trimethyl-siloxy)titanium	$[(\text{CH}_3)_3\text{SiO}]_4\text{Ti}$	404.7		0.900 ₄ ²⁰	1.427 ²⁰		110 ^{10mm}		

t91	1,1,3,3-Tetramethoxy-propane	$[(\text{CH}_3\text{O})_2\text{CH}]_2\text{CH}_2$	164.20		0.997	1.4081 ²⁰		183	54	
t92	Tetramethoxysilane	$(\text{CH}_3\text{O})_4\text{Si}$	152.2	1, 287	1.052 ₄ ²⁰	1.368 ²⁰		121–122	20	
t93	Tetramethyl-ammonium bromide	$(\text{CH}_3)_4\text{N}^+\text{Br}^-$	154.06	4, 51	1.56		d > 230	subl > 360		55 aq
t94	Tetramethyl-ammonium chloride	$(\text{CH}_3)_4\text{N}^+\text{Cl}^-$	109.60	4, 51	1.169 ₄ ²⁰		d > 230	subl > 300		s aq, hot alc
t95	Tetramethyl-ammonium iodide	$(\text{CH}_3)_4\text{N}^+\text{I}^-$	201.06		1.829		d 230			sl s aq; v s abs alc
t96	<i>N,N</i> ,3,5-Tetramethylaniline	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{N}(\text{CH}_3)_2$	149.24	12, 1131	0.913	1.5443 ²⁰		226–228	90	
t97	1,2,3,4-Tetramethylbenzene	$\text{C}_6\text{H}_2(\text{CH}_3)_4$	134.22	5, 430	0.905 ₄ ²⁰	1.5187 ²⁰	–6.2	205.0	68	misc alc, eth
t98	1,2,3,5-Tetramethylbenzene	$\text{C}_6\text{H}_2(\text{CH}_3)_4$	134.22	5, 430	0.8906 ₄ ²⁰	1.5134 ²⁰	–23.7	198.0	63	s alc; v s eth
t99	1,2,4,5-Tetramethylbenzene	$\text{C}_6\text{H}_2(\text{CH}_3)_4$	134.22	5, 431	0.838 ₄ ⁸¹		79.2	196.8	73	v s alc, bz, eth

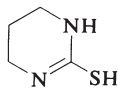
6,7,8,9-Tetrahydro-5*H*-tetrazoloazepine, p26
Tetrahydrothiophene 1,1-dioxide, t106
Tetrahydrothiophene oxide, t107

Tetrahydroxyadipic acid, t84
Tetralin, t73
β-Tetralonehydantoin, b40

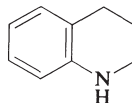
N,N,N',N'-Tetramethyldiaminomethane, t113
N,N,N',N'-Tetramethyl-1,3-diamino-2-propanol, b173



t78



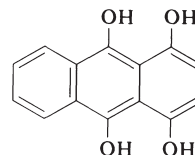
t79



t80



t81



t82

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

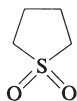
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t100	2,2,3,3-Tetramethylbutane	$(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3$	114.23	1, 165	0.656^{-120}		-120.7	106.5	< 1	
t101	<i>N,N,N',N'</i> -Tetramethyl-1,4-butane-diamine	$(\text{CH}_3)_2\text{N}(\text{CH}_2)_4\text{N}(\text{CH}_3)_2$	144.26	4, 265	0.786^{20}	1.4280^{20}		169	46	s aq, alc, eth
t102	1,1,3,3-Tetramethylbutylamine	$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)_2\text{NH}_2$	129.25	4, 198	0.805	1.4240^{20}		137–143	32	s alc, eth, PE; i aq
t103	1,3,5,7-Tetramethylcyclotetrasiloxane	$[\text{—SiH}(\text{CH}_3)\text{O—}]_4$	240.5		0.9912_4^{20}	1.3870^{20}	-69	134–135		
t104	1,1,4,4-Tetramethyl-1,4-dichlorodisilyl-ethylene	$[(\text{CH}_3)_2\text{Si}(\text{Cl})\text{CH}_2\text{—}]_2$	215.3				37	$198^{734\text{mm}}$	68	
t105	Tetramethyldisiloxane	$[(\text{CH}_3)_2\text{SiH}]_2\text{O}$	134.3		0.757_4^{20}	1.370^{20}		$71^{731\text{mm}}$		
t106	Tetramethylene sulfone		120.71	17 ¹ , 5	1.2614_4^{30}	1.4820^{30}	27.6	285	165	misc aq, acet, bz
t107	Tetramethylene sulfoxide		104.17		1.158	1.5200^{20}			> 112	
t108	<i>N,N,N',N'</i> -Tetramethylethylene diamine	$(\text{CH}_3)_2\text{NCH}_2\text{CH}_2\text{N}(\text{CH}_3)_2$	116.21	4, 250	0.770	1.4179^{20}	-55	120–122	10	
t109	Tetramethyl-germanium	$(\text{CH}_3)_4\text{Ge}$	132.73		1.006^0	1.3871^{20}	-88	43.4		
t110	1,1,3,3-Tetramethylguanidine	$[(\text{CH}_3)_2\text{N}]_2\text{C}=\text{NH}$	115.18					163		
t111	<i>N,N,N',N'</i> -Tetramethyl-1,6-hexane-diamine	$[(\text{CH}_3)_2\text{N}(\text{CH}_2)_3\text{—}]_2$	172.32	4 ¹ , 423	0.806	1.4359^{20}		209–210	73	
t112	Tetramethyllead	$(\text{CH}_3)_4\text{Pb}$	267.33	4, 639	1.995_4^{20}		-27.5	110		misc alc, eth

t113	<i>N,N,N',N'</i> -Tetra- methyl- methanediamine	$(\text{CH}_3)_2\text{NCH}_2\text{N}(\text{CH}_3)_2$	102.18	4, 54	0.749 ²⁰	1.4005		85	< 1	
t114	Tetramethyl ortho- carbonate	$\text{C}(\text{OCH}_3)_4$	136.15	3 ² , 4	1.023	1.3845 ²⁰	−5	114	6	
t115	2,6,10,14-Tetra- methylpentadecane	$[(\text{CH}_3)_2\text{CH}(\text{CH}_2)_3\text{-CH}(\text{CH}_3)\text{CH}_2]_2\text{CH}_2$	268.53		0.7827 ²⁰ ₄	1.4379 ²⁰	−100	167 ^{11mm}		s bz, chl, eth, PE
t116	2,3,5,6-Tetramethyl- phenol	$(\text{CH}_3)_4\text{C}_6\text{HOH}$	150.22	6, 547			108–110	250		
t117	2,2,6,6-Tetramethyl- piperidino-N-oxy- (free radical)		156.25				36–38		67	
t118	<i>N,N,N',N'</i> -Tetra- methyl-1,3-propane- diamine	$(\text{CH}_3)_2\text{N}(\text{CH}_2)_3\text{N}(\text{CH}_3)_2$	130.24	4, 262		1.4234 ²⁰		145–146	31	
t119	Tetramethylpyrazine		136.20	23, 99			84–86	190		
t120	Tetramethylsilane	$(\text{CH}_3)_4\text{Si}$	88.23	4, 625	0.6411 ²⁰ ₄	1.3585 ²⁰	−99.5	26.5	−27	v s alc, eth
t121	1,2,2,3-Tetramethyl- 1,1,3,3-tetra- phenyltrisiloxane	$[(\text{C}_6\text{H}_5)_2\text{Si}(\text{CH}_3)\text{O}]_2\text{-Si}(\text{CH}_3)_2$	484.8		1.07 ²⁰ ₄	1.551 ²⁵		235 ^{0.5mm}	221	

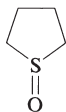
2,2,5,5-Tetramethyl-3,4-dithiahexane, d114
Tetramethylene chlorobromide, b251
Tetramethylethylene glycol, d491

Tetramethylene oxide, t66
Tetramethylene sulfide, t81
Tetramethylolmethane, p20

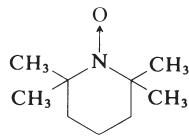
2,2,4,4-Tetramethyl-3-thiapentane, d133
Tetramethylthiuram disulfide, b174



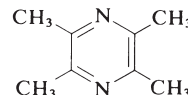
t106



t107



t117



t119

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t122	1,1,3,3-Tetramethyl-2-thiourea	$(\text{CH}_3)_2\text{NC}(=\text{S})\text{N}(\text{CH}_3)_2$	132.23	4 ¹ , 336			75–77	245		
t123	Tetramethyltin	$(\text{CH}_3)_4\text{Sn}$	178.83	4, 631	1.3149 ²⁵	1.5201	–54.8	78		
t124	1,1,3,3-Tetramethylurea	$(\text{CH}_3)_2\text{NC}(=\text{O})\text{N}(\text{CH}_3)_2$	116.16	4, 74	0.9687 ²⁰ ₄	1.4493 ²⁵	–1.2	176	65	misc aq, alc, chl, eth
t124a	Tetranitromethane	$\text{C}(\text{NO}_2)_4$	196.03	1, 80	1.6229 ²⁵ ₄	1.4358 ²⁵	13.5	126	> 112	v s alc, eth, alk
t125	1,4,7,10-Tetraoxa-cyclododecane		176.21		1.089	1.4621 ²⁰	16		> 112	
t126	2,4,8,10-Tetraoxa-spiro[5.5]undecane		160.17	19, 436			52–55	83 ^{1.5mm}		
t127	Tetraphenoxysilane	$(\text{C}_6\text{H}_5\text{O})_4\text{Si}$	400.5		1.141 ⁶⁰ ₄	1.554 ⁶⁰	48–49	237 ^{1mm}		
t128	Tetraphenylboron sodium	$(\text{C}_6\text{H}_5)_4\text{B}^-\text{Na}^+$	342.23				> 300			v s aq, acet; s chl
t129	1,1,4,4-Tetraphenyl-1,3-butadiene	$(\text{C}_6\text{H}_5)_2\text{C}=\text{CHCH}=\text{C}-(\text{C}_6\text{H}_5)_2$	358.49	5, 750			207–209			
t130	1,1,3,3-Tetraphenyl-1,3-dimethyldisiloxane	$[(\text{C}_6\text{H}_5)_2\text{Si}(\text{CH}_3)]_2\text{O}$	410.7		1.076 ²⁵ ₄	1.5866 ²⁶	50	215 ^{0.5mm}	193	
t131	Tetraphenylethylene	$(\text{C}_6\text{H}_5)_2\text{C}=\text{C}(\text{C}_6\text{H}_5)_2$	332.45	5, 743			222–224	420		
t132	Tetraphenylsilane	$(\text{C}_6\text{H}_5)_4\text{Si}$	336.5		1.078 ²⁰ ₄		236–237	228 ^{3mm}		
t133	Tetraphenyltin	$(\text{C}_6\text{H}_5)_4\text{Sn}$	427.11		1.490 ⁰		226	> 420	110	
t134	Tetrapropoxysilane	$(\text{C}_3\text{H}_7\text{O})_4\text{Si}$	264.4		0.916 ²⁰ ₄	1.401 ²⁰		94 ^{5mm}		
t135	Tetrapropylammonium bromide	$(\text{CH}_3\text{CH}_2\text{CH}_2)_4\text{N}^+\text{Br}^-$	266.27	4 ¹ , 364			270 d			s aq
t136	1 <i>H</i> -Tetrazole		70.06	26, 346			156–158	subl		s aq, alc, acet
t137	2-Thenoyltrifluoroacetone		222.18				40–44	98 ^{8mm}		

t138	Theobromine		180.17	26, 457			357	subl 290		0.05 aq; 0.045 alc; s alk; i bz, chl, eth
t139	Thiamine HCl		337.27				d 248			100 aq; 1 alc
t140	Thiazole		85.13	27, 15	1.200 ¹⁷	1.5375 ²⁰		117–118	22	s alc, eth; sl s aq
t141	Thioacetamide	$\text{CH}_3\text{C}(=\text{S})\text{NH}_2$	75.13	2, 232			112–114			16 aq; sl s alc, eth
t142	Thioacetic acid	$\text{CH}_3\text{O}-\text{SH}$	76.12	2, 230	1.065	1.4630 ²⁰	< -17	88–91	< 1	s aq; misc alc, eth
t143	Thiobenzoic acid	$\text{C}_6\text{H}_5\text{CO}-\text{SH}$	138.19	9, 419	1.174	1.6020 ²⁰	15–18	d	> 112	misc eth; v s alc; i aq

Tetrantoin, b40

2,5,8,13-Tetraoxadodecane, b189

3,6,9,12-Tetraoxatridecanol, t53

Tetraphene, b6

2-Thenoic acid, t157

2-Thiabutane, e182

Thiacyclobutane, t345a

1-Thia-3-cyclopentene, 1,1-dioxide, d368

3-Thiaheptane, b451

2-Thiahexane, b463

3-Thiahexane, e210

Thianaphthene, b61

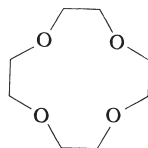
5-Thianonane, d132

2-Thiapentane, m395

3-Thiapentane, d337

Thioanisole, m364

2-Thiobarbituric acid, d388



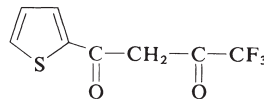
t125



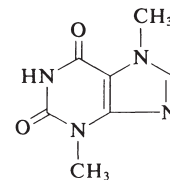
t126



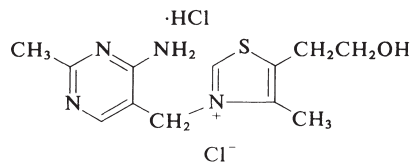
t136



t137



t138



t139



t140

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t144	4,4'-Thiobis(2- <i>tert</i> -butyl-6-methylphenol)		358.54				127	316 ^{40mm}	240	
t145	4,4'-Thiobis(1,3-dihydroxybenzene)	$[(\text{HO})_2\text{C}_6\text{H}_3]_2\text{S}$	250.27	6 ³ , 6291			175–177			
t146	Thiocarbanilide	$\text{C}_6\text{H}_5\text{NHCSNHC}_6\text{H}_5$	228.32	12, 394	1.32 ²⁴		154			v s alc, eth
t147	<i>p</i> -Thiocresol	$\text{HSC}_6\text{H}_4\text{CH}_3$	124.21	6, 416			43–44	195	68	s alc, eth; i aq
t148	2,2'-Thiodiacetic acid	$(\text{HOOCCH}_2)_2\text{S}$	150.15	3, 253			129			s aq, alc
t149	2,2'-Thiodiethanol	$(\text{HOCH}_2\text{CH}_2)_2\text{S}$	122.19	1, 470	1.1824 ²⁰ ₄	1.5203 ²⁰	–16	282	110	misc aq, alc; sl s eth
t150	4,4'-Thiodiphenol	$(\text{HOC}_6\text{H}_4)_2\text{S}$	218.27	6, 860			150–155			
t151	3,3'-Thiodipropionic acid	$(\text{HOOCCH}_2\text{CH}_2)_2\text{S}$	178.21				134			3.4 aq; v s alc
t152	2-Thiohydantoin		116.14	24, 260			231 d			sl s aq; i alc, eth
t153	<i>N</i> -Thionylaniline	$\text{C}_6\text{H}_5\text{N}=\text{SO}$	139.18	12, 578	1.236	1.6270 ²⁰		200		
t154	Thiophene	$\text{C}_4\text{H}_4\text{S}$	84.14	17, 29	1.0573 ²⁵ ₄	1.5257 ²⁵	–38.2	84.2	–1	misc alc, eth; i aq
t155	2-Thiopheneacetic acid	$(\text{C}_4\text{H}_3\text{S})\text{CH}_2\text{COOH}$	142.18	18, 293			63–67	160 ^{22mm}		
t156	2-Thiophenecarbaldehyde	$(\text{C}_4\text{H}_3\text{S})\text{CHO}$	112.15	17, 285	1.200	1.5900 ²⁰		198	77	s eth
t157	2-Thiophenecarboxylic acid	$(\text{C}_4\text{H}_3\text{S})\text{COOH}$	128.15	18, 289			128.5	260		s aq, chl; v s alc, eth
t158	2-Thiophenemethylamine	$(\text{C}_4\text{H}_3\text{S})\text{CH}_2\text{NH}_2$	113.19	18 ⁴ , 7096	1.103	1.5569 ²⁰		99 ^{28mm}	73	
t159	Thiophenol	$\text{C}_6\text{H}_5\text{SH}$	110.18	6, 294	1.0766 ²⁰	1.5897 ²⁰	–14.9	169.1	50	v s alc; misc bz, eth
t160	Thiophenoxyacetic acid	$\text{C}_6\text{H}_5\text{SCH}_2\text{COOH}$	168.21	6, 313			64–66			

t161	Thiopropionic acid	$\text{CH}_3\text{CH}_2\text{CO}-\text{SH}$	90.14	2, 264	1.014	1.4640 ²⁰				
t162	3-Thiosemicarbazide	$\text{H}_2\text{NC}(=\text{S})\text{NHNH}_2$	91.14	3, 195			182–184			s aq, alc
t163	Thiourea	$\text{H}_2\text{NC}(=\text{S})\text{NH}_2$	76.12	3, 180	1.045		176–178			9 aq; s alc; sl s eth
t164	1,4-Thioxane		104.17	19, 3	1.114	1.5095 ²⁰		147	42	
t165	Thioxanthen-9-one		212.27	17, 357			211	273 ^{715mm}		v s bz, chl, hot HOAc
t166	Titanium(IV) isopropoxide	$\text{Ti}[\text{OCH}(\text{CH}_3)_2]_4$	284.26	1 ² , 382	0.955	1.4654 ²⁰	18–20	218 ^{10mm}	22	
t167	Toluene	$\text{C}_6\text{H}_5\text{CH}_3$	92.14	5, 280	0.8660 ²⁰	1.4969 ²⁰	–95.0	110.6	7	misc alc, chl, eth, acet, HOAc
t168	2,4-Toluenediamine	$\text{CH}_3\text{C}_6\text{H}_3(\text{NH}_2)_2$	122.17	13, 124			97–99	283.5		s hot aq, alc, eth
t169	2,5-Toluenediamine	$\text{CH}_3\text{C}_6\text{H}_3(\text{NH}_2)_2$	122.17	13, 144			64	273–274		v s aq, alc, eth
t170	2,6-Toluenediamine	$\text{CH}_3\text{C}_6\text{H}_3(\text{NH}_2)_2$	122.17	13, 148			104–106			s aq, alc
t171	3,4-Toluenediamine	$\text{CH}_3\text{C}_6\text{H}_3(\text{NH}_2)_2$	122.17	13, 148			88–90	156 ^{18mm}		v s aq
t172	Toluene-2,4-diisocyanate	$\text{CH}_3\text{C}_6\text{H}_3(\text{NCO})_2$	174.16	13, 138	1.2244 ²⁰	1.5689 ²⁰	20–21	251	121	d aq, alc; misc bz, acet, eth

Thiocarbanilide, d692
 2,2'-Thiodiethanethiol, b187
 Thiodiethylene glycol, t149
 Thiodiglycol, t149
 Thiodiglycolic acid, t148
 Thioethanolamine, a162
 1-Thioglycerol, m20
 Thioglycolic acid, m14

Thiolactic acid, m21
 Thiomalic acid, m23
 4,4'-Thioresorcinol, t145
 Thiosalicylic acid, m16
 Thiosinamine, a101
 2-Thioxo-4-thiazolidinone, r3
 Threonine, a187
 Tiglic acid, m161

Tioxolone, h104
 TMS, t120
 TMSDEA, t371
 TMSI, t373
 Tolazoline, b102
p-Tolualdehyde, m126
 Tolueneethiols, p128, t147

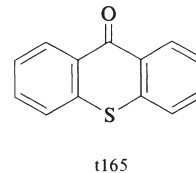
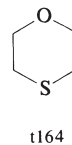
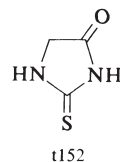
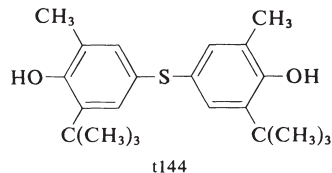


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t173	<i>p</i> -Toluenesulfinic acid	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{H}$	172.20	11, 9			85			v s alc, eth
t174	<i>p</i> -Toluenesulfonamide	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{NH}_2$	171.22	11, 104			137–140			0.2 aq; 3.6 alc
t175	<i>p</i> -Toluenesulfonylhydrazide	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{NHNH}_2$	186.23	11 ² , 66			110 d			
t176	<i>p</i> -Toluenesulfonic acid	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_3\text{H}$	172.20	11, 97				140 ^{20mm}		67 aq; s alc, eth
t177	<i>p</i> -Toluenesulfonyl chloride	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{Cl}$	190.65	11, 103			69–71	134 ^{10mm}		v s alc, bz, eth; i aq
t178	<i>p</i> -Toluenesulfonyl fluoride	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{F}$	174.19	11 ² , 54			41–42	112 ^{16mm}		
t179	<i>p</i> -Toluenesulfonyl isocyanate	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{NCO}$	197.21			1.4355 ²⁰		144 ^{10mm}		
t180	<i>o</i> -Toluidine	$\text{CH}_3\text{C}_6\text{H}_4\text{NH}_2$	107.16	12, 772	0.9984 ²⁰	1.5725 ²⁰	–16.1	200.4	85	1.7 aq; s alc, eth
t181	<i>m</i> -Toluidine	$\text{CH}_3\text{C}_6\text{H}_4\text{NH}_2$	107.16	12, 853	0.989 ²⁰ ₄	1.5681 ²⁰	–30.4	203.4	85	misc alc, eth
t182	<i>p</i> -Toluidine	$\text{CH}_3\text{C}_6\text{H}_4\text{NH}_2$	107.16	12, 880	1.046 ²⁰ ₄	1.5532 ⁵⁹	43.8	200.6	88	7.4 aq; v s alc, eth
t183	1-(<i>o</i> -Toluidino)-1,3-butanedione	$\text{CH}_3\text{C}_6\text{H}_4\text{NHCOCCH}_3$	191.23	12, 823			104–106	143		
t184	<i>o</i> -Tolunitrile	$\text{CH}_3\text{C}_6\text{H}_4\text{CN}$	117.15	9, 466	0.9955 ²⁰ ₄	1.5279 ²⁰	–13	205.2	84	i aq; misc alc, eth
t185	<i>m</i> -Tolunitrile	$\text{CH}_3\text{C}_6\text{H}_4\text{CN}$	117.15	9, 477	0.976 ¹⁵	1.5256 ²⁰	–23	210	86	0.09 aq; v s alc, eth
t186	<i>p</i> -Tolunitrile	$\text{CH}_3\text{C}_6\text{H}_4\text{CN}$	117.15	9, 489	0.9785 ³⁰ ₄		29.5	217.6		i aq; v s alc, eth
t187	<i>o</i> -Toluoyl chloride	$\text{CH}_3\text{C}_6\text{H}_4\text{COCl}$	154.60	9, 464	1.185	1.5549 ²⁰		90 ^{12mm}	76	
t188	<i>m</i> -Toluoyl chloride	$\text{CH}_3\text{C}_6\text{H}_4\text{COCl}$	154.60	9, 477	1.173	1.5485 ²⁰		86 ^{5mm}	76	
t189	<i>p</i> -Toluoyl chloride	$\text{CH}_3\text{C}_6\text{H}_4\text{COCl}$	154.60	9, 484	1.169	1.5535 ²⁰	–2	225–257	82	
t190	<i>m</i> -Tolyl isocyanate	$\text{CH}_3\text{C}_6\text{H}_4\text{NCO}$	133.15	12, 864	1.033	1.5305 ²⁰		76 ^{12mm}	65	s alc, eth; i aq
t191	(<i>p</i> -Tolylsulfonyl)-methyl isocyanide	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_2\text{CH}_2\text{NC}$	195.24				114–115			
t192	<i>p</i> -Tolyltrichlorosilane	$\text{CH}_3\text{C}_6\text{H}_4\text{SiCl}_3$	225.6		1.3 ²⁰ ₄			218–220		

t193	1,2,4-Triacetoxy-benzene	$C_6H_3(OOCCH_3)_3$	252.22	6, 1089			98–100		
t194	Triacetoxyethylsilane	$C_2H_5Si(OOCCH_3)_3$	234.3		1.1428 ²⁰ ₄	1.4123 ²⁰		107–108 ^{8mm}	
t195	Triacetoxyvinylsilane	$(CH_3COO)_3SiCH=CH_2$	232.3		1.167 ²⁰ ₄	1.423 ²⁰		113 ^{1mm}	104
t196	1,3,5-Triacetylbenzene	$C_6H_3(COCH_3)_3$	204.23	7, 866			160–162		17
t197	Triallyl-s-triazine-2,4,6(1H,3H,5H)-trione		249.27			1.5129 ²⁰		152 ^{4mm}	> 112
t198	2,4,6-Triamino-1,3,5-triazine		126.12	26, 245	1.573 ²⁵⁰		> 250	subl	sl s aq; i alc, eth
t199	1H-1,2,4-Triazole		69.07	26, 13			119–121	260 d	s aq, alc
t200	Tribenzylamine	$(C_6H_5CH_2)_3N$	287.41	12, 1038	0.991 ⁹⁵ ₄		91–94		s hot alc, eth
t201	Tribromoacetaldehyde	Br_3CCHO	280.76	1, 626	2.665	1.5850 ²⁰		174	s aq, alc, chl, eth
t202	Tribromoacetic acid	Br_3CCOOH	296.76	2, 220			130–133	245 d	s aq, alc, eth
t203	2,4,6-Tribromoaniline	$Br_3C_6H_2NH_2$	329.83	12, 663	2.35		120–122	300	s hot alc, chl, eth
t204	2,2,2-Tribromoethanol	Br_3CCH_2OH	282.77	1 ² , 338			80–81	93 ^{10mm}	2 aq; s alc, bz, eth
t205	1,1,2-Tribromoethylene	$BrCH=CBr_2$	264.74	1, 191	1.708 ²¹	1.6247 ²⁵		162.5	

Toluic acids, m130, m131, m132
 α -Tolunitrile, p80

p-Tolylacetamide, m355
Triacetin, p201

1,3,5-Triazine-2,4,6-triol, c299
Tributyl borate, t209

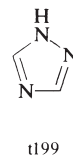
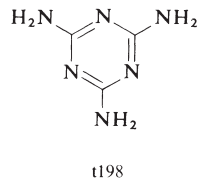
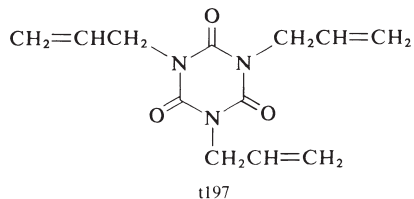


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t206	Tribromomethane	CHBr_3	252.77	1, 68	2.9031 ¹⁵	1.6005 ¹⁵	8.1	149.6	none	0.3 aq; misc eth, MeOH
t207	2,4,6-Tribromophenol	$\text{Br}_3\text{C}_6\text{H}_2\text{OH}$	330.82	6, 203	2.55		94–96	244		s alc, chl, eth; i aq
t208	1,2,3-Tribromopropane	$\text{BrCH}_2\text{CH}(\text{Br})\text{CH}_2\text{Br}$	280.78	1, 112	2.4114 ¹⁵		16–17	219–221		s alc, eth
t209	Tributoxyborane	$(\text{C}_4\text{H}_9\text{O})_3\text{B}$	230.16	1 ² , 398	0.8580 ²⁰	1.4092 ²⁰	–70	233.5	93	hyd aq
t210	Tributylamine	$(\text{C}_4\text{H}_9)_3\text{N}$	185.36	4, 157	0.7784 ²⁰	1.4283 ²⁰	–70	216–217	63	v s alc, eth; s acet
t211	2,4,6-Tri- <i>tert</i> -butylphenol	$[(\text{CH}_3)_3\text{C}]_3\text{C}_6\text{H}_2\text{OH}$	262.44		0.864 ²⁷		131	278		
t212	Tributyl phosphate	$(\text{C}_4\text{H}_9\text{O})_3\text{P}(\text{O})$	266.32	1 ² , 397	0.972 ²⁵	1.4226 ²⁵	< –80	289 d	146	0.04 aq; misc org solv
t213	Tributylphosphine	$(\text{C}_4\text{H}_9)_3\text{P}$	202.32	4 ² , 971	0.812	1.4619 ²⁰		150 ^{50 mm}	40	
t214	Tributyl phosphite	$(\text{C}_4\text{H}_9\text{O})_3\text{P}$	250.32	1 ¹ , 187	0.925 ²⁰	1.4326 ²⁰		125 ^{7 mm}	121	misc alc, bz, eth, PE
t215	Tributyltin chloride	$(\text{C}_4\text{H}_9)_3\text{SnCl}$	325.49		1.200	1.4905 ²⁰		173 ^{25 mm}	> 112	
t216	Trichloroacetic acid	Cl_3CCOOH	163.39	2, 206	1.629 ⁶¹		57–58	196–197		120 aq; v s alc, eth
t217	Trichloroacetonitrile	Cl_3CCN	144.39	2, 212	1.4403 ²⁵	1.4409 ²⁰		85.7	none	
t218	Trichloroacetyl chloride	Cl_3CCOCl	181.83	2, 210	1.629	1.4689 ²⁰		114–116	none	
t219	Trichloroacetyl isocyanate	$\text{Cl}_3\text{CC}(=\text{O})\text{NCO}$	188.40			1.4809 ²⁰		85 ^{20 mm}	65	
t220	2,4,5-Trichloroaniline	$\text{Cl}_3\text{C}_6\text{H}_2\text{NH}_2$	196.46	12, 627			93–95	270		s alc
t221	2,4,6-Trichloroaniline	$\text{Cl}_3\text{C}_6\text{H}_2\text{NH}_2$	196.46	12, 627			73–75	262		s alc, eth
t222	1,2,3-Trichlorobenzene	$\text{C}_6\text{H}_3\text{Cl}_3$	181.45	5, 203	1.69 ²⁵ ₂₅		52.6	221	113	v s bz, CS_2
t223	1,2,4-Trichlorobenzene	$\text{C}_6\text{H}_3\text{Cl}_3$	181.45	5, 204	1.446 ²⁵	1.5707 ²⁰	17	214	110	misc bz, eth, PE

t224	1,3,5-Trichloro- benzene	C ₆ H ₃ Cl ₃	181.45	5, 204		1.5662 ¹⁹	63.4	208.5	107	v s bz, eth, PE
t225	2,2,2-Trichloro-1,1- dimethylethyl chloroformate	ClCOOC(CH ₃) ₂ CCl ₃	239.92				30–32	83– 84 ^{14mm}	none	
t226	1,1,1-Trichloro- ethane	CH ₃ CCl ₃	133.41	1, 85	1.3376 ²⁰ ₄	1.4379 ²⁰	–30.4	74.0	none	0.13 aq; s bz, eth
t227	1,1,2-Trichloro- ethane	ClCH ₂ CHCl ₂	133.41	1, 85	1.4416 ²⁰ ₄	1.4711 ²⁰	–36.6	113.5	none	0.4 aq; misc alc, eth
t228	2,2,2-Trichloro- ethanol	Cl ₃ CCH ₂ OH	149.40	1, 338	1.557 ²⁰ ₂₀	1.4885 ²⁰	17.8	151		8 aq; misc alc, eth
t229	2,2,2-Trichloro- ethyl chloroformate	ClCOOCH ₂ CCl ₃	211.86		1.539	1.4703 ²⁰		171–172	none	
t230	1,1,2-Trichloro- ethylene	ClCH=CCl ₂	131.39	1, 187	1.4649 ²⁰ ₄	1.4775 ²⁰	–84.8	86.7	none	0.1 aq; misc alc, chl, eth
t231	Trichloroethylsilane	C ₂ H ₃ SiCl ₃	163.5		1.2373 ²⁰ ₄	1.4256 ²⁰	–106	100.5	27	
t232	Trichlorofluoro- methane	Cl ₃ CF	137.4		1.485 ²¹	1.384 ²⁰	–111	23.8		0.14 aq; s alc, eth
t233	α,α,2-Trichloro- 6-fluorotoluene	ClC ₆ H ₃ (F)CHCl ₂	213.47	5 ³ , 701	1.446	1.5506 ²⁰		228–230	> 112	
t234	Trichloroisocyanuric acid		232.41	25, 256			249–251			

Tributylin, g19

β,β,β-Trichloroethoxycarbonyl chloride, t229

Trichloromethane, c126

Trichlorophenylsilane, p155

3,3,3-Trichloropropylene oxide, e13

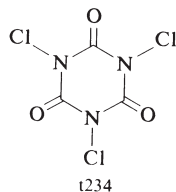


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

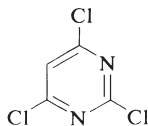
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t235	Trichloromethane-sulfonyl chloride	Cl_3CSCl	185.89	3, 135	1.700_4^{20}	1.5436^{20}		146–148	none	
t236	Trichloromethane sulfonyl chloride	$\text{Cl}_3\text{CSO}_2\text{Cl}$	217.88	3 ² , 16			139			s alc, eth
t237	1,1,1-Trichloro-2-methyl-2-propanol	$(\text{CH}_3)_2\text{C}(\text{OH})\text{CCl}_3$	177.46	1, 382			99	167		s alc, bz, chl, eth
t238	Trichloromethylsilane	CH_3SiCl_3	149.48		1.275_4^{20}	1.4108^{20}	−90	66	5	
t238a	1,2,4-Trichloro-5-nitrobenzene	$\text{Cl}_3\text{C}_6\text{H}_2\text{NO}_2$	226.45	5, 246	1.790^{20}		49–55	288		v s bz, eth
t239	Trichloronitromethane	Cl_3CNO_2	164.38	1, 76	1.6558_4^{20}	1.4611^{20}	−64	112		misc alc, bz; s eth
t240	2,4,5-Trichlorophenol	$\text{Cl}_3\text{C}_6\text{H}_2\text{OH}$	197.45	6 ² , 180			67	253		615 acet; 163 bz; 525 eth; s alc; i aq
t241	2,4,6-Trichlorophenol	$\text{Cl}_3\text{C}_6\text{H}_2\text{OH}$	197.45	6, 190	1.4901_4^{75}		69	246	none	525 acet; 113 bz; 354 eth; v s alc; i aq
t242	(2,4,5-Trichlorophenoxy)acetic acid	$\text{Cl}_3\text{C}_6\text{H}_2\text{OCH}_2\text{COOH}$	255.49	6 ³ , 702			153			s alc; v sl s aq
t243	2-(2,4,5-Trichlorophenoxy)propionic acid	$\text{Cl}_3\text{C}_6\text{H}_2\text{O}-\text{CH}(\text{CH}_3)\text{COOH}$	269.51				181.6			0.14 aq; 16 acet; 0.16 bz; 7.1 eth
t244	1,2,3-Trichloropropane	$\text{ClCH}_2\text{CH}(\text{Cl})\text{CH}_2\text{Cl}$	147.43	1, 106	1.3880^{20}	1.4834^{20}	−14.7	156.9	82	misc alc, eth; i aq
t245	1,1,1-Trichloro-2-propanol	$\text{CH}_3\text{CH}(\text{OH})\text{CCl}_3$	163.43	1, 365			50	162	82	2.9 aq; v s alc, eth

t246	2,4,6-Trichloro- pyrimidine		183.43	23, 90		1.5700 ²⁰	23–25	210–215	> 112	
t247	Trichlorosilane	HSiCl ₃	135.45		1.3417 ₄ ²⁰	1.400 ²⁰	–1.28	31–32	–20	d aq; s bz, chl
t248	α,α,α-Trichlorotoluene	C ₆ H ₃ CCl ₃	195.48	5, 300	1.3756 ₄ ²⁰	1.5570 ²⁰	–5.0	220.8	97	s alc, bz, eth
t249	α,2,6-Trichloro- toluene	Cl ₂ C ₆ H ₃ CH ₂ Cl	195.48				36–39	119 ^{14mm}		v s alc, eth
t250	2,4,6-Trichloro- 1,3,5-triazine		184.41	26, 35			148	190 ^{720mm}		i aq; s alc
t251	1,1,2-Trichloro- trifluoroethane	Cl ₂ CFCClF ₂	187.38	1 ³ , 157	1.5635 ²⁵	1.3557 ²⁵	–36.4	47.6	none	0.017 aq
t252	Trichlorovinyl- silane	H ₂ C=CHSiCl ₃	161.49		1.243 ₄ ²⁰	1.4300 ²⁰	–95	90–93	–9	
t253	Tricyclo[5.2.1.0 ^{2,6}]- decane		136.24	5, 164			77–79	193	40	
t254	Tricyclo[5.2.1.0 ^{2,6}]- decan-8-one		150.22	7 ² , 133	1.063	1.5025 ²⁰		132 ^{30mm}		
t255	1,3,5-Tricyclohexyl- hexahydro- <i>s</i> - triazine		333.57				74–75	97 ^{6mm}		

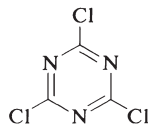
Tricine, t428

Tricyclo[3.3.1.1^{3,7}]decane, a67

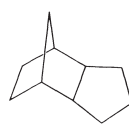
Tricyclo[5.2.1.0^{2,6}]decane-4,8-dimethanol, b185



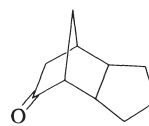
t246



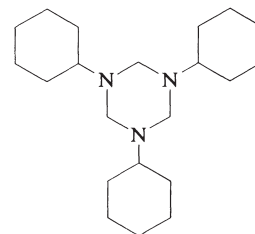
t250



t253



t254



t255

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

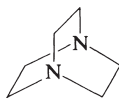
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t256	Tridecane	$\text{CH}_3(\text{CH}_2)_{11}\text{CH}_3$	184.37	1, 171	0.7563^{20}_4	1.4256^{20}	−5.4	235.4	79	v s alc, eth
t257	Tridecanoic acid	$\text{CH}_3(\text{CH}_2)_{11}\text{COOH}$	214.35	2, 364			41–42	$236^{100\text{mm}}$		v s alc, eth; i aq
t258	1-Tridecene	$\text{CH}_3(\text{CH}_2)_{10}\text{CH}=\text{CH}_2$	182.35	1, 225	0.7653^{20}	1.4334^{20}	−23.1	232.8	79	s alc; v s eth
t259	Triethanolamine	$(\text{HOCH}_2\text{CH}_2)_3\text{N}$	149.19	4, 285	1.1242^{20}_4	1.4835^{25}	21.6	335.4	185	misc aq, alc, acet; 4.5 bz; 1.6 eth; s chl
t260	Triethoxyborane	$(\text{CH}_3\text{CH}_2\text{O})_3\text{B}$	145.99	1, 335	0.864^{20}_{20}	1.3740^{20}		117–118	11	d aq
t261	Triethoxyethylsilane	$(\text{C}_2\text{H}_5\text{O})_3\text{SiC}_2\text{H}_5$	192.3		0.8963^{20}_4	1.3955^{20}		158–159		
t261a	Triethoxymethylsilane	$\text{CH}_3\text{Si}(\text{OC}_2\text{H}_5)_3$	178.30	4, 629	0.895^{20}_4	1.3845^{20}		141–143	23	s alc
t261b	Triethoxysilane	$(\text{C}_2\text{H}_5\text{O})_3\text{SiH}$	164.28	1, 334	0.875^{20}_4	1.3762		131.5	26	
t262	Triethoxyvinylsilane	$(\text{C}_2\text{H}_5\text{O})_3\text{SiCH}=\text{CH}_2$	190.32		0.903^{20}_4	1.3978^{20}		160–161	34	
t263	Triethylaluminum	$(\text{C}_2\text{H}_5)_3\text{Al}$	114.17	4, 643	0.832 ²⁵		−58	194		d aq, air
t264	Triethylamine	$(\text{C}_2\text{H}_5)_3\text{N}$	101.19	4, 99	0.7326^{25}_4	1.3980^{25}	−114.7	89.6	−6	5.5 aq; misc alc, eth; s acet, EtAc
t265	Triethylantimony	$(\text{C}_2\text{H}_5)_3\text{Sb}$	208.94	4, 618	1.324^{16}	1.42	−29	159.5		
t266	Triethylarsine	$(\text{C}_2\text{H}_5)_3\text{As}$	162.11	4, 602	1.150^{20}_{20}			$140^{736\text{mm}}$		i aq; misc alc, eth
t267	Triethylbismuthine	$(\text{C}_2\text{H}_5)_3\text{Bi}$	296.17	4, 622	1.82			$107^{79\text{mm}}$		i aq; v s alc, eth
t268	Triethylborane	$(\text{C}_2\text{H}_5)_3\text{B}$	98.00	4, 641			explodes when heated in air −92.9	95		i aq; d air
t269	Triethylenediamine		112.18				158	174		45 aq; 13 acet; 77 alc; 51 bz
t270	Triethylene glycol	$(\text{HOCH}_2\text{CH}_2\text{OCH}_2\text{—})_2$	150.17	1, 468	1.1274^{15}_4	1.4578^{15}	−4.3	285	165	misc aq, alc, bz
t271	Triethylene glycol dibenzoate	$(\text{C}_6\text{H}_5\text{COOCH}_2\text{—})_2$ $\text{CH}_2\text{OCH}_2\text{—})_2$	358.39		1.2715^{30}	1.5252^{50}	47			
t272	Triethylenetetramine	$(\text{H}_2\text{NCH}_2\text{CH}_2\text{NHCH}_2\text{—})_2$	146.24	4, 255	0.982	1.4971^{20}	12	266–267	143	

t273	<i>N,N,N'</i> -Triethyl-ethylenediamine	(C ₂ H ₅) ₂ NCH ₂ CH ₂ -NHC ₂ H ₅	144.26	4 ² , 691	0.804	1.4311 ²⁰		55 ^{13mm}	32	
t274	Triethylgallium	(C ₂ H ₅) ₃ Ga	156.91		1.0576 ³⁰		−82.3	142.6		
t275	1,3,5-Triethylhexahydro- <i>s</i> -triazine		171.29	26, 2	0.894	1.4595 ²⁰		207–208		
t276	Triethylindium	(C ₂ H ₅) ₃ In	202.01		1.260 ²⁰	1.538 ²⁰	−32	144		
t277	Triethyl ortho-acetate	CH ₃ C(OC ₂ H ₅) ₃	162.23	2, 129	0.8847 ²⁵ ₄	1.3950 ²⁵		142	55	misc alc, chl, eth
t278	Triethyl ortho-formate	HC(OC ₂ H ₅) ₃	148.20	2, 20	0.891 ²⁰ ₄	1.3919 ²⁰	−76	146	30	d aq; s alc, eth
t279	Triethyl ortho-propionate	CH ₃ CH ₂ C(OC ₂ H ₅) ₃	176.26	2, 240	0.876	1.3995 ²⁰		155–160	60	v s alc, eth
t280	Triethyl phosphate	(C ₂ H ₅ O) ₃ P(O)	182.16	1, 332	1.0725 ¹⁹	1.4045 ²⁰		215–216		s aq(d), alc, eth
t281	Triethylphosphine	(C ₂ H ₅) ₃ P	118.16	4, 582	0.800 ¹⁵ ₄		−88	129	pyro-phoric	i aq; misc alc, eth
t282	Triethyl phosphite	(C ₂ H ₅ O) ₃ P	166.2	1, 330	0.969 ²⁰ ₄	1.4131 ²⁰		65 ^{24mm}	55	i aq(hyd); misc alc, acet, bz, eth, PE
t283	Triethyl phosphono-acetate	(CH ₃ CH ₂ O) ₂ P(O)-CH ₂ COOC ₂ H ₅	224.19	4 ¹ , 573	1.130	1.4310 ²⁰		145 ^{9mm}	> 112	

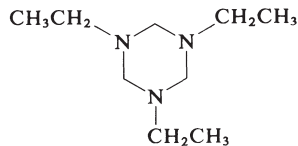
Tridecylbenzene, p156
 3-Triethoxysilylpropylamine, a279
 Triethyl borate, t260

Triethylenediamine, d45
 Triethylene glycol, e127
 Triethylene glycol dimethyl ether, b189

O,O,O-Triethyl phosphorothioate, t285



t269



t275

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t284	Triethylsilane	$(\text{C}_2\text{H}_5)_3\text{SiH}$	116.28	4, 625	0.731_4^{20}	1.412^{20}		107–108		i aq; misc alc, eth
t285	Triethyl thio-phosphate	$(\text{C}_2\text{H}_5\text{O})_3\text{P}(\text{S})$	198.22	1, 333	1.082	1.4480^{20}		$100^{16\text{mm}}$	107	
t286	2,2,2-Trifluoro-acetamide	CF_3CONH_2	113.04	2 ² , 186			75	162.5		
t287	Trifluoroacetic acid	CF_3COOH	114.02	2 ² , 186	1.4890^{20}	1.2850^{20}	−15.3	71.8		misc aq
t288	Trifluoroacetic anhydride	$[\text{CF}_3\text{C}(\text{O})]_2\text{O}$	210.03	2 ² , 186	1.487	> 1.30	−65	39		
t289	α,α,α -Trifluoro-acetophenone	$\text{C}_6\text{H}_5\text{COCF}_3$	174.12		1.240	1.4595^{20}		165–166	41	
t290	α,α,α -Trifluoro- <i>m</i> -cresol	$\text{CF}_3\text{C}_6\text{H}_4\text{OH}$	162.11	6 ¹ , 187	1.333	1.4588^{20}	−1.8	178–179	73	
t291	1,1,1-Trifluoroethane	CH_3CF_3	84.04				−111.3	−47.3		
t292	2,2,2-Trifluoro-ethanol	$\text{CF}_3\text{CH}_2\text{OH}$	100.04		1.3842_4^{20}	1.2907^{22}	−43.5	74.1	29	
t293	2,2,2-Trifluoro-ethyl acrylate	$\text{CF}_3\text{CH}_2\text{OOCCH}=\text{CH}_2$	154.0		2.142_4^{25}	1.3981^{25}		$46^{125\text{mm}}$		
t294	2,2,2-Trifluoro-ethyl trifluoro-acetate	$\text{CF}_3\text{CH}_2\text{OOC}(\text{CF}_3)_2$	196.0		1.4725_4^{18}	1.2812^{18}	−65.5	55		
t295	Trifluoromethane	HCF_3	70.01	1, 59	1.52^{-100}		−155.2	−82.2		75 mL aq; 500 mL alc
t296	Trifluoromethane-sulfonic acid	$\text{CF}_3\text{SO}_3\text{H}$	150.07	3 ³ , 34	1.695^{25}	1.3250^{25}	34	162	none	v s aq; misc eth
t297	Trifluoromethane-sulfonic anhydride	$(\text{CF}_3\text{SO}_2)_2\text{O}$	282.13	3 ⁴ , 35	1.677	1.3212^{20}		84		d aq, alc
t298	3-(Trifluoromethyl)-benzonitrile	$\text{CF}_3\text{C}_6\text{H}_4\text{CN}$	171.12	9, 478	1.2813^{20}	1.4505^{20}	14.5	189	72	

t299	3-(Trifluoromethyl)-benzyl chloride	$\text{CF}_3\text{C}_6\text{H}_4\text{CH}_2\text{Cl}$	194.59		1.254	1.4605		70 ^{12mm}		
t300	α,α,α -Trifluorotoluene	$\text{C}_6\text{H}_5\text{CF}_3$	146.11	5, 290	1.1886 ²⁰	1.4145 ²⁰	−29	102	12	
t301	Trihexylamine	$[\text{CH}_3(\text{CH}_2)_5]_3\text{N}$	269.52	4, 188				263–265	> 112	v s alc, eth; i aq
t302	Trihexylchlorosilane	$[\text{CH}_3(\text{CH}_2)_5]_3\text{SiCl}$	319.1		0.871 ²⁰ ₄	1.456 ²⁰		155 ^{5mm}		
t303	Trihexylsilane	$[\text{CH}_3(\text{CH}_2)_5]_3\text{SiH}$	284.60			1.448 ²⁰		160 ^{5mm}		
t304	1,2,3-Trihydroxybenzene	$\text{C}_6\text{H}_3(\text{OH})_3$	126.11	6, 1071	1.45		131–133			59 aq; 77 alc; 62 eth
t305	1,3,5-Trihydroxybenzene	$\text{C}_6\text{H}_3(\text{OH})_3$	126.11	6, 1092			218–220	subl d		1 aq; 10 alc; s eth
t306	3,4,5-Trihydroxybenzoic acid	$(\text{HO})_3\text{C}_6\text{H}_2\text{COOH}$	170.12	10, 470			d 235			1.1 aq; 17 alc; 1 eth; 20 acet; i bz, chl, PE
t307	Triisobutylaluminum	$[(\text{CH}_3)_2\text{CHCH}_2]_3\text{Al}$	198.33		0.781 ²⁵		6	86 ^{10mm}	pyrophoric	
t308	Triisodecyl phosphite	$[(\text{CH}_3)_2\text{CH}(\text{CH}_2)_7\text{O}]_3\text{P}$	502.80		0.886 ²⁵ ₁₃	1.454 ²⁵	< 0	180 ^{0.1mm}	235	
t309	Triisopropanolamine	$[\text{CH}_3\text{CH}(\text{OH})\text{CH}_2]_3\text{N}$	191.27		0.9996 ⁵⁰ ₂₀		46	305.4	152	v s aq
t310	Triisopropoxyborane	$[(\text{CH}_3)_2\text{CHO}]_3\text{B}$	188.08	1, 363	0.815	1.3764 ²⁰		139–141	17	
t311	Triisopropoxyvinylsilane	$[(\text{CH}_3)_2\text{CHO}]_3\text{Si}-\text{CH}=\text{CH}_3$	232.4		0.863 ²⁵ ₄	1.396 ²⁵		179–181		
t312	1,3,5-Triisopropylbenzene	$\text{C}_6\text{H}_3[\text{CH}(\text{CH}_3)_2]_3$	204.36	5, 458	0.845	1.4884 ²⁰		232–236	86	
t313	Triisopropyl phosphite	$[(\text{CH}_3)_2\text{CHO}]_3\text{P}$	208.24	1, 363	0.914 ²⁰ ₄	1.4101 ²⁰		64 ^{11mm}	73	i aq (sl hyd)

2,2,2-Trifluoroethyl mesylate, m438
 2-(Trifluoromethyl)aniline, a129
 3-(Trifluoromethyl)aniline, a130
m-Trifluoromethylphenol, t290

4,4,4-Trifluoro-1-(2-thienyl)-1,3-butanedione, t137
 α,α,α -Trifluorotoluidines, a129, a130, a131
 α,α,α -Trifluorotolunitrile, t298

Triglyme, b189
 Tri-(2-hydroxyethyl)amine, t259
 1,2,6-Trihydroxyhexane, h65
 Triiodomethane, i36

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

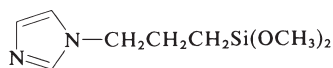
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t314	3,4,5-Trimethoxybenzaldehyde	$(\text{CH}_3\text{O})_3\text{C}_6\text{H}_2\text{CHO}$	196.20	8, 391			73–75	165 ^{10mm}		
t315	1,2,3-Trimethoxybenzene	$\text{C}_6\text{H}_3(\text{OCH}_3)_3$	168.19	6, 1081	1.112		43–45	241		
t316	3,4,5-Trimethoxybenzoic acid	$(\text{CH}_3\text{O})_3\text{C}_6\text{H}_2\text{COOH}$	212.20	10, 481			168–171	227 ^{10mm}		v s alc, eth; s chl
t317	3,4,5-Trimethoxybenzoyl chloride	$(\text{CH}_3\text{O})_3\text{C}_6\text{H}_2\text{COCl}$	230.65	10, 487			79–81	185 ^{18mm}		
t318	3,4,5-Trimethoxybenzyl alcohol	$(\text{CH}_3\text{O})_3\text{C}_6\text{H}_2\text{CH}_2\text{OH}$	198.22	6, 1159	1.233	1.5459 ²⁰		228 ^{25mm}	> 112	
t319	Trimethoxyborane	$(\text{CH}_3\text{O})_3\text{B}$	103.91	1, 287	0.920 ²³ ₄	1.3568 ²⁰	–34	67–68	–1	hyd aq; misc alc, eth
t320	Trimethoxyboroxine	$[\text{—OB}(\text{OCH}_3)\text{—}]_3$	173.53		1.195	1.3996 ²⁰	10	130	10	
t321	1,3,3-Trimethoxybutane	$(\text{CH}_3\text{O})_2\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{OCH}_3$	148.20	1 ³ , 3214	0.940	1.4096 ²⁰		63 ^{20mm}	45	
t321a	Trimethoxy(methyl)silane	$\text{CH}_3\text{Si}(\text{OCH}_3)_3$	136.23		0.9548 ²⁰ ₄	1.3696 ²⁰		102–103	21	
t322	1,3,3-Trimethoxypropane	$\text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}(\text{OCH}_3)_2$	134.18	1, 820	0.942	1.4004 ²⁰		45–46 ^{17mm}		
t323	(Trimethoxysilyl)propyldiethylenetriamine	$(\text{CH}_3\text{O})_3\text{Si}(\text{CH}_2)_3\text{NHCH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{NH}_2$	265.4		1.03 ²⁰ ₄	1.463 ²⁰				
t324	N-[3-Trimethoxysilylpropyl]ethylenediamine	$(\text{CH}_3\text{O})_3\text{Si}(\text{CH}_2)_3\text{NHCH}_2\text{CH}_2\text{NH}_2$	222.4		1.010	1.4450 ²⁰		146 ^{15mm}	> 112	
t325	N-(Trimethoxysilylpropyl)imidazole		230.3		1.00 ²⁰ ₄	1.45 ²⁵				
t326	3-(Trimethoxysilyl)propyl methacrylate	$(\text{CH}_3\text{O})_3\text{SiCH}_2\text{CH}_2\text{CH}_2\text{OOC}(\text{CH}_3)=\text{CH}_2$	249.3		1.045 ²⁰ ₄	1.429 ²⁵		190	92	

t327	Trimethylaluminum	$(\text{CH}_3)_3\text{Al}$	72.09	4, 643	0.752 ²⁰	1.432 ¹²	15.4	20 ^{8mm}	pyro- phoric -6	s alk; v sl s alc
t328	Trimethylamine	$(\text{CH}_3)_3\text{N}$	59.11	4, 43	0.636		-117.1	2.9		41 aq; misc alc; s bz, chl, eth
t329	Trimethylamine- <i>N</i> -oxide	$(\text{CH}_3)_3\text{N}(\text{O})$	75.11				257			s aq, MeOH
t330	2,4,6-Trimethyl- aniline	$(\text{CH}_3)_3\text{C}_6\text{H}_2\text{NH}_2$	135.21	12, 1160	0.963	1.5510 ²⁰		233	96	
t331	1,3,3-Trimethyl-6- azabicyclo[3.2.1]- octane		153.27		0.902	1.4716 ²⁰		194	75	
t332	3,3,5-Trimethyl-1- azacycloheptane		141.26		0.852	1.4563 ²⁰		180	67	
t333	1,2,3-Trimethyl- benzene	$\text{C}_6\text{H}_3(\text{CH}_3)_3$	120.20	5, 399	0.894 ²⁰ ₄	1.5139 ²⁰	-25.4	176.1	48	i aq; s alc, eth
t334	1,2,4-Trimethyl- benzene	$\text{C}_6\text{H}_3(\text{CH}_3)_3$	120.20	5, 400	0.8756 ²⁰ ₄	1.5048 ²⁰	-43.9	169.4	48	s alc, bz, eth
t335	1,3,5-Trimethyl- benzene	$\text{C}_6\text{H}_3(\text{CH}_3)_3$	120.20	5, 406	0.8637 ²⁰ ₄	1.4994 ²⁰	-44.7	164.7	44	misc alc, bz, eth

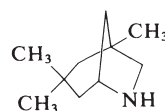
Trimellitic acid, b29
 Trimesic acid, b30
 Trimesoyl chloride, b32
 Trimethylacetaldehyde, d596

Trimethylacetamide, d597
 Trimethylacetic acid, d598
 Trimethylacetic anhydride, d599
 Trimethylacetyl chloride, d600

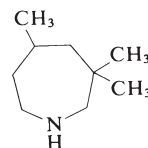
endo-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol,
 b216



t325



t331



t332

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t336	Trimethyl 1,2,4-benzenetricarboxylate	$C_6H_3(COOCH_3)_3$	252.22	9 ¹ , 429	1.261	1.5214 ²⁰	38–40	194 ^{12mm}	> 112	
t337	2,2,3-Trimethylbutane	$(CH_3)_2CHC(CH_3)_3$	100.20	1 ² , 121	0.6901 ²⁰ ₄	1.3894 ²⁰	–24.9	80.9		s alc, eth
t338	2,3,3-Trimethyl-2-butanol	$(CH_3)_3CC(CH_3)_2OH$	116.20	1 ² , 447	0.8380 ²⁵ ₄	1.4233 ²²	15–17	130.5		misc alc, eth
t339	1,1,3-Trimethylcyclohexane	$C_6H_9(CH_3)_3$	126.24			1.4296 ²⁰		136.6		
t340	3,5,5-Trimethylcyclohex-2-ene-1-one		138.2	7, 65	0.925 ²⁰ ₂₀	1.478 ²⁰	–8.1	215.2	96	1.2 aq
t341	2,2,6-Trimethyl-1,3-dioxen-4-one		142.15	19 ³ , 1604	1.088	1.4622 ²⁰	12–13	65– 67 ^{2mm}		
t342	4,4'-Trimethylenebis-(1-methylpiperidine)		238.42		0.896	1.4820 ²⁰	13	215 ^{50mm}	110	
t343	4,4'-Trimethylenedipiperidine		210.37				65–68			
t344	4,4'-Trimethylenedipyridine		198.27				57–60			
t345	Trimethylene oxide		58.08	17, 6	0.8930 ²⁵ ₄	1.3895 ²⁵		50	< 1	misc aq
t345a	Trimethylene sulfide		74.15	17 ¹ , 3	1.025 ²⁰	1.5102 ²⁰	–73.3	95.0	< 1	
t346	2,2,5-Trimethylhexane	$(CH_3)_2CHCH_2CH_2-C(CH_3)_3$	128.26	1 ³ , 516	0.7072 ²⁰	1.3997 ²⁰	–105.8	124.1		v s org solv
t347	3,5,5-Trimethyl-1-hexanol	$(CH_3)_3CCH_2CH(CH_3)-CH_2CH_2OH$	144.25		0.8236 ²⁰ ₄	1.4300 ²⁵	< –70	194		s alc, eth
t348	Trimethylhydroquinone	$(CH_3)_3C_6H(OH)_2$	152.19	6, 931			172–174			s aq; v s alc, bz, eth

t348a	2,6,8-Trimethyl-4-nonanol	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{CH}_3)\text{-CH}_2\text{CH}(\text{OH})\text{CH}_2\text{-CH}(\text{CH}_3)_2$	186.33		0.8193		225	93	
t349	2,6,8-Trimethyl-4-nonanone	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{CH}_3)\text{-CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}(\text{CH}_3)_2$	184.31		0.818 ₂₀ ²⁰	-75	218.4		
t350	α -(-)-1,3,3-Trimethyl-2-norbornanol		154.25	6, 70	0.9641 ₄ ²⁰	48	201	73	s alc, eth

Trimethyl borate, t319

Trimethylchlorosilane, c255

$\alpha,\alpha,4$ -Trimethyl-3-cyclohexene-1-methanol, t7

3,5,5-Trimethylcyclohex-2-en-1-one, i82

1,2,2-Trimethyl-1,3-cyclopentenedicarboxylic acid, c5

Trimethylene chlorobromide, b257

Trimethylene chlorohydrin, c214

Trimethylenediamine, p193

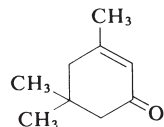
Trimethylene dibromide, d93

Trimethylene glycol, p195

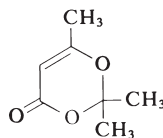
Trimethylethylene, m159

Trimethylgermanium bromide, b363

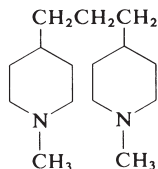
3,3,5-Trimethylhexahydroazepine, t332



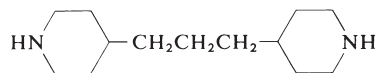
t340



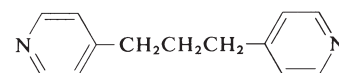
t341



t342



t343



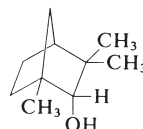
t344



t345



t345a



α form
t350

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

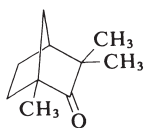
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t351	(+)-1,3,3-Tri-methyl-2-norbor-nanone		152.24	7, 96	0.948 ¹⁸	1.4635 ¹⁸	5–6	192–193	52	v s alc, eth
t352	Trimethyl orthoacetate	$\text{CH}_3\text{C}(\text{OCH}_3)_3$	120.15	1 ² , 128	0.9428 ²⁵ ₄	1.3859 ²⁵		105		v s alc, eth
t353	Trimethyl orthoformate	$\text{HC}(\text{OCH}_3)_3$	106.12	2, 19	0.9676 ²⁰ ₄	1.3790 ²⁰		100.6	15	
t354	2,4,4-Trimethyl-1-oxazoline		113.16		0.887	1.4213 ²⁰		112–113	12	
t355	2,2,3-Trimethyl-pentane	$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{-CH}_2\text{CH}_3$	114.23	1 ¹ , 62	0.7160 ²⁰ ₄	1.4030 ²⁰	–112.3	109.8		s eth; sl s alc
t356	2,2,4-Trimethyl-pentane	$(\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{CH}_3)_3$	114.23	1 ² , 127	0.6919 ²⁰ ₄	1.3915 ²⁰	–107.4	99.2	–7	s bz, chl, eth
t357	2,3,4-Trimethyl-pentane	$(\text{CH}_3)_2\text{CH}[\text{CH}(\text{CH}_3)]_2\text{CH}_3$	114.24	1 ³ , 500	0.7190 ²⁰ ₄	1.4042 ²⁰	–109.2	113.5		s alc, org solv
t358	2,2,4-Trimethyl-1,3-pentanediol	$(\text{CH}_3)_2\text{CHCH}(\text{OH})\text{-C}(\text{CH}_3)_2\text{CH}_2\text{OH}$	146.22	1 ³ , 2225	0.928 ⁵⁵ ₁₅	1.4513 ¹⁵	46	229	113	1.8 aq; 75 alc; 22 bz; 25 acet
t359	2,4,4-Trimethyl-1-pentene	$(\text{CH}_3)_3\text{CCH}_2\text{-C}(\text{CH}_3)=\text{CH}_2$	112.22	1 ³ , 849	0.7150 ²⁰ ₄	1.4112 ²⁰	–93	101.4	< 1	
t360	2,3,5-Trimethyl-phenol	$(\text{CH}_3)_3\text{C}_6\text{H}_2\text{OH}$	136.19	6, 518			92–95	230–231		
t361	2,3,6-Trimethyl-phenol	$(\text{CH}_3)_3\text{C}_6\text{H}_2\text{OH}$	136.19				62–64			
t362	2,4,6-Trimethyl-phenol	$(\text{CH}_3)_3\text{C}_6\text{H}_2\text{OH}$	136.19	6, 158			68–71	220		
t363	Trimethyl phosphate	$(\text{CH}_3\text{O})_3\text{P}(\text{O})$	140.08	1, 286	1.197	1.3958 ²⁰	–46	197	none	100 aq; s alc
t364	Trimethyl phosphite	$(\text{CH}_3\text{O})_3\text{P}$	124.08	1, 285	1.046 ²⁰ ₄	1.4080 ²⁰	< –78	111–112	40	d aq; misc alc, acet, bz, PE

t365	Trimethyl phosphonoacetate	$(\text{CH}_3\text{O})_2\text{P}(\text{O})\text{CH}_2\text{COCH}_3$	182.11		1.125	1.4370 ²⁰		118 ^{0.85mm}	> 112	
t366	1,2,4-Trimethylpiperazine		128.22		0.851 ²⁵ ₂₅	1.4480 ²⁵	< -50	151 ^{746mm}		s aq, alc, acet, bz
t367	2,4,6-Trimethylpyridine	$(\text{C}_5\text{H}_2\text{N})(\text{CH}_3)_3$	121.18	20, 250	0.9166 ²² ₄	1.4979 ²⁰	-43	170.5	57	3.5 aq; misc eth; s alc, bz, chl
t368	<i>N</i> -(Trimethylsilyl)acetamide	$\text{CH}_3\text{CONHSi}(\text{CH}_3)_3$	131.25				52-54	185-186	57	
t369	<i>N</i> -(Trimethylsilyl)aniline	$(\text{CH}_3)_3\text{SiNHC}_6\text{H}_5$	165.3		0.940 ²⁰ ₄	1.522 ²⁰		207-208		
t370	Trimethylsilyl bromoacetate	$\text{BrCH}_2\text{COOSi}(\text{CH}_3)_3$	211.14		1.284	1.4421 ²⁰		57-58 ^{9mm}	28	
t371	<i>N</i> -(Trimethylsilyl)diethylamine	$(\text{CH}_3)_3\text{SiN}(\text{C}_2\text{H}_5)_2$	145.33					127 ^{738mm}		
t372	2-(Trimethylsilyl)ethanol	$(\text{CH}_3)_3\text{SiCH}_2\text{CH}_2\text{OH}$	118.25		0.825	1.4246 ²⁰		71-73 ^{35mm}	50	
t373	<i>N</i> -(Trimethylsilyl)imidazole		140.26		0.956	1.4751 ²⁰		99 ^{14mm}	80	
t374	3-(Trimethylsilyloxy)allene	$(\text{CH}_3)_3\text{SiOCH}_2\text{CH}=\text{CH}_2$	130.3		0.7830 ³⁰ ₄	1.4075 ²⁵		100-102		

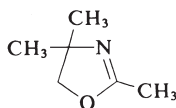
Trimethylolpropane, c156
Trimethylsilyl cyanide, c298

Trimethylsilyldiethylamine, d343
Trimethylsilyl iodide, i55

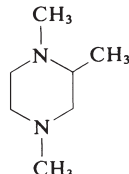
Trimethylsilylnitrile, c298



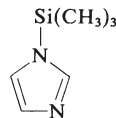
t351



t354



t366



t373

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t375	Trimethylsilyl-phenoxide	$(\text{CH}_3)_3\text{SiOC}_6\text{H}_5$	166.3		0.9256 ₄ ²⁰	1.4782 ²⁰	−55	81 ^{23mm}		
t376	Trimethylsilyl trifluoroacetate	$(\text{CH}_3)_3\text{SiOOCFCF}_3$	186.2		1.077 ₄ ²⁰	1.3880 ²⁰		89–90		
t377	Trimethylsulfonium iodide	$[(\text{CH}_3)_3\text{S}]\text{I}$	204.07				215–220	subl		
t378	Trimethylsulfonium iodide	$[(\text{CH}_3)_3\text{S}(\text{O})]\text{I}$	220.07				175 d			
t379	Trimethylvinyl-oxyasilane	$(\text{CH}_3)_3\text{SiOCH}=\text{CH}_2$	116.2		0.772 ₄ ²⁰	1.389 ²⁰		74–75		
t380	Trimethylvinyl-silane	$(\text{CH}_3)_3\text{SiCH}=\text{CH}_2$	100.2		0.690 ₄ ²⁰	1.3920 ²⁰		55	< 1	
t381	2,4,6-Trinitro-aniline	$(\text{O}_2\text{N})_3\text{C}_6\text{H}_2\text{NH}_2$	228.12	12, 763	1.762 ¹⁴		188–190	explodes		s hot acet; sl s alc
t382	1,2,4-Trinitro-benzene	$\text{C}_6\text{H}_3(\text{NO}_2)_3$	213.11	5, 271	1.73 ¹⁶		61–62	explodes		5.5 alc; 7.1 eth; i aq
t383	1,3,5-Trinitro-benzene	$\text{C}_6\text{H}_3(\text{NO}_2)_3$	213.11	5, 271	1.688 ₄ ²⁰		122.5	explodes		0.035 aq; 1.9 alc; 1.5 eth; 6.2 bz
t384	2,4,7-Trinitro-9-fluorenone		315.20	7 ² , 410			175–176			v s bz, acet; sl s aq
t385	Trinitromethane	$\text{HC}(\text{NO}_2)_3$	151.04	1, 79	1.597 ₄ ²⁴		15	47 ^{22mm}		s aq, alk
t386	2,4,6-Trinitro-toluene	$(\text{O}_2\text{N})_3\text{C}_6\text{H}_2\text{CH}_3$	227.13	5, 347	1.654 ₄ ²⁰		80.1	explodes		1.5 alc; 4 eth; s bz, acet; 0.01 aq
t387	Trioctylamine	$[\text{CH}_3(\text{CH}_2)_7]_3\text{N}$	353.68	4, 196	0.809	1.4485 ²⁰		365–367	> 112	
t388	s-Trioxane		90.08	19, 381	1.170 ⁶⁵		64	115	45	17.2 aq; v s alc, bz, eth, EtAc
t389	Tripentaerythritol		372.41				245 d			
t390	2,4,6-Triphenoxy-s-triazine		357.37				232–234			

t391	Triphenoxyvinylsilane	$(C_6H_5O)_3SiCH=CH_2$	334.5		1.130 ₄ ²⁵	1.562 ²⁵		210 ^{7mm}		
t392	Triphenylamine	$(C_6H_5)_3N$	245.33	12, 181	0.774 ₀ ⁰		125–127	347–348		s acet, eth; sl s alc
t393	Triphenylantimony	$(C_6H_5)_3Sb$	353.07	16, 891	1.4343 ²⁵		52–54	377		v s bz, eth; sl s alc
t394	Triphenylarsine	$(C_6H_5)_3As$	306.24	16, 828	1.2225 ⁴⁸	1.6139 ⁴⁸	60–62	233 ^{14mm}		v s bz, eth; s alc
t395	1,3,5-Triphenylbenzene	$(C_6H_5)_3C_6H_3$	306.41	5, 737	1.205		172–174	460		v s bz; s abs alc, eth
t396	Triphenylene		228.29	5, 720	1.302		199	425		s alc; v s bz, eth
t397	Triphenylmethane	$(C_6H_5)_3CH$	244.34	5, 698	1.0134 ₄ ⁹⁹		93.4	360		v s hot alc, eth; 49 chl; 7 bz; s PE; i aq
t398	Triphenylmethanol	$(C_6H_5)_3COH$	260.34	6, 713	1.199 ₄ ⁰		164.2	360		v s alc, bz, eth; i aq
t399	Triphenyl phosphate	$(C_6H_5O)_3P(O)$	326.29	6, 179			49–51	244 ^{10mm}	223	misc alc; s bz, acet, chl, eth; i aq

2,4,6-Trinitrophenol, p173
Triolein, g22

Trioxymethylene, t388
Tripalmitin, g23

Triphenylmethyl bromide, b366

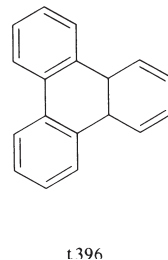
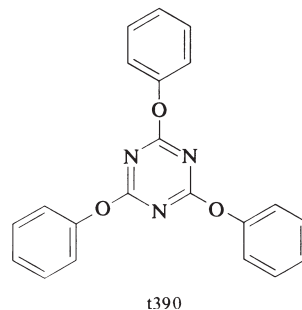
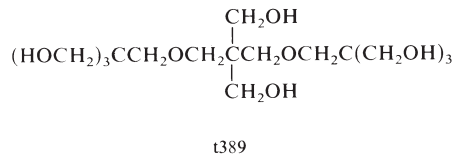
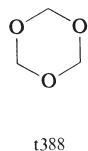
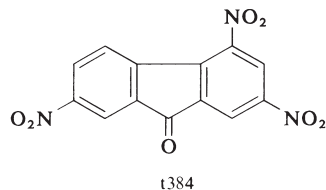


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

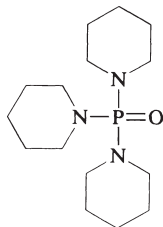
No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
t400	Triphenylphosphine	(C ₆ H ₅) ₃ P	262.29	16, 759	1.075 ₄ ⁸¹		80.5	377	181	v s eth; s bz, chl, HOAc; sl s alc; i aq
t401	Triphenylphosphine selenide	(C ₆ H ₅) ₃ P(Se)	341.25				187–189			
t402	Triphenylphosphine sulfide	(C ₆ H ₅) ₃ P(S)	294.36	16, 784			162–164			
t403	Triphenyl phosphite	(C ₆ H ₅ O) ₃ P	310.29	6, 177	1.184 ₁₅ ²⁵	1.5903 ²⁰	22–24	360	218	s alc, bz, chl, eth
t404	Triphenylsilane	(C ₆ H ₅) ₃ SiH	260.41	16 ² , 605			42–44	152 ^{2mm}		
t405	Tripiperidino-phosphine oxide		299.40	20, 88			40–42	273 ^{50mm}		
t406	Tripropoxyborane	(CH ₃ CH ₂ CH ₂ O) ₃ B	188.08	1 ² , 369	0.8576 ₄ ²⁰	1.3948 ²⁰		175		v s alc; misc eth
t407	Tripropylamine	(CH ₃ CH ₂ CH ₂) ₃ N	143.27	4, 139	0.753	1.4160 ²⁰	–93	155–158	36	s aq, alc, eth
t408	Tripropylene glycol	H(OCH ₂ CH ₂ CH ₂) ₃ OH	192.3		1.018	1.442 ²⁵		267.2	141	s aq
t409	Tripropylene glycol butyl ether	HO(CH ₂ CH ₂ CH ₂ O) ₃ -(CH ₂) ₃ CH ₃	248.4		0.934 ₂₅ ²⁵	1.430 ²⁵		276	135	
t410	Tripropylene glycol ethyl ether	HO(CH ₂ CH ₂ CH ₂ O) ₃ -CH ₂ CH ₃	220.3		0.0948 ₂₅ ²⁵	1.427 ²⁵		486	132	
t411	Tripropylene glycol isopropyl ether	HO(CH ₂ CH ₂ CH ₂ O) ₃ -CH(CH ₃) ₂	234.8		0.0942 ₂₅ ²⁵	1.428 ²⁵		112.7	124	
t412	Tripropylene glycol-methyl ether	HO(CH ₂ CH ₂ CH ₂ O) ₃ CH ₃	206.3		0.967 ₂₅ ²⁵	1.428 ²⁵	–42	242.4	127	misc aq, alc, eth
t413	Tripropyl orthoformate	HC(OCH ₂ CH ₂ CH ₃) ₃	190.28		0.8805 ₄ ²⁰	1.4072 ²⁰		108 ^{5mm}		
t414	Tris(butoxyethyl) phosphate	(C ₄ H ₉ OCH ₂ CH ₂ O) ₃ P(O)	398.48		1.006	1.4359 ²⁰		228 ^{4mm}	> 112	
t415	Tris(2-chloroethoxy)silane	(ClCH ₂ CH ₂ O) ₃ SiH	267.6		1.2886 ₄ ²⁰	1.4577 ²⁰		118 ^{2mm}		

t416	Tris(2-chloro-ethyl) phosphate	$(\text{ClCH}_2\text{CH}_2\text{O})_3\text{P}(\text{O})$	285.49	$1^2, 337$	1.390	1.4721^{20}		330	232	
t417	Tris(2-chloro-ethyl) phosphite	$(\text{ClCH}_2\text{CH}_2\text{O})_3\text{P}$	269.49		1.353_4^{20}	1.4863^{20}		$115^{2\text{mm}}$	190	misc alc, bz, eth
t418	Tris(2,6-dichloro-phenyl) phosphate	$(\text{Cl}_2\text{C}_6\text{H}_3\text{O})_3\text{P}(\text{O})$	533.09				208–210			
t419	Tris(dimethylamino)-methane	$\text{CH}[\text{N}(\text{CH}_3)_2]_3$	145.25		1.4360^{20}		42– $43^{12\text{mm}}$			
t420	Tris(dimethylamino)-methylsilane	$[(\text{CH}_3)_2\text{N}]_3\text{SiCH}_3$	175.4		0.850_4^{22}	1.432^{22}	– 11	$56^{17\text{mm}}$		
t421	Tris(2-ethylhexyl) phosphite	$[\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2\text{CH}_3)-\text{CH}_2\text{O}]_3\text{P}$	418.6		0.902_4^{20}	1.4494^{20}		$164^{0.3\text{mm}}$	185	i aq
t422	Tris(heptafluoropropyl)-s-triazine		585.1		1.7158^{25}	1.7158^{25}		165		
t423	Tris(hydroxymethyl)amino-methane	$(\text{HOCH}_2)_3\text{CNH}_2$	121.14	4, 303			172	$220^{10\text{mm}}$		

Triphenylsilyl azide, a320
Tripropyl borate, t406

Tripropylsilyl chloride, c258
TRIS, t423

Tris(dimethylamino)silyl chloride, c257a
1,1,1-Tris(hydroxymethyl)ethane, h141



t405



t422

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent		
t424	2-[Tris(hydroxymethyl)methylamino]-1-ethanesulfonic acid	(HOCH ₂) ₃ CNHCH ₂ -CH ₂ SO ₃ H	229.25	1, 520			223–225					
t425	1,1,1-Tris(hydroxymethyl)ethane	CH ₃ C(CH ₂ OH) ₃	120.15				226					
t426	3-[N-Tris(hydroxymethyl)methylamino]-2-hydroxypropane-sulfonic acid	(HOCH ₂) ₃ CNHCH ₂ -CH(OH)CH ₂ SO ₃ H	259.3									
t427	3-[Tris(hydroxymethyl)-methylamino]-1-propanesulfonic acid	(HOCH ₂) ₃ CNHCH ₂ CH ₂ -CH ₂ SO ₃ H	243.28				240 d					
t428	N-[Tris(hydroxymethyl)methyl]-glycine	(HOCH ₂) ₃ CNHCH ₂ COOH	179.17	4 ³ , 462			184 d	145 ^{16mm}	65	53		
t429	Tris(2-methoxyethoxy)methylsilane	CH ₃ Si(OCH ₂ CH ₂ OCH ₃) ₃	268.4				1.045 ²⁰ ₄				1.420 ²⁰	
t430	Tris(2-methoxyethoxy)vinylsilane	H ₂ C=CHSi(OCH ₂ -CH ₂ OCH ₃) ₃	280.38				1.034 ²⁵ ₄				1.427 ²⁵	284–286
t431	Tris(2-methylallyl)-amine	[H ₂ C=C(CH ₃)CH ₂] ₃ N	173.91				0.794				1.4575 ²⁰	83–85 ^{15mm}
t432	Tris(pentafluoroethyl)-s-triazine		435.1		1.6506 ²⁵	1.3131 ²⁵		121–122				

t433	1,3,5-Trithiane		138.27	19, 382			216–218			s bz; sl s alc, eth
t434	Trithiocarbonic acid	(HS) ₂ C(S)	110.21	3, 221	1.483 ₄ ²⁰	1.8225 ²⁰	–26.9	57.8		d aq, alc; sl s eth
t435	1,2,4-Trivinylcyclohexane	(H ₂ C=CH) ₃ C ₆ H ₉	162.28		0.836	1.4780 ²⁰		88 ^{20mm}	68	
t436	L-(–)-Tryptophan		204.23	22, 546			280–285 d			1 aq; s hot alc, alk; i eth, chl
t437	L-Tyrosine	(HO)C ₆ H ₄ CH ₂ - CH(NH ₂)COOH	181.19	14, 605			> 300 d			0.03 aq; 0.01 alc; s alk; i eth
t438	L-Tyrosine hydrazide	HOC ₆ H ₄ CH ₂ CH(NH ₂)- CONHNH ₂	195.22	14 ¹ , 665			196–198			
u1	Undecanal	CH ₃ (CH ₂) ₉ CHO	170.30	1, 712	0.825	1.4322 ²⁰	–4	115 ^{5mm}	96	i aq; s alc, eth
u2	Undecane	CH ₃ (CH ₂) ₉ CH ₃	156.31	1, 170	0.7402 ²⁰	1.4173 ²⁰	–25.6	195.9	60	i aq; misc alc, eth
u3	Undecanoic acid	CH ₃ (CH ₂) ₉ COOH	186.30	2, 358	0.8907	1.4294 ⁴⁵	28.5	228 ^{160mm}		s alc, chl, eth; i aq
u4	1-Undecanol	CH ₃ (CH ₂) ₁₀ OH	172.31	1, 427	0.8324 ²⁰	1.4402 ²⁰	15.9	242.8	> 112	0.02 aq; s alc
u5	2-Undecanone	CH ₃ (CH ₂) ₈ COCH ₃	170.30	1, 173	0.829	1.4280 ²⁰	11–12	231–232	88	s alc, bz, chl, eth, acet; i aq
u6	6-Undecanone	CH ₃ (CH ₂) ₄ - CO(CH ₂) ₄ CH ₃	170.30	1, 174	0.831	1.4280 ²⁰	14.6	228	88	i aq; v s alc, eth
u7	10-Undecenal	H ₂ C=CH(CH ₂) ₈ CHO	168.28		0.810	1.4427 ²⁰			92	
u8	1-Undecene	CH ₃ (CH ₂) ₈ CH=CH ₂	154.29	1, 225	0.763 ₄ ²⁰	1.4261 ²⁰	–49.2	192.7		i aq; misc alc, eth

Tris(7-methylnonyl) phosphite, t308

Trityl alcohol, t398

Tryptamine, a170

Tyramine, a173

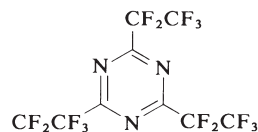
Umbelliferone, h109

Undecyl alcohol, u4

Undecyl-10-en-1-oic acid, u9

Undecylenic aldehyde, u7

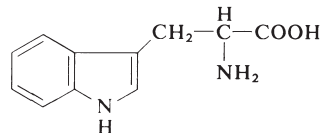
Undecylic aldehyde, u1



t432



t433



t436

TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
u9	10-Undecenoic acid	$\text{H}_2\text{C}=\text{CH}(\text{CH}_2)_8\text{COOH}$	184.28	2, 458	0.907_4^{24}	1.4493^{20}	24.5	$137^{2\text{mm}}$	148	s alc, chl, eth; i aq
u10	10-Undecen-1-ol	$\text{H}_2\text{C}=\text{CH}(\text{CH}_2)_9\text{OH}$	170.30	1,452	0.850^{15}	1.4500^{20}	-2	245	93	
u11	10-Undecenoyl chloride	$\text{H}_2\text{C}=\text{CH}(\text{CH}_2)_8\text{COCl}$	202.73	2, 459	0.944	1.4532^{20}		$122^{10\text{mm}}$	93	
u12	Urea	$(\text{H}_2\text{N})_2\text{CO}$	60.06	3, 42	1.32_4^{18}		132.7	d > mp		100 aq; 20 alc
u13	Uric acid		168.11	26, 513	1.893^{20}		> 300	d		s alk; i aq, alc, eth
u14	Uridine		244.20	31, 23			165			s aq; hot alc, pyr
v1	L-Valine	$(\text{CH}_3)_2\text{CH}-\text{CH}(\text{NH}_2)\text{COOH}$	117.15	4, 427	1.230		315	subl		8.8 aq; v sl s alc, eth
v2	Vinyl acetate	$\text{H}_2\text{C}=\text{CHOOCCCH}_3$	86.09	2 ¹ , 63	0.9318_4^{20}	1.3959^{20}	-92.8	72.5	-6	2 aq; misc alc, eth
v3	5-Vinylbicyclo-[2.2.1]-2-heptene		120.19		0.84	1.4802	-80	141		
v4	Vinyl crotonate	$\text{CH}_3\text{CH}=\text{CHCOOCH}=\text{CH}_2$	112.13	2 ³ , 1263	0.940	1.4488^{20}		$50^{10\text{mm}}$	27	
v5	Vinylcyclohexane	$\text{C}_6\text{H}_{11}\text{CH}=\text{CH}_2$	110.20	5 ¹ , 35		1.4463^{20}		128	21	
v6	4-Vinyl-1-cyclohexene		108.18	5 ¹ , 63	0.830_4^{20}	1.4640^{20}	-101	126-127	20	
v7	1-Vinylimidazole		94.12	23 ⁴ , 569	1.039	1.5308^{20}		78- $79^{13\text{mm}}$	81	
v8	5-Vinyl-2-norbornene		120.20		0.8411	1.4802^{20}	-80	141	27	
v9	2-Vinylpyridine	$(\text{C}_5\text{H}_4\text{N})\text{CH}=\text{CH}_2$	105.14	20, 256	0.975	1.5490^{20}		158-159	43	v s alc, chl, eth
v10	4-Vinylpyridine	$(\text{C}_5\text{H}_4\text{N})\text{CH}=\text{CH}_2$	105.14	20 ² , 170	0.975	1.5500^{20}		$65^{15\text{mm}}$	51	sl s hot aq, hot alc
v11	N-Vinyl-2-pyrrolidinone		111.14		0.980	1.5120^{20}		$93^{13\text{mm}}$	93	
x1	Xanthene		182.22	17, 73			101	310-312		s bz, eth; sl s alc, aq
x2	Xanthen-9-carboxylic acid		226.23	12 ² , 279			217 d			s hot alc, eth
x3	9-Xanthenone		196.21	17, 354			174	$350^{730\text{mm}}$		0.5 alc; v s chl

Uracil, p268
 5-Ureidohydantoin, a77
 Urethane, e91
 Valeraldehyde, p27
 Valeric acid, p36
 γ -Valerolactone, p40
 Valerone, d531
 Valeronitrile, p33
 Valeryl chloride, p44
 Valinols, a213, a214

Vanillic acid, h132
 Vanillin, h131
o-Vanillin, h130
 Vanillyl alcohol, h135
 Veratraldehyde, d430
 Veratric acid, d434
 Veratrole, d431
 Veronal, d280
 Vinylacetic acid, b403
 Vinyl bromide, b284

Vinyl 2-butenate, v4
 Vinyl chloride, c109
 Vinylidene chloride, d178
 Vinyltrimethylsilane, t380
 Vinyltris (2-methoxyethoxy)silane, t430
 Vitamin B₁, t139
 Vitamin B₂, r4
 Vitamin C, a312
 Xanthone, x3

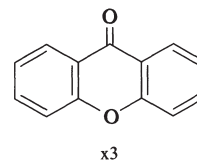
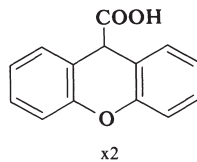
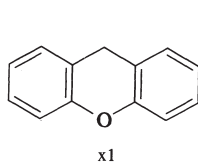
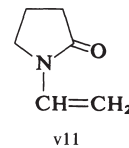
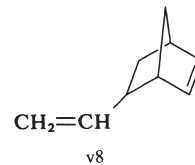
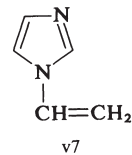
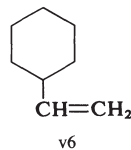
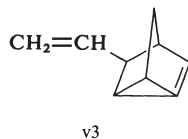
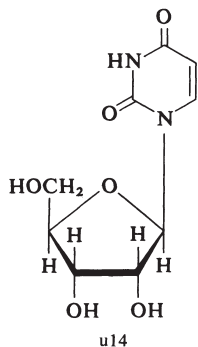
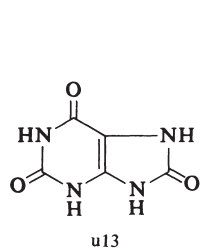


TABLE 1.15 Physical Constants of Organic Compounds (*continued*)

No.	Name	Formula	Formula weight	Beilstein reference	Density	Refractive index	Melting point	Boiling point	Flash point	Solubility in 100 parts solvent
x4	o-Xylene	$C_6H_4(CH_3)_2$	106.17	5, 362	0.8802 ₄ ²⁰	1.5054 ²⁰	−25.2	144.4	32	misc alc, eth; 0.017 aq
x5	m-Xylene	$C_6H_4(CH_3)_2$	106.17	5, 370	0.8684 ₄ ¹⁵	1.4972 ²⁰	−47.9	139.1	25	misc alc, eth; 0.02 aq
x6	p-Xylene	$C_6H_4(CH_3)_2$	106.17	5, 382	0.8611 ₄ ²⁰	1.4958 ²⁰	13.3	138.4	30	v s eth; s alc; 0.02 aq
x7	Xylitol	$HOCH_2(CHOH)_3CH_2OH$	152.15	1, 531			95–97			s aq
x8	D-(+)-Xylose		150.13	31, 47	1.535 ⁰		144–145			117 aq; s hot alc, pyr
x9	m-Xylylenediamine	$C_6H_4(CH_2NH_2)_2$	136.20	13, 186	1.032	1.5709 ²⁰		265 ^{745mm}	> 112	

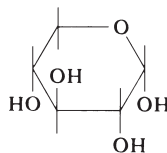
Xylene- α, α' -diol, b18

Xylenols, d579, d580, d581, d582, d583, d584

o-Xylyl bromide, b368

Xylyl chlorides, c258, c259, c260

p-Xylylene glycol, b18



x8

SECTION 2

INORGANIC AND ORGANOMETALLIC COMPOUNDS

Table 2.1 Physical Constants of Inorganic Compounds	2.2
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This section summarizes the properties of various chemical compounds commonly encountered in organic chemistry that are often referred to either as inorganic or organometallic. In some cases, the distinction is artificial and the reader should refer to Section 1 if the expected compound is not presented here. Most compounds containing metals are collected here, rather than in Section 1.

TABLE 2.1 Physical Constants of Inorganic Compounds

Explanation of column headings

Names, while following the IUPAC nomenclature, are generally alphabetized by the central atom to facilitate their location. An example of the table organization is given below for Al_3C_4 , aluminum tetracarbide. It is entered in Table 2.1 as follows:

Main heading	Aluminum
<i>Subgrouping</i>	carbide
Actual table listing	Aluminum (tetra-) carbide (tri-)

Solvates are listed under the entry for the anhydrous salt. Hydrazine hydrate, $\text{H}_2\text{N}-\text{NH}_2\cdot\text{H}_2\text{O}$ is listed under hydrazine. Magnesium sulfate heptahydrate (epsom salt) is listed under **Magnesium**, using the subgroup sulfate 7-water. Inorganic acids are entered under hydrogen. For example, HF is listed under **Hydrogen**, using the subgroup fluoride. Where an elemental designation would be confusing or inappropriate, the compound is listed alphabetically as in the case of **hydroxylamine**, HONH_2 .

Abbreviations used in the Table

>, greater than	ca, approximately	g, gas	pyr, pyridine
α , alpha position	chl, chloroform	glyc, glycerol	s, soluble
a, acid	conc, concentrated	h, hot	satd, saturated
abs, absolute	cub, cubic	hex, hexagonal	sl, slightly
acetone, acet	d, decompose(s)	hyd, hydrolysis	soln, solution
alc, alcohol	dil, dilute	i, insoluble	solv, solvent(s)
alk, alkali, (aq NaOH)	DMF,	ign, ignites	subl, sublimates
anhyd, anhydrous	dimethylformamide	lq, liquid	tetr, tetragonal
aq, aqueous	eth, diethyl ether	MeOH, methanol	THF, tetrahydrofuran
aq reg, aqua regia	EtOH, ethanol	min, mineral	tr, transition
atm, atmosphere	expl, explodes,	misc, miscible	v, very
bz, benzene	explosive	org, organic	vac, <i>vacuo</i> or vacuum
c, solid state	fcc, face-centered cubic	PE, petroleum ether	viol, violently

Formula Weights are based on the International Atomic Weights of 1973 and are computed to the nearest hundredth of an a.m.u.

Density values are given at room temperature unless otherwise indicated by a superscript figure indicating a temperature in $^{\circ}\text{C}$. Thus, 2.487^{15} indicates a density of 2.487 for the named substance at 15°C . For gases density values are given in grams per liter ($\text{g}\cdot\text{L}^{-1}$).

Melting Point values are recorded in $^{\circ}\text{C}$. In certain cases decomposition is indicated with the letter “d” that either precedes or follows the number. The value 250d indicates that the substance melts at 250°C with decomposition. The value d 250 indicates that decomposition only occurs at 250°C and higher temperatures. Where a value such as “ $-6\text{H}_2\text{O}$, 150” is given, it indicates a loss of 6 moles of water per formula weight of the compound at a temperature of 150°C .

Boiling Point values are given at atmospheric pressure (760 mm of mercury) unless otherwise indicated; a value of 82 means that the boiling point is 82°C at 760 mm Hg. A value of 82^{15} means that the boiling point is 82°C when the pressure is 15 mmHg. The specification “subl 550” indicates that the compound sublimates at 550°C .

Solubility is given in parts by weight (of the formula weight) per 100 parts by weight of the solvent. If the solvent is unspecified, it is water. If no temperature is specified, the solubility is for the substance at room temperature. Other temperatures (in $^{\circ}\text{C}$) are indicated by superscript. The symbols of the common mineral acids represent aqueous solutions of those acids.

TABLE 2.1 Physical Constants of Inorganic Compounds

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Aluminum	Al	26.98	2.70	660.1	2450	s HCl, H ₂ SO ₄ , alk
acetylacetonate	Al(C ₅ H ₇ O ₂) ₃	324.31	1.27	subl 193 (vac)	314	i aq; v s alc; s bz, eth
ammonium bis(sulfate) 12-water	AlNH ₄ (SO ₄) ₂ ·12H ₂ O	453.33	1.64	−12 H ₂ O, 250	d > 280	15 aq; i alc
bis(acetylsalicylate)	Al(OOCC ₆ H ₄ O-COCH ₃) ₂ OH	402.30				v sl s aq, alc, eth
bromide	AlBr ₃	266.71	2.64 ¹⁰	97.5	253.3	d viol aq; s alc, acet, bz CS ₂
butoxide, <i>sec</i> -	Al(C ₄ H ₉ O) ₃	246.33	0.967		200–206 ³⁰ mm	v s org solv (flash point 27 °C)
butoxide, <i>tert</i> -	Al(C ₄ H ₉ O) ₃	246.33	1.025 ²⁰ ₀	subl 180		v s org solv
(tetra-) carbide, tri-	Al ₄ C ₃	143.96	2.36	2100	d > 2200	d to CH ₄ in aq (fire hazard)
chlorate	Al(ClO ₃) ₃	277.35				v s aq; s alc
chloride	AlCl ₃	133.34	2.44	194 ^{2.5} atm	subl 181	70 aq (viol); 100 ¹² abs alc; s CCl ₄ , eth; sl s bz
chloride 6-water	AlCl ₃ ·6H ₂ O	241.43	2.40	d 100		83 ²⁰ aq; 25 abs alc; s eth
ethoxide	Al(C ₂ H ₅ O) ₃	162.14	1.42 ²⁰ ₀	134	205 ¹⁴ mm	s hot aq (d); v sl a alc, eth
fluoride	AlF ₃	83.98	2.882 ²⁵ ₄	1040	subl 1276	0.562 ⁵ aq; i a, alk, alc, acet
hydroxide	Al(OH) ₃	78.00	2.42	−H ₂ O, 300		i aq; s a, alk
iodide	AlI ₃	407.71	3.98 ²⁵	191	360	s aq(d); s alc, CS ₂ , eth
isopropoxide	Al(C ₃ H ₇ O) ₃	204.25	1.0346 ²⁰ ₀	118.5	135 ¹⁰ mm	d aq; s alc, bz, chl, PE
nitrate 9-water	Al(NO ₃) ₃ ·9H ₂ O	375.13		73	d 135	64 ²⁵ aq; 100 alc; s acet
oxide	Al ₂ O ₃	101.96	3.965	2054	2980	i aq; v sl s a, alk
phenoxide	Al(C ₆ H ₅ O) ₃	306.27	1.23	d 265		d aq; s alc, chl, eth
potassium bis (sulfate) 12-water	AlK(SO ₄) ₂ ·12H ₂ O	474.39	1.757 ²⁰	−9H ₂ O, 92	−12H ₂ O, 200	11.4 ²⁰ aq
propoxide	Al(C ₃ H ₇ O) ₃	204.25	1.0578 ²⁰ ₀	106	248 ¹⁴ mm	d aq; s alc
sodium bis(sulfate) 12-water	AlNa(SO ₄) ₂ ·12H ₂ O	458.28	1.675 ²⁰	61		110 ¹⁵ aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Aluminum						
stearate	$\text{Al}(\text{C}_{18}\text{H}_{35}\text{O}_2)_3$	877.42	1.010	103		i aq; s alc, bz, alk
sulfate	$\text{Al}_2(\text{SO}_4)_3$	342.15	2.710	d 770		36.4 ²⁰ aq; sl s alc
sulfate 18-water	$\text{Al}_2(\text{SO}_4)_3 \cdot 18\text{H}_2\text{O}$	666.45	1.69 ¹⁷	d 86.5		87 ⁰ aq; i alc
tetrahydroborate	$\text{Al}(\text{BH}_4)_3$	71.53		−64.5	44.5	d aq
Amidosulfuric acid	$\text{H}_2\text{NSO}_3\text{H}$	97.09	2.126	205	d	14.7 aq
Ammonia	NH_3	17.03	0.7188 ²⁰ $\text{g} \cdot \text{L}^{-1}$	−77.75	−33.42	89.9 aq; 13.2 ²⁰ alc; s eth, org solv
− <i>d</i> ₃ or [² H]	ND_3 or N^2H_3	20.05	0.8437 ²⁰ $\text{g} \cdot \text{L}^{-1}$	−74.33	−31.05	
Ammonium						
acetate	$\text{NH}_4\text{C}_2\text{H}_3\text{O}_2$	77.08	1.17 ²⁰	114	d	148 ⁴ aq; 7.9 ¹⁵ MeOH; s alc
benzoate	$\text{NH}_4\text{C}_7\text{H}_5\text{O}_2$	139.16	1.260	d 198	subl 160	20 ¹⁵ aq; 2.8 alc; s glyc; i eth
boranate, tetrafluoro-	NH_4BF_4	104.84	1.87 ¹⁵	subl		25 ¹⁶ aq
bromide	NH_4Br	97.95	2.429	452 (under pressure)	d 397 (vac)	76 ²⁰ aq; s acet, alc, eth
carbamate	$\text{NH}_4\text{COONH}_2$	78.07		subl 60		v s aq; sl s alc; i eth
carbonate 1-water	$(\text{NH}_4)_2\text{CO}_3 \cdot \text{H}_2\text{O}$	114.10		d 20		100 ¹⁵ aq; i alc
cerate(IV), hexanitrat-	$(\text{NH}_4)_2[\text{Ce}(\text{NO}_3)_6]$	548.23				135 ²⁰ aq; s alc, HNO_3
chloride	NH_4Cl	53.49	1.527	subl 340		26 ¹⁵ aq; 0.6 ¹⁹ abs alc; i acet, eth
chromate	$(\text{NH}_4)_2\text{CrO}_4$	152.08	1.91 ¹²	d 180		34 ²⁰ aq; sl s MeOH, acet; i alc
chromium(III) bis(sulfate) 12-water	$\text{NH}_4\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	478.34	1.72	94		7.2 ⁰ aq
citrate	$(\text{NH}_4)_3\text{C}_6\text{H}_5\text{O}_7$	243.22	1.48	d		100 aq; sl s alc
copper(II) tetrachloride 2-hydrate	$\text{Cu}(\text{NH}_4)_2\text{Cl}_4 \cdot 2\text{H}_2\text{O}$	277.46	1.993	−2H ₂ O, 110	d > 120	40 ²⁰ aq; s alc
dichromate(VI)	$(\text{NH}_4)_2\text{Cr}_2\text{O}_7$	252.06	2.155 ²⁵ ₄	d 170		36 ²⁰ aq; s alc (flammable)

dithiocarbamate	$\text{NH}_4\text{S}—\text{CS}—\text{NH}_2$	110.19	1.451 ²⁰	d 99		v s aq; s alc; sl s eth
diuranate(VI)	$(\text{NH}_4)_2\text{U}_2\text{O}_7$	624.22				v sl s aq, alk; s acids
fluoride	NH_4F	37.04	1.009 ²⁵	subl		100 ⁰ aq; s alc
formate	NH_4OOCH	63.06	1.280	116	d 180	143 ²⁰ aq; s alc, eth
hexadecanoate	$\text{NH}_4\text{OOC}(\text{CH}_2)_{14}\text{CH}_3$	273.45		21–22		s aq; sl s bz; i alc, acet
hexafluoroaluminate	$(\text{NH}_4)_3\text{AlF}_6$	195.10	1.78	d > 100		v s aq
hydrogen carbonate	NH_4HCO_3	79.06	1.58	d 35	subl	22 ²⁰ aq; i alc, acet
hydrogen citrate	$(\text{NH}_4)_2\text{HC}_6\text{H}_5\text{O}_7$	226.19	1.48			100 aq; sl s alc
hydrogen difluoride	NH_4HF_2	57.04	1.50	125.6		v s aq; sl s alc
hydrogen oxalate 1-water	$\text{NH}_4\text{HC}_2\text{O}_4 \cdot \text{H}_2\text{O}$	125.08	1.556	— H_2O , 170		s aq; i bz, eth
hydrogen phosphate	$(\text{NH}_4)_2\text{HPO}_4$	132.05	1.619	d 155		69 ²⁰ aq; i alc, acet
hydrogen phosphate, di-	$\text{NH}_4\text{H}_2\text{PO}_4$	115.03	1.803 ¹⁹	d 190		37 ²⁰ aq; sl s alc; i acet
hydrogen sulfate	NH_4HSO_4	115.11	1.78	146.9	d 350	100 aq; i alc, acet
hydrogen sulfide	NH_4HS	51.11	1.17	d 25		128 ⁰ aq; s alc; sl s acet; i bz
hydrogen sulfite	NH_4HSO_3	99.10	2.03	subl 150 (in N_2)		72 ⁰ aq
hydroxide	NH_4OH	35.05		—77		misc aq
iodide	NH_4I	144.95	2.514 ²⁵	subl 551	220 (vac)	172 ²⁰ aq; v s alc, acet
iron(II) bis(sulfate) 6-water	$\text{Fe}(\text{NH}_4)_2(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	392.14	1.864 ²⁰	d 100		36 ²⁰ aq; i alc
molybdate(VI)(6-) 4-water, hepta- nitrate	$(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$	1235.86	2.498	— H_2O , 90	d 190	43 aq; s a; i alc
octadecanoate	$\text{NH}_4\text{OOC}(\text{CH}_2)_{16}\text{CH}_3$	301.50	1.725 ²⁵	169.6	210 ¹¹ mm	192 ²⁰ aq; 3.8 ²⁰ alc; 17 ²⁰ MeOH
octanoate	$\text{NH}_4\text{OOCCH}_7\text{H}_{15}$	161.24		21–22		sl s aq; s alc; i acet
oxalate 1-water	$(\text{NH}_4)_2\text{C}_2\text{O}_4 \cdot \text{H}_2\text{O}$	142.11	1.50	d on standing		v s aq, alc, acet; sl s eth
palladate(II) tetrachloro-	$(\text{NH}_4)_2\text{PdCl}_4$	284.29	2.170	d 70		5.1 ²⁰ aq
perchlorate	NH_4ClO_4	117.50	1.95	d		v s aq; i abs alc
peroxodisulfate	$(\text{NH}_4)_2\text{S}_2\text{O}_8$	228.18	1.982	d 240		22 ²⁰ aq; s MeOH; sl s alc, acet
phosphate, hexafluoro-	NH_4PF_6	163.00	2.180 ¹²	d 120	expl 180	58 ⁰ aq
phosphinate	$\text{NH}_4\text{PH}_2\text{O}_2$	83.03	1.634	d		75 ²⁰ aq; s alc, acet
picrate	$\text{NH}_4\text{C}_6\text{H}_2\text{N}_3\text{O}_7$	246.14	1.719	200	d 240	100 aq; 5 alc; i acet
platinate(IV), hexachloro-	$(\text{NH}_4)_2\text{PtCl}_6$	443.89	3.065	d	expl 423	1.1 ²⁰ aq; sl s alc
silicate, hexafluoro-	$(\text{NH}_4)_2\text{SiF}_6$	178.14	2.011	d		0.5 ²⁰ aq
						18.6 ²⁰ aq; i alc, acet

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Ammonium						
sulfamate	$\text{NH}_4\text{SO}_3\text{NH}_2$	114.13		131	d 160	v s aq; sl s alc
sulfate	$(\text{NH}_4)_2\text{SO}_4$	132.14	1.769 ²⁰	d > 280		43.5 ²⁵ aq; i alc, acet
sulfide	$(\text{NH}_4)_2\text{S}$	68.14		d		v s aq; s alc
DL-tartrate	$(\text{NH}_4)_2\text{C}_4\text{H}_4\text{O}_6$	184.15	1.601	d		58 ¹⁵ aq; sl s alc
tetraborate 4-water	$(\text{NH}_4)_2\text{B}_4\text{O}_7 \cdot 4\text{H}_2\text{O}$	263.44				s aq; i alc
thiocyanate	NH_4SCN	76.12	1.305	149.6	d 170	128 ⁰ aq; v s alc; s acet
thiosulfate	$(\text{NH}_4)_2\text{S}_2\text{O}_3$	148.20	1.679	d 150		v s aq
vanadate(V)(1-)	NH_4VO_3	116.98	2.326	d 200		0.48 ²⁰ aq
Antimony						
(III) chloride	SbCl_3	228.11	3.14 ²⁰	73.4	223.5	10 ²⁰ aq; s alc, bz, chl
(V) chloride	SbCl_5	299.02	2.336 ²⁰	3.5	140	d aq; s HCl, chl, CCl_4
(III) fluoride	SbF_3	178.75	4.379 ²⁰	292	376	444 ²⁰ aq
(V) fluoride	SbF_5	216.74	2.99 ²³	8.3	141	d viol aq; s HOAc; forms solids with alc, bz, CS_2 , eth
hydride	SbH_3	124.77	4.36 ¹⁵	-91.5	-18.4	20 ⁰ mL aq; s CS_2
(III) oxide	Sb_2O_3	291.50	5.2	655	1425	v sl s aq; s HCl, KOH
(V) oxide	Sb_2O_5	323.50	2.78	-O ₂ , >300		v sl s aq; sl s warm KOH, eth
potassium oxide tartrate 0.5-water	$\text{K}(\text{SbO})\text{C}_4\text{H}_4\text{O}_6 \cdot 0.5\text{H}_2\text{O}$	333.93	2.607	d 100		8.3 ²⁰ aq; 6.7 glyc; i alc
(III) sulfide	Sb_2S_3	339.69	4.64	546		0.002 ²⁰ aq d; s H_2SO_4
(V) sulfide	Sb_2S_5	403.82				i aq; s HCl, d NaOH
Argon						
	Ar	39.95	1.7824 g · L ⁻¹	-189.38	-185.87	3.36 ²⁰ mL aq
Arsenic						
	As	74.92	5.72	817 ²⁸ atm	subl 612	i aq; s HNO_3
(III) chloride	AsCl_3	181.28	2.1497 ²⁵	-16	130.2	d aq; misc chl, CCl_4 , eth; s alc
(III) oxide dimer	As_4O_6	395.68	4.15	313	465	1.8 ²⁰ aq; s alc

(V) oxide	As ₂ O ₅	229.84	4.32	d 800		66 ²⁰ aq; s alc
(III) sulfide	As ₂ S ₃	246.04	3.46	300–325	707	i aq; s alk; slowly s hot HCl
Barium						
acetate 1-water	Ba(C ₂ H ₃ O ₂) ₂ ·H ₂ O	273.46	2.19	d 150		76 ²⁰ aq; 0.14 alc
benzenesulfonate	Ba(O ₃ SC ₆ H ₅) ₂	451.70				s aq; sl s alc
carbonate	BaCO ₃	197.35	4.43	d 1360		0.002 aq; s a
chlorate 1-water	Ba(ClO ₃) ₂ ·H ₂ O	322.26	3.18	–H ₂ O, 120	–O ₂ , 250	34 ²⁰ aq
chloride	BaCl ₂	208.25	3.856	962	2029	36 ²⁰ aq
fluoride	BaF ₂	175.34	4.89	1368	2272	0.16 ²⁰ aq
hydrogen phosphate	BaHPO ₄	233.32	4.165 ¹⁵	d 410		0.01 aq; s a
hydroxide 8-water	Ba(OH) ₂ ·8H ₂ O	315.48	2.18 ¹⁶	78		3.9 ²⁰ aq
manganate(VI)(2-)	BaMnO ₄	256.28	4.85			v sl s aq
nitrate	Ba(NO ₃) ₂	261.35	3.24	575	d	9 ²⁰ aq
nitrite 1-water	Ba(NO ₂) ₂ ·H ₂ O	247.37	3.173 ²⁰	d 115		73 ²⁰ aq; i alc
oxide	BaO	153.34	5.72	2013	3088	3.5 ²⁰ aq
perchlorate 3-water	Ba(ClO ₄) ₂ ·3H ₂ O	390.29	2.74	d 400		198 ²⁵ aq; s MeOH; sl s alc, acet
permanganate	Ba(MnO ₄) ₂	375.21	3.77	d 200		62 ¹¹ aq
peroxide	BaO ₂	169.34	4.96	450	–O ₂ , 800	1.5 ⁰ aq
sulfate	BaSO ₄	233.40	4.50 ¹⁵	1580		0.0002 aq
sulfide	BaS	169.40	4.25 ¹⁵	2227		7.9 ²² aq d
sulfite	BaSO ₃	217.40		d		0.02 ²⁰ aq
thiocyanate 2-water	Ba(SCN) ₂ ·2H ₂ O	289.53	2.286 ¹⁸	d 160		170 ²⁵ aq
thiosulfate 1-water	BaS ₂ O ₃ ·H ₂ O	267.48	3.5 ¹⁸	d 220		0.21 ²⁰ aq
Beryllium						
	Be	9.01	1.86	1277	2484	i q; s a, alk
bromide	BeBr ₂	168.83	3.465 ²⁵	506–509	521	v s aq; s alc; 19 pyr
chloride	BeCl ₂	79.92	1.899 ²⁵	399	482	42 aq; s alc, eth, CS ₂ , pyr; i bz
fluoride	BeF ₂	47.01	1.986 ²⁵ ₄	552	1175	v s aq but slow
hydride	BeH ₂	11.03		–H ₂ , 220		d slowly aq; d rapidly a
hydroxide	Be(OH) ₂	43.03	1.92	134 d		s hot conc a, alk
iodide	BeI ₂	262.82	4.2	480	482	hyd aq; s alc, eth, CS ₂
oxide	BeO	25.01	3.01	2408(α)	3787	s conc H ₂ SO ₄
sulfate 4-water	BeSO ₄ ·4H ₂ O	177.14	1.713 ¹¹	–4H ₂ O, 270	d 580	39 ²⁰ aq; i alc

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Bismuth						
chloride, tri-	BiCl_3	315.34	4.75	ca 232	447	d aq; s HCl, alc, eth, acet
fluoride, penta-	BiF_5	303.98	5.4 ²⁵	151	230	d viol aq giving O_3
hydroxide	$\text{Bi}(\text{OH})_3$	260.00	4.36	— H_2O , 100		d aq; s a
(III) nitrate 5-water	$\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$	485.07	2.83	d 30		d aq; s, acet
(III) oxide	Bi_2O_3	495.96	8.76	817	1890	i aq; s a
Boron						
bromide, tri-	BBr_3	250.57	2.695 ⁰	—46.0	91.3	d aq
chloride, tri-	BCl_3	117.19	1.35 ¹²	—107	18	d aq, alc
fluoride, tri-	BF_3	67.81	2.99 g·L ⁻¹	—127.1	—100.4	105 ⁰ mL aq; s bz, chl, CCl_4
fluoride-1-diethyl ether	$\text{BF}_3 \cdot \text{O}(\text{C}_2\text{H}_5)_2$	141.94	1.125 ²⁵	—60.4	125.7	d aq
fluoride-1-methanol	$\text{BF}_3 \cdot \text{CH}_3\text{OH}$	131.89	1.203		59 ⁴ mm	
oxide	B_2O_3	69.62	2.46	450	2065	sl s aq
Bromine	Br_2	159.81	3.1028	—7.3	58.75	3.6 ²⁰ aq; v s alc, chl, eth, CS_2
fluoride, tri-	BrF_3	136.90	2.803 ²⁵	8.77	125.74	d viol aq; d alk
Cadmium						
acetate	$\text{Cd}(\text{C}_2\text{H}_3\text{O}_2)_2$	230.50	2.341	256	d	v s aq
chloride	CdCl_2	183.32	4.047	568	961	120 ²⁵ aq
iodide	CdI_2	366.21	5.670 ³⁰	387	796	85 ²⁰ aq; s alc, acet, eth
oxide	CdO	128.40	8.15	subl 1497		i aq; s a
sulfate-water (3/8)	$3\text{CdSO}_4 \cdot 8\text{H}_2\text{O}$	769.56	3.09	— H_2O , 40	forms mono-hydrate 80	94.4 ²⁵ ; i alc
sulfide	CdS	144.46	4.82 hex		sub 1380 (in N_2)	3.13 ¹⁸ aq; s a
Calcium						
acetate	$\text{Ca}(\text{C}_2\text{H}_3\text{O}_2)_2$	158.17	d > 160			37 ⁰ aq; i alc, acet, bz
arsenate(V)	$\text{Ca}_3(\text{AsO}_4)_2$	398.08	3.620			0.013 ²⁵ aq

bromide	CaBr ₂	199.90	3.353	765	806–812	143 ₂₀ aq; v s alc, acet
carbide, di-	CaC ₂	64.10	2.22		2300	d aq giving C ₂ H ₂
carbonate	CaCO ₃	100.09	2.930	d 900		0.0013 ²⁰ ; s a
chlorate	Ca(ClO ₃) ₂	206.99		340		178 aq; s alc, acet
chloride	CaCl ₂	110.99	2.15	772	1940	75 ²⁰ ; s alc, acet
chloride 6-water	CaCl ₂ ·6H ₂ O	219.08	1.71	–6H ₂ O, 200		536 ²⁰ aq; s alc
citrate 4-water	Ca(C ₆ H ₅ O ₇) ₂ ·4H ₂ O	570.51		–4H ₂ O, 120		0.85 ¹⁸ aq; 0.0065 ¹⁸ alc
cyanamide	CaCN ₂	80.11	2.29 ²⁰ ₄	1340	subl 1150	i aq; no known solv
cyanide	Ca(CN) ₂	92.12		d 350		d aq
diphosphate	Ca ₂ P ₂ O ₇	254.10	3.09	1230		i aq; s a
fluoride	CaF ₂	78.08	3.180	1418	2510	0.002 ²⁰ aq; sl s a
formate	Ca(OOCH) ₂	130.12	2.015	d		16.6 ²⁰ aq; i alc
glycerophosphate	Ca[C ₃ H ₅ (OH) ₂]PO ₄	210.16		d > 170		1.7 ²⁰ aq, i alc
hydrogen phosphate, di- 1-water	Ca(H ₂ PO ₄) ₂ ·H ₂ O	252.07	2.220 ¹⁸ ₄	–H ₂ O, 109	d 203	1.8 ³⁰ aq
hydroxide	Ca(OH) ₂	74.09	2.24	–H ₂ O, 522		0.17 ¹⁰ aq; s a
hypochlorite	Ca(OCl) ₂	142.99	2.35	100 d		d aq evolving Cl ₂ ; i alc
iodate 6-water	Ca(IO ₃) ₂ ·6H ₂ O	497.98		d 35		0.24 ²⁰ aq; i alc
lactate 5-water	Ca(C ₃ H ₅ O ₃) ₂ ·5H ₂ O	308.30		–3H ₂ O, 100	–5H ₂ O, 120	5.4 ¹⁵ aq; v sl s alc
nitrate	Ca(NO ₃) ₂	164.09	2.504 ¹⁸	561		152 ³⁰ aq
nitrite 4-water	Ca(NO ₂) ₂ ·4H ₂ O	204.5	1.674 ⁰ ₀	–2H ₂ O, 44		84.5 ¹⁸ aq; sl s alc
oleate	Ca(C ₁₈ H ₃₃ O ₂) ₂	603.01		83–84	d 140	0.04 aq; s bz, chl; v sl s alc
oxide	CaO	56.08	3.25	2927	3500	0.13 ²⁵ aq; s a
palmitate	Ca(C ₁₆ H ₃₁ O ₂) ₂	550.93		d 155		0.003 aq; sl s bz, chl; i alc, eth
pantothenate (vitamin B ₃)	Ca[O ₂ CH ₂ CH ₂ HO- CH(OH)C(CH ₃) ₂ - CH ₂ OH] ₂	476.55		d 195–196		35 aq; sl s alc, acet
peroxide	CaO ₂	72.08	2.92 ²⁵ ₄	d 275		sl s aq; s a
phenoxide	Ca(OC ₆ H ₅) ₂	226.28				sl s aq, alc
phosphate	Ca ₃ (PO ₄) ₂	310.18	3.14	1730		0.03 ²⁵ ; s a; i alc
salicylate 2-water	Ca(C ₇ H ₅ O ₃) ₂ ·2H ₂ O	350.34		–2H ₂ O, 120	d 240	2.8 ¹⁵ aq; 0.015 ¹⁶ EtOH
selenate 2-water	CaSeO ₄ ·2H ₂ O	219.07	2.68 ²⁰ ₄	–2H ₂ O, 200	d 698	9.2 ²⁵ aq
stearate	Ca(C ₁₈ H ₃₅ O ₂) ₂	607.04		179–180		0.004 ¹⁵ aq; s hot pyr; i chl, eth

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Calcium						
succinate 3-water	$\text{CaC}_4\text{H}_6\text{O}_4 \cdot 3\text{H}_2\text{O}$	212.22				1.28 ²⁰ aq; s a; i alc
sulfate	CaSO_4	136.14	2.960	1400		0.20 aq; s a
sulfate hemihydrate	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$	145.15		−H ₂ O, 163		0.3 ²⁰ aq; s a, glyc
sulfate 2-water	$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$	172.17	2.32	−2H ₂ O, 163		0.26 ²⁰ aq; s a, glyc
sulfite 2-water	$\text{CaSO}_3 \cdot 2\text{H}_2\text{O}$	156.17		−2H ₂ O, 100		0.004 aq; s a; sl s alc
DL-tartrate 4-water	$\text{CaC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$	260.21		−4H ₂ O, 200		0.0045 ²⁵ aq; sl s alc
tetrahydridoaluminate	$\text{Ca}(\text{AlH}_4)_2$	102.10				ign moist air; d viol aq, alc
thiocyanate 3-water	$\text{Ca}(\text{SCN})_2 \cdot 3\text{H}_2\text{O}$	210.29		d 160		150 aq; v s alc
Carbon						
(graphite)	C	12.01	2.25 ²⁰	4000 ^{63.5 atm}	3930	i aq, alc
bromide, tetra-	CBr_4	331.65	3.42	90.1	190	i aq; s alc, chl, eth
chloride, tetra-	CCl_4	153.82	1.5867 ²⁰ ₂₀	−22.9	76.7	i aq; s alc, chl, eth
hydride, tetra-	CH_4	16.04	0.415 ^{−164}	−182.48	−161.49	i aq; s bz
iodide, tetra-	CI_4	519.63	4.34	d 171		sl hyd aq; s alc, bz, eth
oxide, mono-	CO	28.01	0793 (lq)	−205.05	−191.49	2.1 mL aq; s alc, bz
			1.250 g · L ^{−1} (gas)			
oxide di-	CO_2	44.01	1.56 ^{−79} (c)	−56.2	−78.44	31 ¹⁵ mL aq
			1.975 g · L ^{−1}	solid subl		
(tri-) oxide, di-	C_3O_2	68.03	1.114 ⁰ ₄	−112.19	6.4	d aq to malonic acid
selenide, di-	CSe_2	169.93	2.663 ²⁵ ₄	−43	125.1	i aq; d alc, pyr; misc CCl_4 ; s acet, eth
sulfide, di-	CS_2	76.14	1.261 ²²	−111.6	46.26	0.29 ²⁰ aq; s alc, eth

Carbonic acid	$\text{H}_2\text{CO}_3(\text{CO}_2 + \text{H}_2\text{O})$	62.03				known in soln only
Carbonyl						
chloride	COCl_2	98.92	1.392	−127.8	7.6	hyd aq; s bz
fluoride	COF_2	66.01	1.139^{-114}	−114.0	−83.3	hyd aq
sulfide	COS	60.07	1.073^0 $\text{g} \cdot \text{L}^{-1}$	−138.81	−50.23	54^{20} mL aq; s alc, CS_2
Cerium						
(III) chloride	CeCl_3	246.48	3.92	8.7	1730	100^{20} aq; 30 alc; s acet
(IV) fluoride	CeF_4	216.12	4.80	>650	d >550	i aq; s a
(IV) oxide	CeO_2	172.13				i aq; s a
(IV) sulfate	$\text{Ce}(\text{SO}_4)_2$	332.24	3.91	d 195		hyd aq; s H_2SO_4
Cesium						
bromide	CsBr	212.81	4.44	635	1300	107^{18} aq
carbonate	Cs_2CO_3	325.82		d 610		260^{15} aq; 11^{20} alc; s eth
chloride	CsCl	168.36	3.988	645	1324	187^{20} aq; 34^{25} MeOH; v s alc
fluoride	CsF	151.90	4.115	703	1231	322^{18} aq
hydroxide	CsOH	149.91	3.675	272	990	386^{15} aq; s alc
iodide	CsI	259.81	4.510	621	ca 1280	77^{20} aq; s EtOH; i acet
nitrate	CsNO_3	194.91	3.685^{20}_4	414	d 849	23^{20} aq; s acet; v sl s alc
oxalate	$\text{Cs}_2\text{C}_2\text{O}_4$	353.82	3.230^{15}			313 aq
selenate	Cs_2SeO_4	408.77	4.4528^{20}_4			244^{12} aq
sulfate	Cs_2SO_4	361.87	4.243	1019		179^{20} aq; i alc, acet, pyr
Chlorine						
fluoride, tri-	ClF_3	92.45	1.825^{11}	−76.28	11.74	hyd viol aq; glass wool and org matter ign
(di-) oxide	Cl_2O	86.91	3.02^2	−120.6	2.1	3.5^{20} aq (hyd to HClO); s CCl_4
oxide, di-	ClO_2	67.46	1.642^0	−59.6	10.9	11.2^{10} aq
(di-) oxide, hepta-	Cl_2O_7	182.90	1.805^{25}	−91.5	83.6	d aq; expl on concussion or contact with flame or I_2
Chlorosulfonic acid	HSO_3Cl	116.52	1.753^{20}_4	−80	158	d viol aq to $\text{HCl} + \text{H}_2\text{SO}_4$
Chromium						
(II) acetate	$\text{Cr}(\text{C}_2\text{H}_3\text{O}_2)_2$	170.10				sl s aq, alc; i eth
carbonyl, hexa-	$\text{Cr}(\text{CO})_6$	220.06	1.77^{18}	d 130	expl 210	i aq, alc, eth

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Chromium						
(II) chloride	CrCl ₂	122.90	2.878	815	1300	v s aq
(III) chloride	CrCl ₃	158.35	2.76 ¹⁵	877	subl 947	i aq, alc, acet, eth
(III) fluoride	CrF ₃	108.99	3.8	1100	subl	i aq, alc; s HF
(III) nitrate 9-water	Cr(NO ₃) ₃ ·9H ₂ O	400.15		60	d 100	208 ¹⁵ aq; s alc
(III) oxide	Cr ₂ O ₃	152.02	5.21	2330	3000	i aq, alc
(IV) oxide	CrO ₂	83.99	4.89	−O ₂ , 300		i aq; s HNO ₃
(VI) oxide	CrO ₃	99.99	2.70	198	d 250	167 ²⁰ aq; may ign org materials
(III) phosphate 6-water	CrPO ₄ ·6H ₂ O	255.06	2.121 ¹⁴	100		i aq; v s a, alk; sl s HOAc
(II) sulfate 7-water	CrSO ₄ ·7H ₂ O	274.17				23 ⁹ aq
(III) sulfate 18-water	Cr ₂ (SO ₄) ₃ ·18H ₂ O	716.45	1.7	d 100		220 ²⁰ aq
Chromyl						
chloride	CrO ₂ Cl ₂	154.90	1.92	−96.5	117	d aq; s eth
Cobalt						
(II) acetate 4-water	Co(C ₂ H ₃ O ₂) ₂ ·4H ₂ O	249.08	1.705 ¹⁹	−4H ₂ O, 140		s aq; 2.1 ¹⁵ MeOH
(III) acetate	Co(C ₂ H ₃ O ₂) ₃	236.07		d 100		s aq, alc, HOAc
(II) bromide	CoBr ₂	218.75	4.909 ²⁵	678 (in N ₂)		112 ²⁰ aq
(II) carbonate	CoCO ₃	118.94	4.13	d		0.18 ¹⁵ aq; s a
(II) chloride	CoCl ₂	129.84	3.356	740	1087	53 ²⁰ aq
(II) fluoride	CoF ₂	96.93	4.46	1127	1739	1.36 ²⁰ aq; s a
(III) fluoride	CoF ₃	115.93	3.88			d aq; i alc, bz, eth
(II) hydroxide	Co(OH) ₂	92.95	3.597 ¹⁵	d		0.0018 aq; s a
(II) iodide	CoI ₂	312.74	5.68	505 d	570 (vac)	203 aq
(II) nitrate 6-water	Co(NO ₃) ₂ ·6H ₂ O	291.04	1.87	55	d 74	155 ³⁰ aq; v s alc
(II) oxalate	CoC ₂ O ₄	146.95	3.021 ²⁵	d 250		0.002 ¹⁸ aq; s a
(II) oxide	CoO	74.93	6.45	1805		i aq; s a

(II,III) oxide	Co_3O_4	240.80	6.07	d 900		i aq; v sl s a
(II) sulfate 7-water	$\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$	281.10	2.03_4^{25}	96.8	$-7\text{H}_2\text{O}$, 420	65^{20} aq; sl s alc
Copper						
(II) acetate hydrate	$\text{Cu}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot \text{H}_2\text{O}$	199.65	1.882	115	d 240	8 aq; 0.48 MeOH; sl s eth, glyc
(II) acetate–metaarsenite	$\text{Cu}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 3\text{Cu}(\text{AsO}_2)_2$	1013.77				i aq; s a, NH_4OH
(I) bromide	CuBr	143.45	4.98	488	1318	v sl s aq; s a
(II) bromide	CuBr_2	223.31	4.710_4^{20}	498		126 aq; s alc, acet, pyr; i bz, eth
(II) chlorate 6-water	$\text{Cu}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$	338.53		65	d 100	242^{18} aq; v s alc; s acet
(I) chloride	CuCl	98.99	4.14	430	1212	0.024 aq; s HCl
(II) chloride	CuCl_2	134.44	3.386_4^{25}	d 300		73^{20} aq; s alc, acet
(II) chloride 2-water	$\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$	170.47	2.54	$-2\text{H}_2\text{O}$, 100	d	76^{25} aq; v s alc; s acet
(I) cyanide	CuCN	89.56	2.92	473 (in N_2)	d	0.00026 aq; s HCl, KCN
(II) fluoride	CuF_2	101.54	4.23	770	1449	0.075 aq; s a
formate	$\text{Cu}(\text{OOCH})_2$	153.55	1.831			12.5 aq
hydroxide	$\text{Cu}(\text{OH})_2$	97.55	3.368	160		i aq; s a
(I) iodide	CuI	190.44	5.62	588	1207	i aq; s HCl, KI
(II) nitrate 3-water	$\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$	241.60	2.05	114.5	d 170	138^0 aq; v s alc
(II) oleate	$\text{Cu}(\text{OOC}_{17}\text{H}_{33})_2$	626.43				i aq; sl s alc; s eth
(I) oxide	Cu_2O	143.08	6.0	1236	$-\text{O}_2$, 1800	i aq; s HCl
(II) oxide	CuO	79.54	6.315_4^{14}	d 1122		i aq, alc; s a
(II) perchlorate	$\text{Cu}(\text{ClO}_4)_2$	262.43	2.225^{23}	82.3	d 130	146^{30} aq; s eth; i bz, CCl_4
(II) stearate	$\text{Cu}(\text{OOC}_{17}\text{H}_{35})_2$	630.46		ca 250		i aq, alc, eth; s pyr, hot bz
(II) sulfate	CuSO_4	159.61	3.603	805 d		14.3^0 aq
(II) sulfate 5-water	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$	249.68	2.284_4^{16}	$-5\text{H}_2\text{O}$, 150		32^{20} aq; s MeOH, glyc; sl s EtOH
Cyanogen						
azide	$\text{NC}—\text{CN}$	52.04	$2.335 \text{ g} \cdot \text{L}^{-1}$	-27.84	-21.15	420^{20} mL aq; 230 mL alc
	$\text{NC}—\text{N}_3$	68.04		detonates		s acetonitrile; can be handled safely only in solv
bromide	CNBr	105.93	2.015_4^{20}	51.4	61.35	v s aq, alc, eth
chloride	CNCl	61.48	1.186	-6.90	13.0	s aq, alc, eth
iodide	CNI	152.92		146–147	subl 140	s aq, alc, eth
Deuterium						
oxide	D_2 or $^2\text{H}_2$	4.03	0.169^{mp} (lq)	-252.89	-248.24	sl s aq
	D_2O or $^2\text{H}_2\text{O}$	20.03	1.1056^{20}	3.82	101.43	misc aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Disulfuryl dichloride	S ₂ O ₃ Cl ₂	215.03	1.818 ¹¹	−37.5	152.5	d aq, a
Diphosphoric(V) acid	H ₄ P ₂ O ₇	117.98		61		s aq
Fluorine	F ₂	38.00	1.554 ²⁵ g·L ^{−1}	−219.70	−188.20	d aq viol
Fluoroboric acid	HF ₃	87.81		d 130		v s aq
Fluorosulfonic acid	HSO ₃ F	100.07	1.743 ¹⁵	−87.3	165.5	s aq
−d or [H]	DSO ₃ F or ² HSO ₃ F	101.08		−89	163	s aq
Germane	GeH ₄	76.62	1.523 ^{−142}	−165.9	−88.5	sl s hot HCl
Gold						
(III) chloride	AuCl ₃	303.33	3.9	254 d	subl 265	68 ²⁰ aq
Helium	He	4.00	0.1784 ⁰ g·L ^{−1}	−272.2 ²⁵ atm	−268.935	0.861 ²⁰ mL aq
			0.1249 (lq)			
Hydrazine	H ₂ NNH ₂	32.05	1.0083 ²⁰	1.54	113.8	misc aq, alc
hydrate	H ₂ NNH ₂ ·H ₂ O	50.16	1.038 ²¹	−51.7	119.4	misc aq, alc
Hydrazinium						
(1+) chloride	H ₂ NNH ₃ Cl	68.51		92.6	d 240	v s aq
(2+) chloride	ClH ₃ NNH ₃ Cl	104.97	1.4226 ²⁰	198	d 200	v s aq; sl s alc
(2+) sulfate	(H ₃ NNH ₃)SO ₄	130.13	1.378	254	d	3.4 ²⁰ aq; i alc
Hydrogen	H ₂	2.02	0.0899 g·L ^{−1}	−259.76	−252.76	1.9 mL aq
azide	HN ₃	43.03	1.126	−80	37	v s aq (v expl)
borate (1−)	HBO ₂	43.83	2.486	236		v sl s aq
borate(3−), ortho-	H ₃ BO ₃	61.83	1.435 ¹⁵	171.0	d 300	6.4 ³⁰ aq
bromide	HBr	80.92	3.388 ²⁰ g·L ^{−1}	−86.81	−66.71	193 ²⁵ aq; s alc
			2.160 ^{−66} (lq)			
bromide	48% HBr + H ₂ O		1.49 g·L ^{−1}	−11	126	v s aq (constant boiling)
bromide-d	DBr or ² HBr	81.92	3.39 ²⁰ g·L ^{−1}	−87.46	−66.5	v s aq

chloride	HCl	36.46	$1.526^{20} \text{ g} \cdot \text{L}^{-1}$ 1.187^{-85} (lq)	−114.18	−85.00	72^{20} aq
chloride	20.24% HCl + H ₂ O		1.097		110	v s aq (constant boiling)
cyanide	HCN	27.06	$0.901 \text{ g} \cdot \text{L}^{-1}$ 1.2675^{10} (lq)	−13.24	25.70	v s aq
fluoride	HF	20.01	$0.922^0 \text{ g} \cdot \text{L}^{-1}$ 0.957^{19} (lq)	−83.57	19.52	v s aq
fluoride	35.35% HF + H ₂ O				120	v s aq (constant boiling)
iodide	HI	127.92	$5.37^{20} \text{ g} \cdot \text{L}^{-1}$ 2.799^{-35} (lq)	−50.79	−35.35	70^0 aq
iodide	57% HI + H ₂ O		1.70^{15}		127	v s aq (constant boiling)
nitrate	HNO ₃	63.02	1.5027	−41.59	83	v s aq
nitrate	69% HNO ₃ + H ₂ O		1.41^{20}		120.5	misc aq (constant boiling)
oxide	H ₂ O	18.02	1.000^4	0.00	100.00	
oxide-d ₂	D ₂ O or ² H ₂ O	20.03	1.1045	3.82	101.43	misc aq
perchlorate 2-water	HClO ₄ ·2H ₂ O	136.49	1.67^{20}	−17.8	203	v s aq (commercial 72% a)
periodate(1−)	HIO ₄	191.91		subl 110	d 138	440^{25} aq
periodate(5−)	H ₅ IO ₆	227.94		130	d 140	113 aq
peroxide	H ₂ O ₂	34.02	1.4649^0	−0.40	151.2	misc aq; s alc, eth
phosphate(V) (1−)	HPO ₃	79.98	2.2−2.5	subl		s aq
phosphate(V) (3−)	H ₃ PO ₄	98.00	1.88	42.3	d 213	v s aq (commercial 85% a)
phosphide	PH ₃	34.00	1.529 $\text{g} \cdot \text{L}^{-1}$	−133.81	−87.78	26^{17} mL aq ; s alc, eth
selenide	H ₂ Se	80.98	2.12^{-42}_4	−65.73	−42	9.5^{20} mL aq
sulfide	H ₂ S	34.08	1.1906 $\text{g} \cdot \text{L}^{-1}$	−85.52	−60.33	0.334^{25} mL aq
telluride	H ₂ Te	129.63	6.234 $\text{g} \cdot \text{L}^{-1}$	−49	−2	d aq
tungstate(VI) (2−)	H ₂ WO ₄	249.86	5.5	−H ₂ O, 100		i aq; s alk, HF
Hydroxylamine	HONH ₂	33.03	1.332	33.1	$58^{22 \text{ mm}}$	s aq, alc
Hydroxylammonium						
chloride	HONH ₃ Cl	69.49	1.680^{20}	150.5	d	83^{17} aq ; 4.4^{20} alc
sulfate	(HONH ₃) ₂ SO ₄	164.14		d 170		69^{20} aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Iodic acid	HIO ₃	175.91	4.629 ⁰	d 110 to H ₃ IO ₆	d 195 to I ₂ O ₅	310 ¹⁶ aq
Iodine	I ₂	53.82	4.660 ²⁰	113.60	184.24	0.029 ²⁰ aq; s alc, bz, chl, CS ₂ , CCl ₄ , eth
bromide	IBr	206.81	4.4157 ⁰	42	116.d	s aq, alc, eth
chloride	ICl	162.36	3.20	27.38	97.8	d aq; s alc, eth
chloride, tri-	ICl ₃	233.26	3.202	101 d		d aq; s alc, bz, eth
fluoride, penta-	IF ₅	221.90	3.252	8.5	102	d aq
fluoride, hepta-	IF ₇	259.89	2.8 ⁶ g · L ⁻¹	4.5	5.5	
(di-) oxide, penta-	I ₂ O ₅	333.81	4.799 ²⁵	d 275		187 ¹³ aq
Iron	Fe	55.85	7.86	1537	2872	i aq; s a
(II) bromide	FeBr ₂	215.67	4.636	691	934	117 ²⁰ aq
(III) bromide	FeBr ₃	295.57		subl		s aq
carbonyl, penta-	Fe(CO) ₅	195.00	1.49	-21	103	i aq; s alc, bz, eth
(II) chloride	FeCl ₂	126.75	3.16 ²⁵	677	1024	63 ²⁰ aq; v s alc, acet; i eth
(III) chloride	FeCl ₃	162.21	2.898	304	332	74 ⁰ aq
(III) ferrate(II), hexacyano-	Fe ₄ [Fe(CN) ₆] ₃	859.25	1.80	d		i aq; s HCl
(II) fluoride	FeF ₂	93.84	4.09	1100	1837	sl s aq; s a
(III) fluoride	FeF ₃	112.84	3.87	subl 927		0.091 ²⁵ aq; s a; i alc, bz
(II) iodide	FeI ₂	309.66	5.315	587	1093	s aq
(III) nitrate 9-water	Fe(NO ₃) ₃ · 9H ₂ O	404.02	1.684 ²¹	47	d 100	138 ²⁰
(II) oxalate 2-water	FeC ₂ O ₄ · 2H ₂ O	179.90	2.28	d 150–160		0.044 ¹⁸ aq; s a
(II) oxide	FeO	71.85	5.7	1377	d 3414	i aq; s a
(III) oxide	Fe ₂ O ₃	159.69	5.24	1462 d		i aq; s HCl
(II, III) oxide	Fe ₃ O ₄	231.54	5.1	1597		i aq; s a
(II) sulfate 7-water	FeSO ₄ · 7H ₂ O	278.04	1.89			48 ²⁰ aq

(III) sulfate	$\text{Fe}_2(\text{SO}_4)_2$	399.88	3.097 ¹⁸	d 1178		sl s aq (hyd); sl s alc
(III) sulfate 9-water	$\text{Fe}_2(\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$	562.01	2.1	d 175		440 aq
Krypton	Kr	83.80	3.736	– 157.2	– 153.4	5.94 ²⁰ mL aq
			$\text{g} \cdot \text{L}^{-1}$			
Lead	Pb	207.21	11.34 (fcc)	327.50	1753	i aq; s HNO_3
(II) acetate 3-water	$\text{Pb}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 3\text{H}_2\text{O}$	379.33	2.55	d 200		46 ¹⁵ aq
(IV) acetate	$\text{Pb}(\text{C}_2\text{H}_3\text{O}_2)_4$	443.37	2.228 ¹⁷	175		d aq; s chl
(II) azide	$\text{Pb}(\text{N}_3)_2$	291.23		expl 350		0.023 ¹⁸ aq; s HOAc
(II) carbonate	PbCO_3	267.20	6.6	d 340		i aq; s a, alk
(II) chromate(VI) (2–)	PbCrO_4	323.18	6.12 ¹⁵	844	d	i aq; s a
(IV) fluoride	PbF_4	283.21	6.7	600		hyd aq
(II) nitrate	$\text{Pb}(\text{NO}_3)_2$	331.23	4.53 ²⁰	d 200		56 ²⁰ aq; 1.3 MeOH
(II) oleate	$\text{Pb}(\text{C}_{18}\text{H}_{33}\text{O}_2)_2$	770.12				i aq; s alc, bz, eth
(II) oxide	PbO	223.21	9.53	886	1516	0.0017 ²⁰ ; s HNO_3
(IV) oxide	PbO_2	239.21	9.375	d 752		i aq; s HCl
(II) phosphate	$\text{Pb}_3(\text{PO}_4)_2$	811.59	6.9	1014		i aq; s HNO_3 , alk
(II) stearate	$\text{Pb}(\text{C}_{18}\text{H}_{35}\text{O}_2)_2$	774.15		ca 125		0.05 ³⁵ aq; s hot alc
(II) sulfate	PbSO_4	303.28	6.2	1090		0.004 aq
Lithium	Li	6.94	0.535 ²⁰	180.6	1340	d aq to LiOH
aluminate, tetrahydrido-	LiAlH_4	37.95	0.917	d 125		d aq, alc; 30 eth (flammable)
amide	LiNH_2	22.96	1.178 ¹⁸	374	d 430	d aq; i bz, eth
benzoate	$\text{LiC}_7\text{H}_5\text{O}_2$	128.05		> 300		33 aq; 7.7 alc
boronate	LiBH_4	21.79	0.666	268	d 380	d aq; s eth, THF
bromate	LiBrO_3	134.85	3.62			179 ²⁰ aq
bromide	LiBr	86.84	3.464	550	1289	164 aq; s alc, eth
carbonate	Li_2CO_3	73.89	2.11 ⁰	720	d	1.3 ²⁰ aq; i alc; s a
chloride	LiCl	42.40	2.068	610	1383	77 ²⁰ aq; s alc, acet
fluoride	LiF	25.94	2.640 ²⁰	846	1717	0.13 ²⁵ aq; s a
hydride	LiH	7.95	0.780	688.7	d 950	d aq; no known solv (flammable)
hydroxide	LiOH	23.95	2.54	471.2	1626	12.4 ²⁰ aq
iodide	LiI	133.84	4.061	467	1178	165 ²⁰ aq; v s alc
iodide 3-water	$\text{LiI} \cdot 3\text{H}_2\text{O}$	187.89	3.5	73	– 3H ₂ O, 300	200 aq; 200 alc
nitrate	LiNO_3	68.94	2.38	261		70 ²⁰ aq; s alc

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Lithium						
perchlorate	LiClO ₄	106.40	2.43 ²⁵	236	d 400	56 ²⁰ aq
sulfate	Li ₂ SO ₄	109.88	2.22	860		34.5 ²⁰ aq
Magnesium						
amide	Mg(NH ₂) ₂	24.31	1.74 ²⁰	650	1105	i aq; s a
bromide	MgBr ₂	56.37	1.39 ²⁵ ₄	ign in air		d viol aq giving NH ₃
bromide 6-water	MgBr ₂ ·6H ₂ O	184.13	3.72	711	1158	101 ²⁰ aq
carbonate	MgCO ₃	292.22	2.00	165 d		160 ²⁰ aq; s alc
chloride	MgCl ₂	84.32	2.958	d 402		0.01 aq; s a
hydride	MgH ₂	95.23	2.41	714	1437	54.6 ²⁰ aq
hydroxide	Mg(OH) ₂	26.34	1.45	d 287 (vac)	ign air	d viol aq, alc
oleate	Mg(C ₁₈ H ₃₃ O ₂) ₂	58.33	2.36	268 d		i aq; s a
oxide	MgO	293.61				i aq; s alc, eth, PE
perchlorate	Mg(ClO ₄) ₂	40.52	3.58	2825	3260	i aq; s a
sulfate 7-water	MgSO ₄ ·7H ₂ O	223.23	2.21 ²⁰	d 251		49.6 aq
sulfite 6-water	MgSO ₃ ·6H ₂ O	246.49	1.67	−6H ₂ O, 120	−7H ₂ O, 250	27.2 aq; s alc
		212.47	1.725	−6H ₂ O, 200	d	66 ²⁵ aq
Manganese						
acetate 4-water	Mn(C ₂ H ₃ O ₂) ₂ ·4H ₂ O	245.08	1.589			38 ⁵⁰ aq; s alc
bromide 4-water	MnBr ₂ ·4H ₂ O	286.82		54d		200 aq; s alc
carbonate	MnCO ₃	114.94	3.125	d		0.0065 ²⁵ aq; s a
(di-) carbonyl, deca-	Mn ₂ (CO) ₁₀	389.99	1.75 ²⁵	155 (CO atm)	d 110	i aq; s org solv
chloride 4-water	MnCl ₂ ·4H ₂ O	197.91	2.01	−4H ₂ O, 198		143 aq; s alc; i eth
(III) fluoride	MnF ₃	111.93	3.54	d 600		hyd aq; s a
nitrate 6-water	Mn(NO ₃) ₂ ·6H ₂ O	287.05	1.8	25.8		v s aq, alc
(IV) oxide	MnO ₂	86.94	5.026	d 530		i aq; s HCl
sulfate hydrate	MnSO ₄ ·H ₂ O	169.01	2.95	−H ₂ O, 400		70 ²⁰ aq

Mercury	Hg	200.59	13.594 ²⁰	−38.86	356.60	i aq; s HNO ₃
(II) acetate	Hg(C ₂ H ₃ O ₂) ₂	318.70	3.28	178		25 ¹⁰ aq; 7.5 ¹⁵ MeOH
(II) bromide	HgBr ₂	360.44	6.05	241	subl > 241	0.56 ²⁰ aq; 20 ²⁵ alc
(I) chloride	Hg ₂ Cl ₂	472.09	7.150	subl 382	d	0.00027 aq; s aqua regia
(II) chloride	HgCl ₂	271.52	5.44	277	304	6.6 ²⁰ aq; 33 alc; 4 eth
(II) cyanide	Hg(CN) ₂	252.65	3.996	d 320		9.3 ²⁰ aq; 8 alc; 25 MeOH
(II) fluoride	HgF ₂	238.61	8.95 ¹⁵	645	647	hyd aq; s HF
(II) iodide	HgI ₂	454.45	6.28	259	350	0.006 ²⁵ aq; 1 alc; 1.7 acet
(II) nitrate	Hg(NO ₃) ₂	324.63	4.3	79	d	v s aq; s acet
(II) oxide	HgO	216.61	11.14	d 476		0.005 ²⁵ aq; s a
(I) sulfate	Hg ₂ SO ₄	497.29	7.56	d		0.06 ²⁵ aq; s HNO ₃
(II) sulfate	HgSO ₄	296.68	6.47	d		d aq; s a
(II) sulfide, red	HgS	232.68	8.10	subl 583		i aq; s aqua regia
Molybdenum						
carbonyl, hexa-	Mo(CO) ₆	264.02	1.96	subl 102	156.4	s bz
(V) chloride	MoCl ₅	273.21	2.928	194	264	hyd aq; s conc a
(VI) oxide	MoO ₃	143.95	4.696 ²⁶	801	1155	0.22 ²⁸ aq; s alk, NH ₃
sulfide, di-	MoS ₂	160.08	5.06 ¹⁵	2375	subl 450	i aq; s aqua regia
Molybdic acid hydrate	H ₂ MoO ₄ •H ₂ O	179.97	3.124 ¹⁵	−H ₂ O, 70		0.133 ¹⁸ ; s alk
Molybdic phosphoric acid	H ₇ [P(Mo ₂ O ₇) ₆]•28H ₂ O	2365.71	2.53	78		hyd aq
Neon	Ne	20.18	0.8899 ⁰ g•L ^{−1}	−248.6	−246.1	1.05 ²⁰ mL aq
Nickel	Ni	58.71	8.90	1455	2920	i aq; s HNO ₃
acetylacetonate	Ni(C ₅ H ₇ O ₂) ₂	256.93	1.455 ¹⁷	229	235	s aq, alc, bz, chl
bromide	NiBr ₂	218.53	5.098	963	subl	131 ²⁰ aq
chloride 6-water	NiCl ₂ •6H ₂ O	237.70				111 ²⁰ aq
dimethylglyoxime	Ni(HC ₂ H ₆ N ₂ O ₂) ₂	288.91		subl 250		i aq; s abs alc, a
formate 2-water	Ni(OOCH) ₂ •2H ₂ O	184.78	2.154 ²⁰	−2H ₂ O, 130	d 180	s aq; i alc
nitrate 6-water	Ni(NO ₃) ₂ •6H ₂ O	290.81	2.05	56.7	136.7	150 ²⁰ aq
sulfate 6-water	NiSO ₄ •6H ₂ O	262.86	2.07	53.3		40 ²⁰ aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Niobium						
(V) chloride	NbCl ₅	270.20	2.75	204	250	s HCl, CCl ₄
(V) fluoride	NbF ₅	187.91	2.70 ⁸⁰	80	235	hyd aq, alc
(V) oxide	Nb ₂ O ₅	265.82	4.6	1512		i aq; s HF, hot H ₂ SO ₄
Nitrogen	N ₂	28.01	1.165 ²⁰ g·L ⁻¹	-210.00	-195.81	1.52 ²⁰ mL aq
[¹⁵ N]	¹⁵ N ₂	30.01	1.25 ²⁰ g·L ⁻¹	-209.95	-195.73	
chloride, tri-	NCl ₃	120.37	1.653 ²⁰	-27	71	i aq; s bz, CS ₂ , CCl ₄
(di-) oxide	N ₂ O	44.02	1.8433 ²⁰ g·L ⁻¹	-90.85	-88.47	130 ⁰ mL aq; s alc
oxide	NO	30.01	1.2488 ²⁰ g·L ⁻¹	-163.64	-151.76	7 ⁰ mL aq
(di-) oxide, tetra-	N ₂ O ₄	92.02	1.447 ²⁰ ₄	-9.3	21.10 d	d aq; s HNO ₃ , H ₂ SO ₄ , chl
(di-) oxide, penta-	N ₂ O ₅	108.01	2.05 ¹⁵	30	47.0	s aq, chl
Nitrosyl						
chloride	NOCl	65.47	1.592 ⁻⁵	-61.5	-5.5	hyd aq
fluoride	NOF	49.01	2.788 ²⁰ g·L ⁻¹	-132.5	-59.9	hyd aq
Nitryl						
chloride	NO ₂ Cl	81.46	2.81 ¹⁰⁰ g·L ⁻¹	-145	-13.5	d aq
fluoride	NO ₂ F	65.00	2.7 ²⁰ g·L ⁻¹	-166.0	-72.4	d aq
Osmium oxide, tetra-	OsO ₄	254.20	4.91	40.6	130.0	7.24 ²⁵ aq; 375 ²⁵ CCl ₄
Oxygen	O ₂	32.00	1.331 ²⁰ g·L ⁻¹	-218.75	-182.96	36 ²⁵ mL aq

Ozone	O ₃	48.00	1.998 ²⁰ g·L ⁻¹	−192.5	−110.50	49.4 ⁰ mL aq
Palladium	Pd	106.4	12.023	1550	2940	s hot HNO ₃ , H ₂ SO ₄
acetate	Pd(C ₂ H ₃ O ₂) ₂	224.49		205d		i aq, alc; s acet, chl
chloride	PdCl ₂	177.30	4.0 ¹⁸	680	d 680	s aq
nitrate	Pd(NO ₃) ₂	230.42		d		hyd aq; s HNO ₃
oxide	PdO	122.40	8.70 ²⁰	870 d		i aq, a
Perchloryl fluoride	ClO ₃ F	102.46	0.637	−147.74	−46.67	
Phosphine	PH ₃	34.00	1.529	−133.81	−87.78	26 ¹⁷ mL aq; s alc, eth
			g·L ⁻¹			
Phosphinic acid	HPH ₂ O ₂	66.00	1.493 ¹⁹	26.5	d 50	s aq
Phosphonic acid	H ₂ PHO ₃	82.00	1.651 ²¹	ca 73	d 180	v s aq, alc
Phosphoric acid						
meta-	HPO ₃	79.98	2.2–2.5			slowly hyd aq; s alc
ortho-	H ₃ PO ₄	98.00	1.88	42.35		
commercial 85% acid			1.685	anhyd 150	to H ₄ P ₂ O ₇ ca 200; to HPO ₃ > 300	v s aq
fluoro-	H ₂ PO ₃ F	99.99	1.818	−80		
Phosphorus						
(white)	P (P ₄ molecules)	30.97	1.828	44.2	280.3	i aq; 0.025 alc; 1 eth; 2.5 chl, bz; 1.25 CS ₂
(red)	P	30.97	2.34	597	subl 416	i aq (ign in air 260°C)
bromide, tri-	PBr ₃	270.73	2.85 ¹⁵	−40.5	173.2	d aq, alc; s acet, CS ₂
bromide, penta-	PBr ₅	430.56	3.46 ²⁰	d 100		d aq; s CCl ₄ , CS ₂
chloride, tri-	PCl ₃	137.35	1.575 ²⁰	−91	75	d aq, alc; s bz, chl
chloride, penta-	PCl ₅	208.27	2.119 ²⁰	subl 100	166 d	hyd aq; s CCl ₄ , CS ₂
fluoride, penta-	PF ₅	125.98	5.805	−93.8	−84.6	hyd aq
			g·L ⁻¹			
(tetra-) oxide, hexa-	P ₄ O ₄	219.90	2.136 ²⁰	24	175 (in N ₂)	hyd aq; s bz, CS ₂
(tetra-) oxide, deca-	P ₄ O ₁₀	283.88	2.30	340	subl 360	d aq; s H ₂ SO ₄
(tetra-) selenide, tri-	P ₄ Se ₃	360.80	1.31	245	360–400	hyd aq; s bz, chl, acet
(tetra-) sulfide, deca-	P ₄ S ₁₀	444.54	2.09	288	514	hyd aq; s alk, CS ₂

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Phosphoryl chloride, tri-Platinic(IV) acid	POCl ₃	153.35	1.645 ²⁵	2	105	d aq, alc
6-water, hexachloro-Platinum	H ₂ PtCl ₆ · 6H ₂ O	517.92	2.431	60		v s aq, alc
Platinum	Pt	195.09	21.45 ²⁰	1770	3824	i aq; s aqua regia, fused alk
(II) chloride	PtCl ₂	266.00	6.05	d 581		i aq; s HCl, NH ₄ OH
(IV) oxide	PtO ₂	227.09	10.2	450		i aq, aqua regia
Potassium	K	39.10	0.856 ²⁰	63.7	765.5	d to KOH aq; s a
acetate	KC ₂ H ₃ O ₂	98.14	1.57 ²⁵	292		256 ²⁰ aq; 34 alc
bismuthate(4—), heptaiodo-	K ₄ BiI ₇	1253.82				d aq; s alk iodide soln
borate, tetrahydrido-	KBH ₄	53.95	1.11	d 497		21 ²⁵ aq; 3.5 ²⁰ MeOH
bromate	KBrO ₃	167.01	3.27 ¹⁷	350	d 370	6.9 ²⁰ aq
bromide	KBr	119.01	2.75	734	1398	65 ²⁰ aq; 0.4 alc
carbonate	K ₂ CO ₃	138.20	2.29	901	d	111 ²⁰ aq; i alc
chlorate	KClO ₃	122.55	2.238 ²⁰	368	d 368	7.3 ²⁰ aq; 2 glyc
chloride	KCl	74.56	1.988	771	1437	34 ²⁰ aq; 7 glyc
chromate(VI)	K ₂ CrO ₄	194.20	2.732 ¹⁸	975		64 ²⁰ aq; i alc
citrate hydrate	K ₃ C ₆ H ₅ O ₇ · H ₂ O	324.42	1.98	d 230		167 ¹⁵ aq
cobaltate(III) 1.5-water, hexanitrito-	K ₃ [Co(NO ₂) ₆] · 1.5H ₂ O	479.30		d 200		0.089 ¹⁷ aq; v sl s alc
cyanate	KOCN	81.11	2.048	d 700–900		s aq; sl s alc
cyanide	KCN	65.12	1.52 ¹⁶	622	1625	50 aq
dichromate(VI)	K ₂ Cr ₂ O ₇	294.19	2.676 ²⁵	398	d 500	12.3 ²⁰ aq
disulfate(IV)	K ₂ S ₂ O ₅	222.32				s aq (flammable if ground)

ethyldithiocarbonate	$\text{KC}_2\text{H}_5\text{OCSS}$	160.30	1.558 ²²	d 200		v s aq
ferrate(III), hexacyano-	$\text{K}_3[\text{Fe}(\text{CN})_6]$	329.26	1.89	d		84 ²⁰ aq (slow)
fluoride	KF	58.10	2.481	858	1517	95 ²⁰ aq
formate	KOOCH	84.10	1.91	167.5	d 168	337 ²⁰ aq
gluconate	$\text{KC}_6\text{H}_{11}\text{O}_7$	234.24		d 180		v s aq; i alc, bz, chl
hydride	KH	40.11	1.43	417 d		d aq
hydrogen arsenate, di-	KH_2AsO_4	180.02	2.867	288		19 ⁶ aq; 63 gly; i alc
hydrogen carbonate	KHCO_3	100.11	2.17	d 100–200		34 ²⁰ aq
hydrogen difluoride	KHF_2	78.11	2.37	238.7	d 478	30 ²⁰ aq; s alc
hydrogen bisiodate	$\text{KH}(\text{IO}_3)_2$	389.92				1.3 ¹⁵ aq
hydrogen oxalate	KHC_2O_4	128.11	2.044	d		2.5 aq
hydrogen bisoxalate dihydrate, tri-	$\text{KH}_3(\text{C}_2\text{O}_4)_2 \cdot 2\text{H}_2\text{O}$	254.20	1.836	d		1.8 ¹³ aq
hydrogen phosphate	K_2HPO_4	174.18		d		150 aq
hydrogen phosphate, di-	KH_2PO_4	136.09	2.338	400	d	22.6 ²⁰ aq
hydrogen phthalate	$\text{KHC}_8\text{H}_4\text{O}_4$	204.22	1.636 ²⁵	d		10.2 aq; sl s alc
hydrogen sulfate	KHSO_4	136.17	2.24	197	d	48 ²⁰ aq
hydrogen tartrate	$\text{KHC}_4\text{H}_4\text{O}_6$	188.18	1.956			0.5 ²⁰ aq
hydroxide	KOH	56.11	2.044	406	1320	112 ²⁰ aq; 33 alc
iodate	KIO_3	214.02	3.89 ²⁵	560 d		8.1 ²⁰ aq; i alc
iodide	KI	166.02	3.12	681	1345	144 ²⁰ aq; 4,5 alc; 1.2 acet
manganate(VI)	K_2MnO_4	197.12		d 190		s aq (stable in KOH)
nitrate	KNO_3	101.10	2.109 ¹⁶	334.3	d 400	32 ²⁰ aq; 0.16 alc; s glyc
nitrite	KNO_2	85.10	1.915	441	d 250	306 ²⁰ aq
oxalate hydrate	$\text{K}_2\text{C}_2\text{O}_4 \cdot \text{H}_2\text{O}$	184.24	2.127 ⁴	— H_2O , 160	d	36 ²⁰ aq
periodate	KIO_4	230.01	3.618 ¹⁵	582 d		0.42 ²⁰ aq
permanganate	KMnO_4	158.03	2.703	d 240		6.34 ²⁰ aq
peroxide	K_2O_2	110.20		490		d
peroxodisulfate	$\text{K}_2\text{S}_2\text{O}_8$	270.32	2.477	d 100		5.3 ²⁰ aq
phenolsulfonate hydrate	$\text{KC}_6\text{H}_4(\text{OH})\text{SO}_3 \cdot \text{H}_2\text{O}$	240.28	1.87			s aq, alc
phosphate	K_3PO_4	212.28	2.564 ¹⁷	1340		92 ²⁰ aq
selenocyanate	KSeCN	144.08		d 100		s aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Potassium						
silicate(2—)	K ₂ SiO ₃	154.29		976		s aq
silicate, hexafluoro-	K ₂ SiF ₆	220.25	2.27	d		sl s aq
sodium tartrate 4-water	KNaC ₄ H ₄ O ₆ ·4H ₂ O	282.23	1.790	70–80	d 220	54 ¹⁵ aq
sorbate	KC ₆ H ₇ O ₂	150.22	1.363	d 270		110 ²⁰ aq
stannate(IV) 3-water	K ₂ SnO ₃ ·3H ₂ O	298.94	3.197	–3H ₂ O, 140		100 ²⁰ aq
sulfate	K ₂ SO ₄	174.27	2.662	1067	1670	11 ²⁰ aq; 1.3 glyc; i alc
sulfite dihydrate	K ₂ SO ₃ ·2H ₂ O	194.30		d		106 ²⁰ aq
thiocarbonate	K ₂ CS ₂	186.41		d		v s aq
thiocyanate	KSCN	97.18	1.886 ¹⁴	173	d 500	217 ²⁰ aq; 200 acet; 8 alc
thiosulfate	K ₂ S ₂ O ₃	190.33		d 400		acet; 8 alc
titanate(IV), oxobis-(oxalato)diaqua-	K ₂ [TiO(C ₂ O ₄) ₂ (H ₂ O) ₂]	354.18				155 ²⁰ aq
Rhenium(VII) sulfide	Re ₂ S ₇	596.85	4.866	d 460		i aq; s HNO ₃
Rhodium(III) chloride	RhCl ₃	209.28		d 450	subl 850	i aq; s KOH, KCN
Rubidium						
chloride	RbCl	120.94	2.76	715	1381	91 ²⁰ aq; 1.1 MeOH
iodide	RbI	212.37	3.55	640	1304	144 ¹⁸ aq
nitrate	RbNO ₃	147.47	3.11	310		53 ²⁰ aq
sulfate	Rb ₂ SO ₄	267.03	3.613 ²⁰	1060		48 ²⁰ aq
Ruthenium						
(III) chloride	RuCl ₃	207.47	3.11	d 500		i aq; s HCl, alc
(IV) oxide	RuO ₂	133.07	6.97	d		i aq; s fused alk
Selenic acid	H ₂ SeO ₄	144.98	2.9508 ¹⁵	58	260	567 ²⁰ aq (viol)
Selenium	Se	78.96	4.81 ²⁰	221	685	s CS ₂ , KOH, KCN
(IV) oxide	SeO ₂	110.96	3.954 ¹⁵ ₁₅	340	subl 315	38 ¹⁴ aq; 10 ¹² MeOH

(di-) sulfide, hexa-	Se ₂ S ₆	350.28	2.44	121.5		i aq; 1.2 bz; s CS ₂
(tetra-) sulfide, tetra-	Se ₄ S ₄	444.08	3.20	113		i aq; 0.04 bz; s CS ₂
Silane	SiH ₄	32.09	0.68 ⁻¹⁸⁵	-184.7	-111.9	d aq slowly
Silicon	Si	28.09	2.33 ²⁵	1415	2680	s HF + HNO ₃ , fused alk oxides
carbide	SiC	40.07	3.217	subl 2700	d 2972	s fused alk
chloride	SiCl ₄	169.89	1.48 ²⁰	-70	57.6	hyd aq; s bz, CCl ₄ , eth
isothiocyanate, tetra-	Si(NCS) ₄	260.40		143.8	314.2	d aq
oxide, di- (quartz)	SiO ₂	60.08	2.64-2.66	1423	2230	i aq; s HF
oxide-tungsten	SiO ₂ ·12WO ₃ ·26H ₂ O	3310.66				v s aq, alc
trioxide-water						
(1/12/26) (silico-						
tungstic acid)						
telluride, tri-	Si ₂ Te ₃	438.97		892		
Silver	Ag	107.87	10.49 ¹⁵	960.15	2164	i aq; s HNO ₃
acetate	AgC ₂ H ₃ O ₂	166.92	3.259 ¹⁵	d		1.04 ²⁰ aq
azide	AgN ₃	149.89		252	297	i aq; s KCN, HNO ₃ (expl)
carbonate	Ag ₂ CO ₃	275.77	6.077	d 220		0.003 ³⁰ aq
chlorate	AgClO ₃	191.34	4.430 ²⁰	231	d 270	15.3 ²⁰ aq
chloride	AgCl	143.34	5.56	455	1564	0.00019 aq; s NH ₄ OH
chromate(VI)	Ag ₂ CrO ₄	331.77	5.625 ²⁵			0.002 ²⁰ aq; s HNO ₃ , NH ₄ OH
cyanide	AgCN	133.90	3.95	d 320		i aq; s KCN
fluoride	AgF	126.88	5.852 ¹⁶	435	1150	172 ²⁰ aq
(II) fluoride	AgF ₂	145.87	4.57	690	d 700	hyd viol aq
iodate	AgIO ₃	282.80	5.525 ²⁰	> 200	d	0.004 ²⁰ aq
iodide	AgI	234.80	5.683 ³⁰	558	1505	i aq; s KCN
nitrate	AgNO ₃	169.89	4.352 ¹⁹	210	d 440	216 ²⁰ aq
nitrite	AgNO ₂	153.89	4.453	d 140		0.41 ²⁵ aq
oxide	Ag ₂ O	231.76	7.22 ²⁵	d 200		0.002 ²⁵ aq
(II) oxide	AgO	123.88	7.483 ²⁵	d 100		i aq; s alk
permanganate	AgMnO ₄	226.81	4.49	d		0.9 aq; d alc
phosphate, ortho-	Ag ₃ PO ₄	418.62	6.370	849		0.006 aq
sulfate	Ag ₂ SO ₄	311.83	5.45 ³⁰	660	d 1085	0.80 ²⁰ aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Sodium	Na	22.99	0.968 ²⁰	97.82	881.4	d aq to NaOH
acetate	NaC ₂ H ₃ O ₂	82.04	1.528	324		46.5 ²⁰ aq
aluminate, tetrachloro-	NaAlCl ₄	191.80		151		s aq
amide	NaNH ₂	39.02		210	subl 400	d viol aq
aurate(III) dihydrate, tetrachloro-	NaAuCl ₄ ·2H ₂ O	397.80	1.6	d 100		166 ²⁰ aq
azide	NaN ₃	65.01	1.846 ²⁰	d		41 ²⁰ aq; 0.3 alc
benzoate	NaC ₆ H ₅ O ₂	144.11				63 ²⁵ aq; 1.3 alc
bismuthate(V)(1-)	NaBiO ₃	280.00		d		i aq; d a
boranate	NaBH ₄	37.84	1.074	497 d		55 ²⁵ aq; 4 alc; 1.4 pyr; 5 DMF
borate, tetra-	Na ₂ B ₄ O ₇	201.27	2.367	742.5		2.6 ²⁰ aq
borate, tetrafluoro-	NaBF ₄	109.82	2.47 ²⁰	384	d	108 ²⁷ aq
bromate	NaBrO ₃	150.91	3.339 ¹⁷	380 d		36 ²⁰ aq
bromide	NaBr	102.91	3.205 ¹⁸	747	1447	90 ²⁰ aq; 6 alc; 16 MeOH
carbonate	Na ₂ CO ₃	106.00	2.533	850.0	d	21.5 ²⁰ , s glyc
carbonate 10-water	Na ₂ CO ₃ ·10H ₂ O	286.14	1.46	34		50 aq; s glyc
chlorate	NaClO ₃	106.45	2.489	248	d 350	96 ²⁰ aq; 0.77 alc; 25 glyc
chloride	NaCl	58.45	2.164 ²⁰	801	1465	36 ²⁰ aq; 10 glyc
chlorite	NaClO ₂	90.45		d 180–200		34 ¹⁷ aq
chromate(VI)	Na ₂ CrO ₄	161.97	2.723	792		84 ²⁰
citrate 2-water	Na ₃ C ₆ H ₅ O ₇ ·2H ₂ O	294.10		–2H ₂ O, 150		77 ²⁵ aq
cobaltate(III), hexanitrito-	Na ₃ [Co(NO ₂) ₆]	403.98				v s aq
cyanate	NaOCN	65.01	1.893 ²⁰	550		s aq d; 0.22 ⁰ alc
cyanide	NaCN	49.02		562	1530	58.7 ²⁰ aq
cyanoborohydride	NaBH ₃ CN	62.84		d 242		(flammable solid)
dichromate(VI) 2-water	Na ₂ Cr ₂ O ₇ ·2H ₂ O	298.00	2.348 ²⁵	356 anhyd	d 400	208 ²⁰ aq
diethyldithiocarbamate	NaS ₂ CN(C ₂ H ₅) ₂	225.31		94 anhyd		s aq, alc

dimethylarsonate 3-water	$\text{NaO}_2\text{As}(\text{CH}_3)_2 \cdot 3\text{H}_2\text{O}$	214.03		60	$-3\text{H}_2\text{O}$, 120	200 aq; 40 alc
diphosphate(V)	$\text{Na}_4\text{P}_2\text{O}_7$	265.90	2.45	988		2.26 ⁰ aq
dithionate 2-water	$\text{Na}_3\text{S}_2\text{O}_6 \cdot 2\text{H}_2\text{O}$	242.13	2.189	$-2\text{H}_2\text{O}$, 110	d 267	6.05 ²⁰ aq
dithionate(III) (hydro-sulfite)	$\text{Na}_2\text{S}_2\text{O}_4$	174.13		d		22 ²⁰ aq
dodecylsulfate (laurate)	$\text{NaO}_3\text{SOC}_{12}\text{H}_{25}$	288.38				10 aq
ethoxide	NaOC_2H_5	68.06		> 300		d aq; s abs alc
ethylenebis (aminodi-acetate) (EDTA)	$\text{Na}_4\text{C}_2\text{H}_4\text{N}_2(\text{C}_2\text{H}_3\text{O}_2)_4$	380.20				103 aq
ethylsulfate	$\text{NaO}_3\text{SOC}_2\text{H}_5$	148.11				
ferrate(II) 10-water, hexacyano-	$\text{Na}_4[\text{Fe}(\text{CN})_6] \cdot 10\text{H}_2\text{O}$	484.07	1.458	$-10\text{H}_2\text{O}$, 82	d 435	18.8 ²⁰ aq
ferrate(III) 2-water, pentacyanonitrosyl-(nitroprusside)	$\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}] \cdot 2\text{H}_2\text{O}$	297.65	1.72			40 ¹⁶ aq
fluoride	NaF	41.99	2.78	996	1787	4 ²⁰ aq; i alc
formate	NaOOCH	68.02	1.919	253 d		81 ²⁰ aq; s glyc; sl s alc
gluconate	$\text{NaC}_6\text{H}_{11}\text{O}_7$	218.13				59 ²⁵ aq; sl s alc; i eth
glycerophosphate	$\text{Na}_2\text{C}_3\text{H}_5(\text{OH})_2\text{PO}_4$	216.03		d 130		60 aq; i alc
hydride	NaH	24.00	1.396	d 425		d viol aq, alc
hydrogen carbonate	NaHCO_3	84.01	2.20	$-\text{CO}_2$, 270		9.6 ²⁰ aq; i alc
hydrogen phosphate hydrate, di-	$\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$	137.99	2.040	$-\text{H}_2\text{O}$, 100	d 200	71 ⁰ aq
hydrogen phosphate 7-water	$\text{Na}_2\text{HPO}_4 \cdot \text{H}_2\text{O}$	268.07	1.679	d		185 ⁴⁰ aq
hydrogen sulfate	NaHSO_4	120.07	2.435	315	d	28.5 ²⁵ aq; d alc
hydrogen sulfite	NaHSO_3	104.06	1.48	d		29 aq; 1.4 alc
hydrogen sulfide 2-water	$\text{NaHS} \cdot 2\text{H}_2\text{O}$	92.09		55	d	s aq, alc, eth
hydroxide	NaOH	40.01	2.130 ²⁵	322	1557	108 ²⁰ aq; 14 abs alc; 24 MeOH; s glyc
hydroxymethanesulfinate dihydrate	$\text{NaO}_2\text{SCH}_2\text{OH} \cdot 2\text{H}_2\text{O}$	154.12		63–64		v s aq; i abs alc, bz, eth
hypochlorite	NaClO	74.44				53 ²⁰ aq (anhyd v expl)

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Sodium						
iodate	NaIO ₃	197.90	4.277 ²⁰	d		8.1 ²⁰ aq
iodite	NaI	149.92	3.667 ⁰	660	1304	178 ²⁰
lactate	NaOOCCHOHCH ₃	112.07		d		misc aq, alc
methoxide	NaOCH ₃	54.03		> 300		d aq; s alc
molybdate dihydrate	Na ₂ MoO ₄ ·2H ₂ O	241.95	3.28	687	−2H ₂ O, 100	65 ²⁰ aq
nitrate	NaNO ₃	85.01	2.257	308	d 380	88 ²⁰ aq
nitrite	NaNO ₂	69.00	2.168 ⁰	271	d 320	81 ²⁰ aq
oxalate	Na ₂ C ₂ O ₄	134.01	2.27			3.4 ²⁰ aq
oxide	Na ₂ O	61.98	2.27	1132	d 1950	d aq to NaOH
perchlorate	NaClO ₄	122.44	2.499	468		201 ²⁰
periodate	NaIO ₄	213.91	3.865 ¹⁶	d 300		10.3 ²⁰ aq
peroxide	Na ₂ O ₂	77.99	2.805	675	d	v s aq (d)
peroxoborate 4-water	NaBO ₃ ·4H ₂ O	153.88		d 60		2.5 aq
peroxodisulfate(VI)	Na ₂ S ₂ O ₈	238.13		d		55 aq
phosphate 12-water	Na ₃ PO ₄ ·12H ₂ O	380.12	1.62	73.4	−11H ₂ O, 100	28.3 ¹⁵ aq
platinate(IV) 6-water, hexachloro-	Na ₂ PtCl ₆ ·6H ₂ O	561.88	2.50	−6H ₂ O, 110		v s aq; s alc
propionate	NaOOCCH ₂ CH ₃	96.07				100 ²⁵ aq; 4.1 ²⁵ alc
salicylate	NaC ₇ H ₅ O ₃	160.11				95 ²⁰ aq; 11 alc; 25 glyc
selenate(VI)	Na ₂ SeO ₄	188.94	3.098			27 ²⁰ aq
silicate, hexafluoro-	Na ₂ SiF ₆	188.05	2.679	red heat		0.44 ⁰ aq; i alc
stannate(IV) 3-water	Na ₂ SnO ₃ ·3H ₂ O	266.71		d 140		50 ⁰ aq
stearate	NaOOC ₁₇ H ₃₅	306.47		d		sl s aq
sulfate	Na ₂ SO ₄	142.06	2.664	884		19.5 ²⁰
sulfate 10-water	Na ₂ SO ₄ ·10H ₂ O	322.19	1.464	32.4	−10H ₂ O, 100	36 ¹⁵ aq

sulfide	Na ₂ S	78.05	1.856 ₄ ¹⁴	950		15.7 ²⁰ aq
sulfite	Na ₂ SO ₃	126.06	2.633 ¹⁵	d		26 ²⁰ aq
tartrate dihydrate	Na ₂ C ₄ H ₄ O ₆ · 2H ₂ O	230.08	1.818	−2H ₂ O, 120		29 ⁶ aq
tetraphenylborate	NaB(C ₆ H ₅) ₄	342.24				s aq, acet
thiocyanate	NaSCN	81.07		287		134 ²⁰ aq
thiosulfate	Na ₂ S ₂ O ₃	158.11	2.345			s aq; i alc
thiosulfate 5-water	Na ₂ S ₂ O ₃ · 5H ₂ O	248.18	1.685	−5H ₂ O, 100		70 ²⁰ aq (d slowly)
tungstate(VI) dihydrate	Na ₂ WO ₄ · 2H ₂ O	329.86	3.245	−2H ₂ O, 100		88 ⁰
Strontium						
carbonate	SrCO ₃	147.64	3.70	−CO ₂ , 1172		0.001 ²⁵ aq; s a
chloride	SrCl ₂	158.52	3.052	874	2058	52.9 ²⁰ aq
chromate(VI)	SrCrO ₄	203.64	3.895 ¹⁵			0.09 ²⁰ aq; s HCl
hydroxide	Sr(OH) ₂	121.64	3.625	375 (in H ₂)	−H ₂ O, 710	1.77 ²⁰ aq
Sulfamic acid	H ₂ NSO ₃ H	97.09	2.126	d 200		14.7 aq
Sulfinyl						
bromide	SOBr ₂	207.88	2.67	−49.5	139.7	d aq
chloride	SOCl ₂	118.98	1.656 ¹⁵	−104.5	75.8	hyd aq
fluoride	SOF ₂	86.06	3.0 ^{−44}	−110	−43.8	d aq; s bz, chl, eth
Sulfonyl						
chloride	SO ₂ Cl ₂	134.98	1.6674 ²⁰	−46	69.3	d aq; s bz
fluoride	SO ₂ F ₂	102.07	3.72 g · L ^{−1}	−135.8	−55.38	4 mL aq; 24 mL alc; 136 mL CCl ₄ ; 210 mL toluene
Sulfur						
	S	32.07	1.92	106.8	444.60	i aq; 23 ⁰ CS ₂ ; s alc, bz
	S ₈	256.51	1.96 ²⁰	115.21	444.60	i aq; 23 ⁰ CS ₂ ; s alc, bz
(di-) chloride, di-	S ₂ Cl ₂	135.03	1.688 ¹⁵	−80	138.1	hyd aq
fluoride, tetra-	SF ₄	108.07	1.919 ^{−73}	−121	−38	d viol aq; s bz
fluoride, hexa-	SF ₆	146.07	1.88 ^{−50}	−50.8	subl 63.8	sl s aq; s alc, KOH
			g · L ^{−1}			
oxide, di	SO ₂	64.07	2.716 ²⁰	−75.47	−10.01	3937 ²⁰ mL aq; 25 mL alc
			g · L ^{−1}			
			1.46 ^{−10} (lq)			
oxide, tri(III)	SO ₃	80.07	1.9225 ²⁰	16.86	43.4	slowly v s aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Sulfuric acid	H ₂ SO ₄	98.08	1.8318 ²⁰	10.38	335.5	v s aq
chloro-	HOSO ₂ Cl	116.52	1.753 ²⁰	−80	152	d viol aq
fluoro-	FSO ₂ OH	100.07	1.726 ²⁵	−88.98	162.6	d viol aq
Tantalum	Ta	180.95	16.69	2985	5513	i aq; s HF, fused alk
(V) fluoride	TaF ₅	275.95	4.74 ²⁰	95−97	229	s aq
Tellurium	Te	127.60	6.24 ²⁰	450	1009	i aq; s HNO ₃ , KOH
Thallium	Tl	204.37	11.85	303.5	1487	i aq; s HNO ₃
(III) acetate sesquihydrate	Tl(C ₂ H ₃ O ₂) ₃ · 1.5H ₂ O	408.53		182 d		
(I) bromide	TlBr	284.31	7.54	460	825	0.05 ²⁰ aq; s alc
(I) chloride	TlCl	239.85	7.004 ³⁰	429	816	0.33 ²⁰ aq
(I) ethoxide	TlOC ₂ H ₅	249.43	3.493 ²⁰	−3	d 130	sl s alc; s eth
(I) fluoride	TlF	223.39	8.23 ⁴	322	700	78 ¹⁵ aq
(I) nitrate	TlNO ₃	266.40	5.556	206	430	9.6 ²⁰ aq
(III) nitrate 3-water	Tl(NO ₃) ₃ · 3H ₂ O	444.43		102−103		s aq
(I) oxide	Tl ₂ O	424.78	9.52 ¹⁶	300	1080	v s aq (d); s a
(III) oxide	Tl ₂ O ₃	456.78	10.19 ²²	717	−O ₂ , 875	i aq; s a
			(hex)			
(I) sulfate	Tl ₂ SO ₄	504.85	6.77	632	d	4.9 ²⁰ aq
Thiocarbonyl chloride	CSCl ₂	114.98	1.509 ¹⁵		73.5	d aq; s eth
Thiocyanogen	(SCN) ₂	116.16		ca −2		d aq; s alc, CS ₂ , eth
Thionyl, see Sulfinyl						
Tin (silver-white, tetr) (gray, cub)	Sn	118.69	7.28	231.89	2623	i aq; s HCl, H ₂ SO ₄
			5.75	stable −161 to 13.2		
(IV) bromide	SnBr ₄	438.36	3.35 ³³	30	207	hyd aq; s acet
(II) chloride	SnCl ₂	189.61	3.95	247	652	84 ⁰ aq; s alc, eth

(IV) chloride	SnCl ₄	260.53	2.226	−34	115	s aq, eth
(II) diphosphate(V)	Sn ₂ P ₂ O ₇	411.32	4.009 ¹⁶			i aq; s conc a
(II) fluoride	SnF ₂	156.70	4.57 ²⁵	213		30 aq
(IV) fluoride	SnF ₄	194.70	4.780 ¹⁹	subl 705		hyd aq
(IV) oxide	SnO ₂	150.70	6.95	1630	subl 1900	i aq
(II) sulfide	SnS	150.77	5.08	881	1210	i aq; s conc HCl
(IV) sulfide	SnS ₂	182.83	4.5	765		i aq; d by aqua regia
(II) zirconate (IV), hexafluoro-	SnZrF ₆	323.92	4.21			s aq
Titanium	Ti	47.90	4.507	1660	3318	s hot a, HF
(III) chloride	TiCl ₃	154.27	2.71	subl 831 (vac)	d 5000	s aq, alc
(IV) chloride	TiCl ₄	189.73	1.726	−24.10	136.4	s cold aq, alc
hydride, di	TiH ₂	49.92	3.752	d 400		
(IV) isopropoxide	Ti[OCH(CH ₃) ₂] ₄	284.26	0.9711 ²⁰	ca 20	220 ^{10 mm}	
(IV) oxide (rutile)	TiO ₂	79.90	4.23	1857		s HF
(III) sulfate	Ti ₂ (SO ₄) ₃	384.00				s HCl
Trisulfuryl dichloride	ClSO ₂ OSO ₂ OSO ₂ Cl	295.09	1.90 ²⁰	18.7	61 ^{3 mm}	
Tungsten						
(VI) chloride	WCl ₆	396.57	2.721 ²⁸²	281.5	340.5	hyd aq; s CS ₂ , CCl ₄
(VI) oxide	WO ₃	231.86	7.16	1472	1837	i aq; s hot alk
sulfide, di-	WS ₂	247.98	7.5 ¹⁰	d 1250		s HNO ₃ + HF
Uranyl						
(VI) acetate 2-water	UO ₂ (C ₂ H ₃ O ₂) ₂ •2H ₂ O	422.13	2.893 ¹⁵	−2H ₂ O, 110	d 275	7.7 ¹⁵ aq
nitrate 6-water	UO ₂ (NO ₃) ₂ •6H ₂ O	502.13	2.807 ¹³	60.2	d 100	155 ²⁰ aq
Vanadium						
(III) oxide	V ₂ O ₃	149.00	4.87	2067		i aq; s HNO ₃ + HF
(V) oxide	V ₂ O ₅	181.90	3.35	670	1690	0.80 aq; s a, alk
(IV) oxide sulfate	VOSO ₄	163.00				v s aq
Xenon	Xe	131.30	5.8971 ⁰	−111.8	−108.10	10.8 ²⁰ mL aq
			g•L ^{−1}			
fluoride, di-	XeF ₂	169.30	3.13 ²⁵	129.0	subl 114	2.5 ⁰ aq

TABLE 2.1 Physical Constants of Inorganic Compounds (*continued*)

Name	Formula	Formula weight	Density	Melting point, °C	Boiling point, °C	Solubility in 100 parts solvent
Xenon						
fluoride, tetra-	XeF ₄	207.30	3.03 ²⁵	117.1	subl 116	hyd aq; s F ₃ CCOOH
fluoride, hexa-	XeF ₆	245.30	3.411 ²⁵	49.5	75.6	hyd aq
Zinc	Zn	65.37	7.14 ²⁵	419.6	911	i aq; s a, alk
acetate dihydrate	Zn(C ₂ H ₃ O ₂) ₂ · 2H ₂ O	219.49	1.725	237		41.6 ²⁰ aq; 3.3 alc
bromide	ZnBr ₂	225.21	4.22	402	650	446 ²⁰ aq; 200 alc; s eth
carbonate	ZnCO ₃	125.38	4.398	−CO ₂ , 300		0.02 ²⁵ aq; s a, alk
chloride	ZnCl ₂	136.29	2.907 ²⁵	318	732	395 ²⁰ aq; 77 alc; 50 glyc
chromate(VI)	ZnCrO ₄	181.36	3.40			i aq; s a
cyanide	Zn(CN) ₂	117.42	1.852	d 800		0.058 ¹⁸ aq; s KCN, alk
fluoride	ZnF ₂	103.38	5.00 ²⁵	872	1500	1.6 ²⁰ aq
iodide	ZnI ₂	319.22	4.736 ²⁵	446	730	432 ²⁰ aq; 50 glyc
nitrate 6-water	Zn(NO ₃) ₂ · 6H ₂ O	297.47	2.065 ¹⁴	36.4	−6H ₂ O, 131	146 ⁰ aq
oxide	ZnO	81.37	5.67	1970		i aq; s a, alk
peroxide	ZnO ₂	97.38	3.00	d 150		i aq; d slowly
<i>p</i> -phenolsulfonate 8-water	Zn[C ₆ H ₄ (OH)SO ₃] ₂ · 8H ₂ O	555.83		−8H ₂ O, 120		63 aq; 56 alc
phosphate(V)	Zn ₂ (PO ₄) ₂	386.05	3.998 ¹⁵	900		i aq; s a, NH ₄ OH
phosphide	Zn ₃ P ₂	258.09	4.55	> 420	subl 1100 (in H ₂)	d aq; s bz, CS ₂ ; d viol HCl
propionate	Zn(OOCC ₂ H ₅) ₂	211.52				32 aq; 2.8 alc
silicate 6-water, hexafluoro-	ZnSiF ₆ · 6H ₂ O	315.54	2.104	d 100		v s aq
stearate	Zn(OOCC ₁₇ H ₃₅) ₂	632.33		ca 120		i aq, alc, eth; s bz
sulfate	ZnSO ₄	161.44	3.54	1200		53.8 ²⁰ aq
sulfate 7-water	ZnSO ₄ · 7H ₂ O	287.54	1.957	−7H ₂ O, 280	d 500	96 ²⁰ aq; 40 glyc; i alc
sulfide	ZnS	97.43	4.087	1722		i aq; s a
thiocyanate	Zn(SCN) ₂	181.53				0.14 ¹⁸ aq; s alc

Zirconium	Zr	91.22	6.52 ³⁰	1852	4504	s aqua regia
(IV) chloride	ZrCl ₄	233.05	2.803 ¹⁵	437	subl 334	hyd aq; s alc, eth
chloride oxide 8-water	ZrCl ₂ O•8H ₂ O	322.25	1.91	−8H ₂ O, 210		s aq
hydroxide	Zr(OH) ₄	159.25	3.25	−2H ₂ O, 500		s a
(IV) oxide	ZrO ₂	123.22	5.85	2677	4275	s hot H ₂ SO ₄ , HF slowly
silicate(4−)	ZrSiO ₄	183.31	4.56	d 1538		very inert
sulfate 4-water	Zr(SO ₄) ₂ •4H ₂ O	355.41	3.22 ¹⁶	anhyd 380		52.5 ¹⁸ aq

SECTION 3

PROPERTIES OF ATOMS, RADICALS, AND BONDS

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NUCLIDES

TABLE 3.1 Table of Nuclides

Explanation of column headings

Nuclide. Each nuclide is identified by its atomic number Z , equal to the number of protons in the nucleus; the corresponding symbol for that element; and the mass number A , equal to the sum of the numbers of protons Z and neutrons N in the nucleus. Thus, $A = Z + N$, or $N = A - Z$. The m following the mass number (e.g., ^{69m}Zn) indicates an isomer of that nuclide.

Half-Life. For the radioactive nuclides this time period corresponds to that during which loss by disintegration of 50% of the nuclide occurs. The units of time are designated by year (yr), day (d), hour (h), minute (min), and second (s).

Natural Abundance. The isotopic abundances listed are on an “atom percent” basis for the stable nuclides present in naturally occurring elements in the earth’s crust.

Thermal Neutron Absorption Cross Section. The ease with which a given nuclide can absorb a thermal neutron (energy $\leq \frac{1}{40}$ eV) and become of a different nuclide is indicated by the cross section, given here in units of barns (1 barn = 10^{-24} cm²). If the mode of reaction is other than (n, γ), it is so indicated, for example, (n, p) or (n, α), where n = neutron, p = proton, γ = gamma ray, and α = alpha particle (^4_2He).

Major Radiations. In this column are listed the principal mode(s) of decay and the energies of the emanating radiations in million electronvolts (MeV). The gamma-ray (γ) intensities, where given, are given to the nearest whole percentage in parentheses following the numerical energy value for that particular γ . In most cases the radiations listed should be sufficient for identification of the particular nuclide. The following designations are used: negatron (β^-), positron (β^+), conversion electron (e^-), gamma ray (γ), and alpha particle (α).

Nuclide		Half-life	Natural abundance, %	Thermal neutron absorption cross section, barns	Major radiations		
Symbol	Mass						
¹ H	1.007 825	12.26 yr	99.985	0.332	β^- , 0.018 6; no γ		
² H	2.014 102		0.015	0.000 5			
³ H	3.016 050						
⁶ Li	6.015 125		7.42	953(n, α)			
⁷ Li	7.016 004	53.6 d	92.58	0.037	γ , 0.477(10)		
⁷ Be	7.016 929			54,000(n, p)			
⁹ Be	9.012 186	2.5×10^6 yr	100	0.009	β^- , 0.555; no γ		
¹⁰ Be	10.013 534						
¹⁰ B	10.012 939		19.7	3837(n, α)			
¹¹ B	11.009 305		80.3	0.005			
¹¹ C	11.011 432	20.34 min	1.108	0.000 9	β^+ , 0.97; γ , 0.511		
¹³ C	13.003 354	5730 yr			β^- , 0.156; no γ		
¹⁴ C	14.003 242				β^+ , 1.20; γ , 0.511		
¹³ N	13.005 738	9.96 min					
¹⁴ N	14.003 074	29.1 s	99.635	1.81(n, p)	β^- , 4.60; γ , 0.197(97), 1.37(59)		
¹⁹ O	19.003 578				β^+ , 1.74; γ , 0.511		
¹⁸ F	18.000 937	109.7 min			β^+ , 1.820, 0.545; γ , 0.511, 1.275(100)		
²² Na	21.994 437	2.62 yr					

TABLE 3.1 Table of Nuclides (*continued*)

Nuclide		Half-life	Natural abundance, %	Thermal neutron absorption cross section, barns	Major radiations
Symbol	Mass				
²³ Na	22.934 473	14.96h	100	0.53	β^- , 4.17, 1.389; γ , 0.511, 1.275(100)
²⁴ Na	23.990 962				
²⁵ Mg	24.985 839	21.2h	10.11	0.3	β^- , 0.46; e^- , 0.03; γ , 0.031(96), 0.40(30), 0.95(30), 1.35(70)
²⁸ Mg	27.983 875				
²⁶ Al	25.986 891	7.4×10^5 yr	100	0.235	β^- , 8.5; γ , 0.511, 1.12(4), 1.81(100)
²⁷ Al	26.981 539	2.31 min			
²⁸ Al	27.981 905				
³⁰ Si	29.973 763	2.62h	3.12	0.11	β^- , 1.48; γ , 1.26
³¹ Si	30.975 349				
³¹ P	30.973 765	14.28 d	100	0.19	β^- , 1.710 β^- , 0.248; no γ
³² P	31.973 909				
³³ P	32.971 728	24.4 d	4.22	0.27	β^- , 0.167; no γ β^- , 3.0, 1.1; γ , 1.88(95)
³⁴ S	33.967 865	87.9 d			
³⁵ S	34.969 031	2.87 h			
³⁸ S	37.971 230	3.08×10^5 yr	75.53	44	β^- , 0.714; γ , 0.511
³⁵ Cl	34.968 851				
³⁶ Cl	35.968 309				
³⁷ Cl	36.965 898	37.29 min	24.47	0.4	β^- , 4.91; γ , 1.60(38) β^- , 3.45, 2.18, 1.91; γ , 0.246(44) Cl X rays
³⁸ Cl	37.968 005				
³⁹ Cl	38.968 008	55.5 min	0.118	70	β^- , 1.314; β^+ , 0.483; γ , 1.460(11)
³⁷ Ar	32.966 772	35.1 d			
⁴⁰ K	39.964 000	1.26×10^9 yr			
⁴¹ K	40.961 832	12.36 h	6.77	1.2	β^- , 3.52; γ , 0.31, 1.524(18)
⁴² K	41.962 406				
⁴⁴ Ca	43.955 490	165 d	2.06	0.7	β^- , 0.252 β^- , 1.98, 0.67; γ , 0.49(5), 0.815(5), 1.308(74)
⁴⁵ Ca	44.956 189				
⁴⁷ Ca	46.954 538				
⁴⁶ Sc	45.955 919	83.9 d			β^- , 1.48, 0.357, γ , 0.889(100), 1.120(100)

TABLE 3.1 Table of Nuclides (continued)

Nuclide		Half-life	Natural abundance, %	Thermal neutron absorption cross section, barns	Major radiations		
Symbol	Mass						
⁴⁴ Ti	43.959 572	48 yr	4.31	17	γ , 0.068(90), 0.078(98); e^- , 0.065, 0.073		
⁴⁸ V	47.952 259	16.0 d			β^+ , 0.696; γ , 0.511, 0.945(10), 0.983(100), 1.312(97), 2.241(3)		
⁴⁹ V	48.949 522	330 d			Ti X rays		
⁵⁰ Cr	49.946 054	27.8 d			γ , 0.320(9); e^- , 0.315		
⁵¹ Cr	50.944 768						
⁵⁴ Mn	53.940 362	303 d			γ , 0.835(100); e^- , 0.829		
⁵⁵ Mn	54.938 050	2.576 h	100	13.3	β^- , 2.85; γ , 0.847(99), 1.811(29), 2.110(15)		
⁵⁶ Mn	55.938 910						
⁵⁴ Fe	53.939 617	2.60 yr	5.84	2.9	Mn X rays		
⁵⁵ Fe	54.938 299		0.31	1.1			
⁵⁸ Fe	57.933 282						
⁵⁹ Fe	58.934 878	45.6 d	100	19	β^- , 1.57, 0.475; γ , 0.143(1), 0.192(3), 1.095(56), 1.292(44)		
⁵⁷ Co	56.936 296	270 d			γ , 0.014(9), 0.122(87), 0.136(11), 0.692; e^- , 0.115, 0.129		
⁵⁸ Co	57.935 761	71.3 d			β^+ , 0.474; γ , 0.511, 0.810(99), 0.865(1), 1.67(1)		
⁵⁹ Co	58.933 189	5.263 yr		6	β^- , 1.48, 0.314; γ , 1.173(100), 1.332(100)		
⁶⁰ Co	59.933 813						
⁶² Ni	61.928 342	92 yr	3.66	15	β^- , 0.067; no γ		
⁶³ Ni	62.929 664		1.16	1.5			
⁶⁴ Ni	63.927 958						
⁶⁵ Ni	64.930 072	2.564 h	69.1	4.5	β^- , 2.13; γ , 0.368(5), 1.115(16), 1.481(25)		
⁶³ Cu	62.929 592	12.80 h			β^- , 0.573; β^+ , 0.656; e^- , 1.33; γ , 0.511, 1.34(1)		
⁶⁴ Cu	63.929 759						

TABLE 3.1 Table of Nuclides (*continued*)

Nuclide		Half-life	Natural abundance, %	Thermal neutron absorption cross section, barns	Major radiations
Symbol	Mass				
⁶⁴ Zn	63.929 145	> 8 × 10 ¹⁵ yr	48.89	0.46	β^+ , 0.327; e^- , 1.106; γ , 0.511, 1.115(49)
⁶⁵ Zn	64.929 234				
⁶⁸ Zn	67.924 857	13.8 h	18.56	1.0	γ , 0.439(95); e^- , 0.429 Ga X rays
^{69m} Zn					
⁷¹ Ge	70.924 956	11.4 d	100	4.5	β^- , 2.97; γ , 0.559(43), 0.657(6), 1.22(5) 1.44(1), 1.789, 2.10(1)
⁷⁵ As	74.921 595				
⁷⁶ As	75.922 397	26.4 h			
⁷⁷ As	76.920 645	38.7 h			β^- , 0.68; γ , 0.086, 0.239(3), 0.522(1)
⁷⁵ Se	74.922 525	120.4 d			γ , 0.066(1), 0.097(1), 0.121(17), 0.136(57), 0.265(60), 0.280(25), 0.401(12); e^- 0.085, 0.095, 0.109, 0.124, 0.253
⁷⁹ Br	78.918 329	17.6 min	50.52	8.5	β^- , 2.00; β^+ , 0.87; γ , 0.511, 0.618(7), 0.666(1)
⁸⁰ Br	79.918 536				
⁸¹ Br	80.916 292	35.34 h	49.48	3	β^- , 0.444; γ , 0.554(66), 0.619(41), 0.698(27), 0.777(83), 0.828(25), 1.044(29), 1.317(26), 1.475(17)
⁸² Br	81.916 802				
⁸⁵ Kr	84.912 523	10.76 yr		< 15	β^- , 0.67; γ , 0.514 β^- , 1.78; γ , 1.078(9)
⁸⁶ Rb	85.911 193	18.66 d			
⁸⁵ Sr	84.912 989	64.0 d			γ , 0.514(100); e^- , 0.499
⁹⁰ Y	89.907 163	64.0 h		~7	β^- , 2.27; no γ β^- , 0.160; γ , 0.765(100)
⁹⁵ Nb	94.906 832	35.0 d			

TABLE 3.1 Table of Nuclides (continued)

Nuclide		Half-life	Natural abundance, %	Thermal neutron absorption cross section, barns	Major radiations	
Symbol	Mass					
⁹⁹ Mo	98.907 720	66.7h	26.7	12	β^- , 1.23; γ , 0.041(12), 0.181(7), 0.372(1), 0.740(12), 0.780(4)	
^{99m} Tc		6.049h			γ , 0.140(90); e^- , 0.110	
¹⁰³ Ru	102.906 306	39.5d			β^- , 0.70, 0.21; γ , 0.497(88), 0.610(6)	
¹⁰⁸ Pd	107.903 891	13.47h			β^- , 1.028; γ , 0.088(5), 0.129, 0.31, 0.41, 0.60, 0.64	
¹⁰⁹ Pd	108.905 954					
¹⁰⁹ Ag	108.904 756	39.2s	48.65	89	γ , 0.088(5)	
^{110m} Ag					β^- , 1.05; γ , 0.247(1), 0.342(6)	
¹¹¹ Ag	110.905 316	7.5d			γ , 0.088; e^- , 0.062	
¹⁰⁹ Cd	108.904 928	453d			β^- , 1.11; γ , 0.230(1), 0.262(2), 0.49(10), 0.53(26)	
¹¹⁵ Cd	114.905 431	53.5h				γ , 0.393(64); e^- , 0.365, 0.389
^{113m} In		99.8min	57.25	6	β^- , 1.988; β^+ , 0.42; γ , 1.299	
¹¹⁴ In	113.904 905	72s			γ , 0.255(2)	
¹¹³ Sn	112.905 187	115d			β^- , 1.97; β^+ , 0.56; γ , 0.584(66), 0.686(3), 1.14(1), 1.26(1)	
¹²¹ Sb	120.903 816	2.80d				3.3
¹²² Sb	121.905 183					
¹²³ Sb	122.904 213	1.3×10^{16} yr	42.75	3.3	β^- , 2.31; γ , 0.603(97), 0.644(7), 0.72(14), 0.967(2), 1.048(2), 1.31(3), 1.37(5), 1.45(2), 1.692(50), 2.088(7)	
¹²⁴ Sb	123.905 973	60.4d				< 20
¹²⁵ Sb	124.905 232	2.71yr			β^- , 0.61; e^- , 0.114, 0.395; γ , 0.176(6), 0.427(31), 0.463(10), 0.599(24), 0.634(11), 0.66(3)	

TABLE 3.1 Table of Nuclides (*continued*)

Nuclide		Half-life	Natural abundance, %	Thermal neutron absorption cross section, barns	Major radiations
Symbol	Mass				
¹³² Te	131.908 523	77.7h	100	9	β^- , 0.22; e^- , 0.197; γ , 0.053(17), 0.230(90)
¹²⁵ I	124.904 578	60.2d			γ , 0.035(7); e^- , 0.030
¹²⁷ I	126.904 470	24.99min		6.4	β^- , 2.12; γ , 0.441(14), 0.528(1), 0.743, 0.969
¹²⁸ I	127.905 838				
¹³¹ I	130.906 127	8.05 d		~0.7	β^- , 0.806, 0.606; e^- , 0.330; γ , 0.080(3), 0.284(5), 0.364(82), 0.637(7), 0.723(2)
¹³² I	131.907 981	2.26h		190	β^- , 2.12; γ , 0.24(1), 0.52(20), 0.67(44), 0.773(89), 0.955(22), 1.14(6), 1.28(7), 1.40(14), 1.45(1), 1.91(1), 1.99(1)
¹³³ Xe	132.905 815	5.270d			β^- , 0.346; e^- , 0.045, 0.075; γ , 0.081(37)
¹³¹ Cs	130.905 466	9.70d		136	Xe X rays
¹³⁴ Cs	133.906 823	2.046yr			β^- , 0.662; γ , 0.57(23), 0.605(98), 0.796(99), 1.038(1), 1.168(2), 1.365(3)
¹³⁷ Cs	136.906 770	30.0yr		0.11	β^- , 1.176, 0.514; e^- , 0.624, 0.656; γ , 0.662(85)
¹³¹ Ba	130.906 716	12.0d			γ , 0.124(28), 0.216(19), 0.25(5), 0.373(13), 0.496(48), 0.60(3); e^- , 0.118, 0.180, 0.460
¹³³ Ba	132.905 879	7.2yr			γ , 0.080(36), 0.276(7), 0.302(14), 0.356(69), 0.382(8); e^- , 0.266, 0.319

TABLE 3.1 Table of Nuclides (continued)

Nuclide		Half-life	Natural abundance, %	Thermal neutron absorption cross section, barns	Major radiations	
Symbol	Mass					
^{137m} Ba		2.554 min	100	< 20	γ, 0.662(89); e ⁻ , 0.624, 0.656	
¹⁴⁰ Ba	139.910 565	12.80 d			β ⁻ , 1.02; γ, 0.030(11), 0.163(6), 0.305(6), 0.438(5), 0.537(34)	
¹⁴¹ Ce	140.908 219	32.5 d			β ⁻ , 0.581; e ⁻ , 0.104, 0.139; γ, 0.145(48)	
¹⁴⁴ Ce	143.913 591	284 d			β ⁻ , 0.31; γ, 0.080(2), 0.134(11)	
¹⁹⁷ Au	196.966 541	2.697 d		98.8	β ⁻ , 0.962; e ⁻ , 0.329, 0.398; γ, 0.412(95), 0.676(1), 1.088	
¹⁹⁸ Au	197.968 231		26,000			
¹⁹⁹ Au	198.968 773	3.15 d	29.50	~30	β ⁻ , 0.46, 0.30; γ, 0.158(37), 0.208(8); e ⁻ , 0.125, 0.145	
¹⁹⁷ Hg	196.967 360	65 h		~30	γ, 0.77(18), 0.191(2), 0.268	
²⁰³ Hg	202.972 880	46.9 d			β ⁻ , 0.214; e ⁻ , 0.194, 0.264, 0.275; γ, 0.279(77)	
²⁰³ Tl	202.972 353	3.81 yr		11	β ⁻ , 0.766	
²⁰⁵ Tl	203.973 865					
²¹⁰ Pb	209.984 187	20.4 yr	29.50	< 0.03	β ⁻ , 0.061; γ, 0.047(4); α, 3.72	
²⁰⁷ Bi	206.978 438	30.2 yr			γ, 0.570(98), 1.063(77), 1.771(9); e ⁻ 0.482, 0.975, 1.048	
²¹⁰ Po	209.982 876	138.40 d			20	α, 5.305; γ, 0.803
²²⁶ Ra	226.025 360	1602 yr				α, 4.78, 4.60; γ, 0.186(4), 0.26, 0.42, 0.61; e ⁻ , 0.170
²⁴¹ Am	241.056 714	433 yr			700	α, 5.49, 5.44; γ, 0.060(36), 0.101, 0.208, 0.335, 0.37, 0.663, 0.722

ELECTRONEGATIVITY

According to Pauling, electronegativity χ is the relative attraction of an atom for the valence electrons in a covalent bond. It is proportional to the effective nuclear charge and inversely proportional to the covalent radius.

$$\chi = \frac{0.31(n + 1 \pm c)}{r} + 0.50$$

where n is the number of valence electrons, c is any formal valence charge on the atom and the sign before it corresponds to the sign of this charge, and r is the covalent radius. Because electronegativity is concerned with atoms in molecules rather than atoms in isolation, it is not possible to define precise electronegativity values. Pauling determined his set of values from bond energy data based on experimentally measured heats of dissociation and formation. Originally the element fluorine, whose atoms have the greatest attraction for electrons, was given an arbitrary electronegativity of 4.0. A revision of Pauling's values based on newer heat data assigns 3.9 to fluorine. A unit positive charge changes the χ value for an atom by about two-thirds of the electronegativity difference between it and the atom next on its right in the Periodic Table, and a unit negative charge similarly decreases the χ value.

The greater the difference in electronegativity, the greater is the ionic character of the bond. The amount of ionic character I is given by the expression

$$I = 1 - e^{-0.25(\chi_A - \chi_B)^2}$$

The bond is fully covalent when $(\chi_A - \chi_B) < 0.5$ (and $I < 6\%$). A different expression was proposed by Hannay-Smyth.*

$$I = 0.46|\chi_A - \chi_B| + 0.035(\chi_A - \chi_B)^2$$

Other sets of electronegativities of the elements have been proposed. The rather direct, but somewhat limited, method of Mulliken makes use of the ionization potential IP and electron-affinity data (Table 3.3). Numerical values are obtained that coincide with values from other methods if electronegativities are calculated from

$$\chi = \frac{IP + A}{5.6}$$

Electronegativities on the Allred-Rochow scale[†] are given by

$$\chi = 0.359 \frac{Z_{\text{eff}}}{r^2} + 0.744$$

where Z_{eff} is the effective nuclear charge and r is the atomic radius.

Using Pauling's values, electronegativities of the elements are arranged in periodic order in Table 3.2A.

* Hannay-Smyth, *J. Am. Chem. Soc.*, **68**: 171 (1946).

† *J. Inorg. Nucl. Chem.*, **5**: 264, 269 (1958).

TABLE 3.2A Electronegativities of the Elements

H												
2.2												
Li	Be							B	C	N	O	F
1.0	1.5							2.0	2.5	3.0	3.5	4.0
Na	Mg							Al	Si	P	S	Cl
0.9	1.2							1.5	1.8	2.1	2.4	2.8
K	Ca	Sc	Ti–V	Cr–Mn	Fe–Ni	Cu	Zn	Ga	Ge	As	Se	Br
0.9	1.0	1.3	1.6	1.6	1.8	1.9	1.7	1.6	1.8	2.0	2.4	2.7
Rb	Sr	Y	Zr–Nb	Mo–Tc	Ru–Pd	Ag	Cd	In	Sn	Sb	Te	I
0.8	1.0	1.2	1.6	1.8	2.2	1.9	1.5	1.7	1.8	1.9	2.1	2.2
Cs	Ba	La–Lu	Hf–Ta	W–Re	Os–Pt	Au	Hg	Tl	Pb	Bi		
0.7	0.9	1.1	1.3	1.8	2.2	2.4	1.4	1.8	1.8	1.9		

TABLE 3.2B Electronegativities of the Groups

Group	χ	Group	χ	Group	χ
F	4.0	OH	3.7	C≡N	3.3
Cl	2.8	OCH ₃	3.7	C≡CH	3.3
Br	2.7	NO ₂	3.4	CH=CH ₂	3.0
I	2.2	NH ₂	3.4	C ₆ H ₅	3.0
CF ₃	3.4	N(CH ₃) ₂	3.0	COOH	2.8
CCl ₃	3.0			SiH ₃	2.2
CHCl ₂	2.8			PH ₂	2.3
				SH	2.8

Electronegativities have important uses in chemistry in addition to predicting the amount of ionic character in a bond. The bond stretching force constant k (in units of 10^5 dynes · cm^{−1}) can be estimated for stable molecules exhibiting their normal covalences by the expression:

$$k = 1.67 N \left(\frac{\chi_A \chi_B}{d^2} \right)^{3/4} + 0.30$$

where N is the bond order (i.e., the effective number of covalent or ionic bonds acting between the two atoms A and B) and d is the internuclear distance in angstroms.

An estimate of the percent ionic character may be made for organometallic compounds of the type alkyl-metal for metals in common use in organic synthesis. Among the alkali metals (row 1 of the Periodic Table, these are Li (43%), Na (47%), and K (51%)). The percent ionic character for an organomagnesium compound (typically a Grignard reagent), the bond is estimated to be 34% ionic. The more covalent organozinc and organocadmium compounds have correspondingly less ionic character: Zn (18%) and Cd (15%).

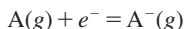
Electronegativities have also been estimated for various common substituent groups. They are arranged in Table 3.2B in clusters of related residues. The values for the individual halogens are from Table 3.2A.

Electronegativity is proportional to the work function ϕ , which is the energy necessary to just remove an electron from the metal surface in thermoelectric or photoelectric emission.

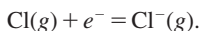
$$\chi = 0.44\phi - 0.15$$

ELECTRON AFFINITY

The *electron affinity* of an atom A is defined as the energy released when an atom and an electron react to form a negative ion in the gas phase at 0 K.



An example is the capture of an electron by chlorine to give chloride anion.



Conceptually related to this is the *ionization potential*, which is the energy for the process



An example is the loss of an electron by an alkali metal to give the alkali metal cation.



The second ionization potential carried this process further, that is, $A^+ \rightarrow A^{2+} + e^-$ and so on for the third or more ionization potentials. Both electron affinities and ionization potentials are typically expressed in electron volts (eV). Data for electron affinities are given in Table 3.3. Uncertainty in the final data figures is given in parentheses.

Source: H. Hotop and W. C. Lineberger, *J. Phys. Chem. Ref. Data*, **4**: 539 (1975). Data for ionization potentials are available in C. E. Moore, *National Bureau of Standards U. S. Publication NSRDS-NBS*, **34** (1970).

TABLE 3.3 Electron Affinities of Elements, Molecules and Radicals

A. Elements

Element	Electron affinity, eV*	Element	Electron affinity, eV*
Aluminum	0.46(3)	Beryllium	<0
Antimony	1.05(5)	Bismuth	1.1(2)
Argon	<0	Boron	0.28(1)
Arsenic	0.80(5)	Bromine	3.364(4)
Astatine	2.8(2)	Cadmium	<0
Barium	<0	Calcium	<0

TABLE 3.3 Electron Affinities of Elements, Molecules and Radicals (*continued*)

A. Elements

Element	Electron affinity, eV*	Element	Electron affinity, eV*
Carbon	1.268(5)	Oxygen	1.462(3)
Cesium	0.4715(5)	Palladium	0.6(3)
Chlorine	3.615(4)	Phosphorus	0.743(10)
Chromium	0.66(5)	Platinum	2.128
Cobalt	0.7(2)	Polonium	1.9(3)
Copper	1.226(10)	Potassium	0.5012(5)
Fluorine	3.399(3)	Radon	<0
Francium	(0.456)	Rare earths	≤0.5 (estimate)
Gallium	0.30(15)	Rhenium	0.15(10)
Germanium	1.2(1)	Rhodium	1.2(3)
Gold	2.3086(7)	Rubidium	0.4860(5)
Hafnium	>0	Ruthenium	1.1(3)
Helium	<0	Scandium	<0
Hydrogen	0.754 209(3)	Selenium	2.0206(3)
Indium	0.30(15)	Silicon	1.385(5)
Iodine	3.061(4)	Silver	1.303(7)
Iridium	1.6(2)	Sodium	0.546(5)
Iron	0.25(20)	Strontium	<0
Krypton	<0	Sulfur	2.0772(5)
Lanthanum	0.5(3)	Tantalum	0.6(4)
Lead	1.1(2)	Technetium	0.7(3)
Lithium	0.620(7)	Tellurium	1.9708(3)
Magnesium	<0	Thallium	0.3(2)
Manganese	<0	Tin	1.25(10)
Mercury	<0	Titanium	0.2(2)
Molybdenum	1.0(2)	Tungsten	0.6(4)
Neon	<0	Vanadium	0.5(2)
Nickel	1.15(10)	Xenon	<0
Niobium	1.0(3)	Yttrium	0.0(3)
Nitrogen	−0.07(8)	Zinc	≈0
Osmium	1.1(3)	Zirconium	0.5(3)

B. Molecules

Molecule	Electron affinity, eV*	Molecule	Electron affinity, eV*
BF ₃	2.65	SF ₆	1.43
<i>p</i> -Benzoquinone	1.34	2,3,5,6-Tetrachloro- benzoquinone	2.40
NO ₂	3.91		
O ₂	0.45	Tetracyanoethylene	2.88

* To convert into kJ · mol^{−1} multiply by 96.48. To convert into kcal · mol^{−1} multiply by 23.06.

TABLE 3.3 Electron Affinities of Elements, Radicals and Molecules (*continued*)

C. Radicals

Radical	Electron affinity, eV*	Radical	Electron affinity, eV*
CH ₃	1.08	OH	1.83
C ₂ H ₅	0.89	CF ₃ O	1.35
C ₆ H ₅	2.20	CH ₃ O	0.38
CCl ₃	1.22	PH ₂	1.60
CF ₃	1.85	SH	2.19
CN	3.17	CH ₃ S	1.32
NH ₂	1.12	SCN	2.17
C ₆ H ₅ NH	1.55	SeCN	2.64
(C ₆ H ₅) ₂ N	1.19	SiF ₃	3.35

* To convert into kJ · mol⁻¹ multiply by 96.48. To convert into kcal · mol⁻¹ multiply by 23.06.

BOND LENGTHS AND STRENGTHS

The bonds most commonly encountered in organic chemistry are those between carbons and between carbon and heteroatoms of the first row of the Periodic Table. Generally and very approximately, single bonds between two carbon atoms are about 1.5 Å in length and have strengths near to, but usually less than, 100 kcal/mole (418 kJ/mol). Likewise, carbon–carbon double bonds are stronger (~150 kcal/mol) and shorter (~1.35 Å). Triple bonds are shorter still (C≡C ≈ 1.2 Å, ~200 kcal/mol). Bonds between carbon and either nitrogen or oxygen are somewhat shorter owing to the heteroatom's electronegativity. A few general examples are shown below and detailed data may be found in the Table 3.4.

General Trends in the Length of Common Organic Chemical Bonds

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
C—C	1.54	C—O	1.43	H—C(sp ³)	1.12
C=C	1.33	C=O	1.20	N—H	1.03
C≡C	1.21	C—N	1.47	O—H	0.97
		C=N	1.28	C—Cl	1.76
		C≡N	1.15		

TABLE 3.4A Bond Lengths between Carbon and other Elements

The numbers in parentheses following a numerical value represent the standard deviation of that value in terms of the final listed digit.
To convert the bond length from angstroms into nanometers, multiply by 0.1; to convert angstroms into picometers, multiply by 100.

Bond type		Bond length, Å*		
Carbon–carbon				
<i>Single bond</i>				
Paraffinic: —C—C—		1.541(3)		
In presence of —C=C— or of aromatic ring		1.53(1)		
In presence of —C=O bond		1.516(5)		
In presence of two carbon–oxygen double bonds		1.49(1)		
In presence of two carbon–carbon double bonds		1.426(5)		
Aryl —C=O		1.47(2)		
In presence of one carbon–carbon triple bond: —C—C≡C—		1.460(3)		
In presence of one carbon–nitrogen triple bond: —C—C≡N		1.464(5)		
In compounds with tendency to dipole formation, e.g., C=C—C=O		1.44(1)		
In aromatic compounds		1.395(3)		
In presence of carbon–carbon double and triple bonds: —C=C—C≡C—		1.426(5)		
In presence of two carbon–carbon triple bonds: —C≡C—C≡C—		1.373(4)		
<i>Double bond</i>				
Single: —C=C—		1.337(6)		
Conjugated with a carbon–carbon double bond: —C=C—C=C—		1.336(5)		
Conjugated with a carbon–oxygen double bond: —C=C—C=O		1.36(1)		
Cumulative: —C=C=C— or —C=C=O		1.309(5)		
<i>Triple bond</i>				
Simple: —C≡C—		1.204(2)		
Conjugated: —C≡C—C=C—, —C≡C—C=O, or —C≡C—aryl		1.206(4)		
Bond type		Bond length, Å		
Carbon–halogen				
	Fluorine	Chlorine	Bromine	Iodine
Paraffinic: R—X	1.379(5)	1.767(2)	1.938(5)	2.139(1)
Olefinic: —C=C—X	1.333(5)	1.719(5)	1.89(1)	2.092(5)
Aromatic: Ar—X	1.328(5)	1.70(1)	1.85(1)	2.05(1)
Acetylenic: —C≡C—X	(1.27)	1.635(5)	1.795(10)	1.99(2)
Bond type				Bond length, Å
Carbon–hydrogen				
<i>Paraffinic</i>				
In methane				1.092
In CD ₄				1.094
In monosubstituted carbon: H—C—Y				1.096(5)
In disubstituted carbon: <div style="display: inline-block; vertical-align: middle; text-align: center;"><div style="display: inline-block; vertical-align: middle; text-align: center;">X H—C— Y</div></div>				1.073(5)

TABLE 3.4A Bond Lengths between Carbon and Other Elements (*continued*)

Bond type	Bond length, Å
Carbon–hydrogen (<i>continued</i>)	
<i>Paraffinic (continued)</i> In trisubstituted carbon: $\begin{array}{c} \text{X} \\ \\ \text{H}-\text{C}-\text{Y} \\ \\ \text{Y} \end{array}$	1.070(7)
<i>Olefinic</i> Simple: $\text{H}-\text{C}=\text{C}-$ Cumulative carbon–carbon double bonds: $\text{H}-\text{C}=\text{C}=\text{C}-$ Cumulative carbon–carbon–oxygen double bonds: $\text{H}-\text{C}-\text{C}=\text{C}=\text{O}$	1.083(5) 1.07(1) 1.08(1)
<i>Aromatic</i>	1.084(5)
<i>Acetylenic</i> (in C_2H_2 , 1.059)	1.055(5)
<i>In small rings</i>	1.081(5)
<i>In presence of a carbon triple bond:</i> $\text{H}-\text{C}\equiv\text{C}-$	1.115(4)
Carbon–nitrogen	
<i>Single bond</i> Paraffinic: 3 covalent nitrogen: RNH_2 , R_2NH , R_3N 4 covalent nitrogen: RNH_3^+ , $\text{R}_3\text{N}-\text{BX}_3$ In $-\text{C}-\text{N}=-$ In aromatic compounds In conjugated heterocyclic systems (partial double bond) In $-\text{N}-\text{C}=\text{O}$ (partial double bond)	1.472(5) 1.479(5) 1.475(10) 1.43(1) 1.353(5) 1.322(5)
<i>Double bond:</i> $-\text{C}=\text{N}-$	1.32
<i>Triple bond</i> (in CN radical, 1.1774): $-\text{C}\equiv\text{N}$	1.157(5)
Carbon–oxygen	
<i>Single bond</i> Paraffinic and saturated heterocyclic: $-\text{C}-\text{O}-$	1.426(5)
Strained, as in epoxides: $\begin{array}{c} \\ -\text{C} \diagup \text{C}- \\ \quad \diagdown \\ \quad \text{O} \end{array}$	1.435(5)
In aromatic compounds, as $\text{Ar}-\text{OH}$ Longer bond in carboxylic acids and esters (HCOOH , 1.312) In conjugated heterocyclics, as furan	1.36(1) 1.358(5) 1.371(16)

TABLE 3.4A Bond Lengths between Carbon and Other Elements (*continued*)

Bond type	Bond length, Å
Carbon–oxygen (<i>continued</i>)	
<i>Double bond</i>	
In CO ⁺	1.115
In CO	1.128
In CO ₂ ⁺	1.177
In HCO	1.198(8)
In carbonyls	1.145(10)
In aldehydes and ketones	1.215(5)
In acyl halides: R—CO—X	1.171(4)
Shorter bond in carboxylic acids and esters	1.233(5)
In zwitterion forms	1.26(1)
In O=C=	1.160(1)
In isocyanates: RN=C=O	1.17(1)
In conjugated systems, as in partial triple bond: O=C—C=C	1.215(5)
In <i>p</i> -quinones	1.15(2)
In metal acetylacetonates	1.28(2)
In calcite: CaCO ₃	1.29(1)
Carbon–selenium	
<i>Single bond</i>	
Paraffinic: —C—Se—	1.98(2)
In presence of fluorine, as in perfluoro compounds: —CF—Se—	1.95(2)
<i>Double bond</i>	
In Se=C=, as SeCS and SeCO	1.709(3)
In CSe radical	1.67
Carbon–silicon	
Alkyl substituent: H ₃ C—Si or H ₂ C—Si	1.870(5)
Aryl substituent: aryl—Si	1.843(5)
Electronegative substituent: R—Si—X	1.854(5)
Carbon–sulfur	
<i>Single bond</i>	
Paraffinic: —C—S—	1.817(5)
In presence of fluorine, as in perfluoro-compounds: —CF—S—	1.835(1)
In heterocyclic systems: partial double bonds	1.718(5)
<i>Double bond</i>	
In S=C: thiophene, S=CR ₂	1.71(1)
In sulfoxides and sulfones	1.80(1)
In presence of second carbon–carbon double bond: S=C—C=C—	1.555(1)
In SC radical [in CS ₂ ⁺ , 1.554(5)]	1.5349(2)

TABLE 3.4A Bond Lengths between Carbon and Other Elements (*continued*)

Bond type	Bond length, Å	Bond type	Bond length, Å
Other elements and carbon			
C—Al	2.24(4)	C—In	2.16(4)
C—As (paraffinic)	1.98(1)	C—Mo	2.08(4)
C—B	1.56(1)	C—Ni	2.107(5)
C—Be	1.93	C—Pb (alkyl)	2.30(1)
C—Bi	2.30	C—Pd	2.27(4)
C—Co	1.83(2)	C—Sb (paraffinic)	2.202(16)
C—Cr	1.92(4)	C—Sn	
C—Fe	1.84(2)	alkyl	2.143(5)
C—Ge		electronegative substituent	2.18(2)
Alkyl	1.98(3)	C—Te	1.904
Aryl	1.945(5)	C—Tl	2.705(5)
C—Hg	2.07(1)	C—W	2.06
in Hg(CN) ₂	1.99(2)		

TABLE 3.4B Bond Lengths between Elements Other than Carbon

Elements	Bond type	Bond length, Å	Elements	Bond type	Bond length, Å
Boron			Hydrogen (<i>continued</i>)		
B—B	B ₂ H ₆	1.77(1)	H—Mg	MgH	1.731
B—Br	BBr ₃	1.87(2)	H—Na	NaH	1.887
B—Cl	BCl ₃	1.72(1)	H—Sb	H ₃ Sb	1.707
B—F	BF ₃ , R ₂ BF	1.29(1)	H—Se	H ₂ Se	1.460
B—H	Boranes	1.21(2)	H—Sn	SnH ₄	1.701
	Bridge	1.39(2)	D—Br	DBr	1.4144
B—N	Borazoles	1.42(1)	D—Cl	DCl	1.2746
B—O	B(OH) ₃ , (RO) ₃ B	1.362(5)	D—I		1.6165
			T—Br		1.4144
			T—Cl		1.2740
Hydrogen			Nitrogen		
H—Al	AlH	1.646	N—Cl	NO ₂ Cl	1.79(2)
H—As	AsH ₃	1.519	N—F	NF ₃	1.36(2)
H—Be	BeH	1.343	N—H	NH ₄ ⁺	1.034(3)
H—Br	HBr	1.408		NH ₃ , RNH ₂	1.012
H—Ca	CaH	2.002		H ₂ NNH ₂	1.038
H—Cl	HCl	1.274		R—CO—NH ₂	0.99(3)
H—F	HF	0.917		HN=C=S	1.013(5)
H—Ge	GeH ₄	1.53	N—D	ND	1.041
H—I	HI	1.609	N—N	HN ₃	1.02(1)
H—K	KH	2.244		R ₂ NNH ₂	1.451(5)
H—Li	LiH	2.595			

TABLE 3.4B Bond Lengths between Elements Other than Carbon (*continued*)

Elements	Bond type	Bond length, Å	Elements	Bond type	Bond length, Å
Nitrogen (<i>continued</i>)			Phosphorus (<i>continued</i>)		
N—O	N ₂ O	1.126(2)	P—H	PH ₃ , PH ₄ ⁺	1.424(5)
	N ₂ ⁺	1.116	P—I	PI ₃	2.52(1)
	NO ₂ Cl	1.24(1)	P—N	Single bond	1.491
	RO—NO ₂	1.36(2)	P—O	Single bond	1.447
N=O	NO ₂	1.188(5)		<i>p</i> ³ bonding	1.67
	N ₂ O	1.186(2)		<i>sp</i> ³ bonding	1.54(4)
	RNO ₂	1.22(1)	P—S	<i>p</i> ³ bonding	2.12(5)
	NO ⁺	1.0619		<i>sp</i> ³ bonding	2.08(2)
N—Si	SiN	1.572		In rings	2.20(2)
Oxygen			P—C	Single bond	1.562
O—H	H ₂ O	0.958		<i>p</i> ³ bonding	1.87(2)
	ROH	0.97(1)	Silicon		
	OH ⁺	1.0289	Si—Br	SiBr ₄ , R ₃ SiBr	2.16(1)
	HOOH	0.960(5)	Si—Cl	SiCl ₄ , R ₃ SiCl	2.019(5)
	D ₂ O	0.9575	Si—F	SiF ₄ , R ₃ SiF	1.561(3)
	OD	0.9699		SiF ₆	1.58
	HO—OH	1.48(1)	Si—H	SiH ₄	1.480(5)
	O ₂ ⁺	1.227		R ₃ SiH	1.476(5)
	O ₂ [−]	1.26(2)	Si—I	SiI ₄	2.34
	O ₂ ^{2−}	1.49(2)		R ₃ SiI	2.46(2)
O—O	O ₃	1.278(5)	Si—O	R ₃ SiOR	1.633(5)
	AlO	1.618	Si—Si	H ₃ SiSiH ₃	2.30(2)
	As ₄ O ₆ (bridges)	1.79	Sulfur		
	BaO	1.940	S—Br	SOBr ₂	2.27(2)
	ClO ₂	1.484	S—Cl	S ₂ Cl ₂	1.585(5)
	OCl ₂	1.68	S—F	SOF ₂	1.585(5)
	MgO	1.749	S—H	H ₂ S	1.333
	OsO ₄	1.66		RSH	1.329(5)
	PbO	1.934		D ₂ S	1.345
			S—O	SO ₂	1.4321
Phosphorus				SOCl ₂	1.45(2)
P—Br	PBr ₃	2.23(1)	S—S	RSSR	2.05(1)
P—Cl	PCl ₃	2.00(2)			
P—F	PFCl ₂	1.55(3)			

TABLE 3.5 Bond Strengths

The quantity $D_0(\text{A—B})$ corresponds to the bond dissociation energy at 0 K, all species considered to be ideal gases, for a bond A—B which is broken through the reaction: $\text{Eq. } \text{AB} \rightarrow \text{A} + \text{B}$

where

$$D_0 = \Delta H_f^\circ(\text{A}) + \Delta H_f^\circ(\text{B}) - \Delta H_f^\circ(\text{AB})$$

D_0 at 298 K, or ΔH_f° , is greater than D_0 at 0 K by an amount which lies between RT and $3/2 RT$, or between 0.6 and 0.9 kcal · mol⁻¹. In polyatomic molecules this difference may be somewhat greater. It is important to note that the bond dissociation energy refers to the enthalpy change ΔH_f in the dissociation process.

The strengths of carbon–carbon bonds are greatest for triple bonds and typically decrease with bond order. Other factors play a role as well. A carbon–carbon single bond between two multiple bonds will share some additional electron density and be correspondingly strengthened. Bonds are weaker than “normal” when cleavage of a bond gives a particularly stable species. For example, cleavage of a single bond in ethylbenzene to give benzyl radical and methyl radical, $\text{C}_6\text{H}_5\text{CH}_2\text{—CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\bullet + \bullet\text{CH}_3$, is favorable because benzyl radical is stable. Thus, the C—C bond strength in this case is only 72 kcal/mol compared to the single bond of propane, which is 85 kcal/mol. Hexamethylethane may dissociate into two *t*-butyl radicals $[(\text{CH}_3)_3\text{C}\bullet]$. The combination of steric crowding and the formation of stabilized radicals makes the C—C bond strength in $(\text{CH}_3)_3\text{C—C}(\text{CH}_3)_3$ only about 68 kcal/mol. A few selected examples follow:

The numbers in parentheses following a numerical value represent the standard deviation of that value in terms of the final listed digit(s).

To convert the tabulated values (in kcal · mol⁻¹) to kJ · mol⁻¹, multiply by 4.184.

Source: T. L. Cottrell, *The Strengths of Chemical Bonds*, 2nd ed., Butterworth, London, 1958; B. deB. Darwent, National Standard Reference Data Series, National Bureau of Standards, no. 31, Washington, 1970; S. W. Benson, *J. Chem. Educ.*, **42**: 502 (1965); and J. A. Kerr, *Chem. Rev.*, **66**: 465 (1966).

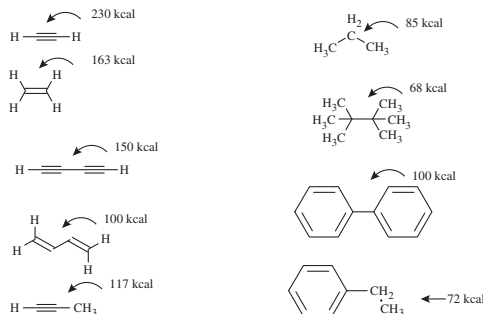
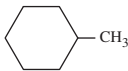


TABLE 3.5 Bond Strengths (*continued*)

Bond	D_0° , kcal · mol ⁻¹	ΔH_f° , kcal · mol ⁻¹	Bond	D_0° , kcal · mol ⁻¹	ΔH_f° , kcal · mol ⁻¹
Boron			Carbon (<i>continued</i>)		
H ₃ B—BH ₃ F ₂ B—F	133(20)	35	CH ₃ —CH ₂ CN CH ₃ —CH(CH ₃)CN CH ₃ —C(C ₆ H ₅)CN(CH ₃) C ₂ H ₅ —CH ₂ CN CH ₃ —CF ₃ CH ₂ F—CH ₂ F CF ₃ —CF ₃ CF ₂ =CF ₂ CF ₃ —CN CH ₂ —CO CH ₃ —CHO CH ₃ CO—CF ₃ CH ₃ CO—COCH ₃ C ₆ H ₅ CO—COC ₆ H ₅ C ₆ H ₅ CH ₂ CO—CH ₂ C ₆ H ₅ C ₆ H ₅ CH ₂ —COOH (C ₆ H ₅ CH ₂) ₂ CH—COOH NC—CN CF ₃ —NF ₂ CH ₃ —NH ₂ C ₆ H ₅ CH ₂ —NH ₂	80.6	73(2) 79(2) 60 76.9(17) 101.2(11) 88(2) 97(2) 76(3) 120 81.9 75 73.8 67(2) 66.4 65.4 68.1 59.4 144(5) 65(3) 79(3) 72(1)
Bromine					
Br—Br Br—CH ₃ Br—CH ₂ Br Br—CHBr ₂ Br—CBr ₃ Br—CCl ₃ Br—CF ₃ Br—CF ₂ CF ₃ Br—CF ₂ CF ₂ CF ₃ Br—CHF ₂ Br—Cl Br—F Br—CN Br—CO—C ₆ H ₅ Br—N Br—NF ₂	45.45(1) 67(2) 49(3) 51(3) 51.6(1) 67.2 68(5)	46.10(1) 68(2) 61(3) 62(4) 50(3) 52(3) 68(3) 68.7(15) 66.5(15) 69 52.3(1) 68.1 91 64 53			

Br—NO	27.8(15)	28.7(15)		
Br—O	55.3(1)	56.2(1)		
Carbon				
HC≡CH		230(2)	CH ₃ —NHC ₆ H ₅	68
H ₂ C=CH ₂		163	CH ₃ —N(CH ₃)C ₆ H ₅	65
CH ₃ —CH ₃		88	C ₆ H ₅ CH ₂ —NHCH ₃	69(1)
CH ₃ —C(CH ₃) ₂ CH ₃		69(2)	C ₆ H ₅ CH ₂ —N(CH ₃) ₂	61(1)
CH ₃ —C(CH ₃) ₃		80	CH ₃ —(N=NCH ₃)	52.5
CH ₃ —C ₆ H ₅		93	C ₂ H ₅ —(N=NC ₂ H ₅)	50.0
CH ₃ —CH ₂ C ₆ H ₅		72	(CH ₃) ₃ C—[N=NC(CH ₃) ₃]	43.5
CH ₃ —CH(CH ₃)C ₆ H ₅		71	C ₆ H ₅ CH ₂ —(N=NCH ₂ C ₆ H ₅)	37.6
C ₂ H ₅ —CH ₂ C ₆ H ₅		71	CF ₃ —(N=NCF ₃)	55.2
C ₃ H ₇ —CH ₂ C ₆ H ₅		67(2)	H ₂ C=NH	154(5)
CH ₃ —(CH=CH ₂)		29	HC≡N	224
CH ₃ —(CH ₂ CH=CH ₂)		72	CH ₃ —NO	41.8(9)
CH ₃ —(C≡CH)		117	C ₂ H ₅ —NO	42.0(13)
(CH ₃) ₃ C—C(CH ₃) ₃		67.5	C ₃ H ₇ —NO	40.1(18)
(CH ₃) ₃ C—C(C ₆ H ₅) ₃		15	(CH ₃) ₂ CH—NO	41.0(13)
(CH ₂ =CH)—(CH=CH ₂)		100	C ₄ H ₉ —NO	51.5(10)
C ₆ H ₅ —C ₆ H ₅		100	C ₆ H ₅ —NO	51.5(10)
(HC≡C)—(C≡CH)		150	Cl ₃ C—NO	32
CH ₃ —CN	119(5)	121(5)	F ₃ C—NO	31
			C ₆ F ₅ —NO	50.5(10)
			NC—NO	29(3)
			CH ₃ —NO ₂	59(3)
			C ₂ H ₅ —NO ₂	62
			CH ₃ —OCH ₃	80

TABLE 3.5 Bond Strengths (*continued*)

Bond	D_0° , kcal · mol ⁻¹	ΔH_f° ₂₉₈ , kcal · mol ⁻¹	Bond	D_0° , kcal · mol ⁻¹	ΔH_f° ₂₉₈ , kcal · mol ⁻¹
Carbon (<i>continued</i>)			Chlorine (<i>continued</i>)		
CH ₃ —OC ₆ H ₅	67	91	Cl—COC ₆ H ₅	57.3(1) 33.3(10) 59.5(5)	74(3)
CH ₃ —OCH ₂ C ₆ H ₅		67	Cl—Cl ⁺		94
C ₂ H ₅ —OC ₆ H ₅		51	Cl—Cl		
C ₆ H ₅ CH ₂ —OCOCH ₃			Cl—ClO		
C ₆ H ₅ CH ₂ —OCOC ₆ H ₅		69	O ₃ Cl—ClO ₄		58
CH ₃ CO—OCH ₃		97	Cl—F		
CH ₃ —O—SOCH ₃		67	O ₃ Cl—F		61
CH ₂ =CHCH ₂ —OSOCH ₃		50	Cl—N		62
C ₆ H ₅ CH ₂ —OSOCH ₃		53	Cl—NCl		67
C=O		256.2(1)	257.3(1)		Cl—NCl ₂
H ₂ C=O		175	Cl—NF ₂		ca 32
OC=O	125.7(1)	127.2(1)	Cl—NH ₂		60(6)
SC=O	148	150	Cl—NO	37.0(15)	38.0(15)
C≡O		257	Cl—NO ₂	33(1)	34(1)
CH ₃ —SH	71(3)	73(3)	Cl—O	64(1)	
CH ₃ —SC ₆ H ₅		68(2)	OCl—O	58(3)	
CH ₃ —SCH ₂ C ₆ H ₅		59(2)	O ₂ Cl—O		48(1)
OC—S	72.9	74.2	Cl—SiCl ₃		111
ĊH ₂ —CH ₃		96	Cl—CH ₃ ⁺		51
ĊH ₂ CH ₂ —CH ₃		25.5	Cl—Cl ⁺		94
(ĊH ₂) ₂ C—CH ₃		51	Fluorine		
ĊHCH—CH ₃		32			
		27.5			
			F—CH ₃		108(5)
			F—C(CH ₃) ₃		105

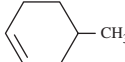
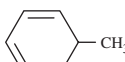


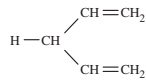

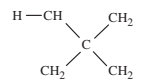
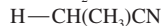
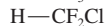
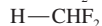
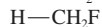
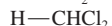
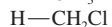
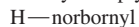
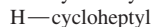
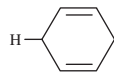
		35	F—C ₆ H ₅ F—CCl ₃ F—CCl ₂ F F—CClF ₂ F—CF ₃ F—COCH ₃ F—F OF—F O ₂ F—F F—N F—NF F—NF ₂ F—NO F—NO ₂ F—F ⁺		116 106(5) 110(6) 117(6) 125(4) 119
		11.5		37(1) 64(3) 18.4 71(10) 75(5) 57(2) 55.2(10) 46(5) >60	
(CH ₃) ₂ C(ĊH ₂)—CH ₃		20			
ÖCH ₂ —CH ₃		12			
(CH ₃) ₂ C(Ö)—CH ₃		7			72(10)
ĊH ₂ CO—CH ₃		30			76(5)
ÖC—CH ₃		11			58(2)
Ö ₂ C—CH ₃		—20			56.3(10)
CH ₃ —CH ₃ ⁺		46			
CH ₂ —CH ₃ ⁺		119			
CH ₂ =CH ₂ ⁺		162			
HC≡CH ⁺		223			
			Gallium		
Chlorine			CH ₃ —Ga(CH ₃) ₃	59.5	
Cl—C	80(10)	80.8	Hydrogen		
Cl—CH ₃		81(5)			
Cl—C(CH ₃) ₃		78.5	H—Br	86.6(1)	87.5(1)
Cl—CH ₂ Cl		74(3)	H—C	80	81.0(5)
Cl—CCl ₃		70(5)	H—CH		108(6)
Cl—CF ₃		86.1(8)	H—CH ₂	112.3(1)	113(1)
Cl—CCl ₂ F		73(2)	H—CH ₃	102(2)	103(2)
Cl—CF ₂ Cl		76(2)	D—CD ₃	104.92(5)	
Cl—CF ₂ CF ₃		82.7(17)	H—(C≡CH)		125(1)
Cl—(CH=CH ₂)		84	H—(C=CH ₂)		102
Cl—CN		105	H—CH ₂ CH ₃		98(1)
Cl—COCl		78.5	H—CH ₂ C≡CH		93.9(12)
Cl—COCH ₃		83.5	H—CH ₂ CH=CH ₂		85




TABLE 3.5 Bond Strengths (*continued*)

Bond	D_0° , kcal · mol ⁻¹	ΔH_f° , kcal · mol ⁻¹	Bond	D_0° , kcal · mol ⁻¹	ΔH_f° , kcal · mol ⁻¹
Hydrogen (<i>continued</i>)			Hydrogen (<i>continued</i>)		
H—cyclopropyl		101(3)	H—Cl	102.3(1)	
H—CH ₂ CH ₂ CH ₃		98(2)	H—CO		30(2)
H—CH(CH ₃) ₂		94.5	H—CHO		87(1)
H—cyclobutyl		95(3)	H—COOH		90
H—CH ₂ CH(CH ₃) ₂		86	H—COCH ₃		87(1)
H—CH(CH ₃)CH ₂ CH ₃		95(1)	H—COCH ₂ CH ₃		87(1)
H—C(CH ₃) ₃		91			92(1)
		81(1)	H—COC ₆ H ₅		87(1)
		80(1)	H—COCF ₃		91(2)
		82(1)	H—F	135(1)	135.8
		99(1)	H—H	103.25	104.19
			H—D	104.07(1)	105.00
			D—D	105.05(1)	105.96
			H—I	70.4(1)	71.3(1)
			H—N	85(2)	85(2)
			H—NH	89(2)	90(2)
			H—NH ₂	103(2)	104(2)
			H—NHCH ₃		103(2)
H—C(CH ₃) ₂ CH=CH ₂		79	H—N(CH ₃) ₂		95(2)
H—cyclopentyl		94.5(10)	H—NHC ₆ H ₅		80(3)
H—CH ₂ C(CH ₃) ₃		100(1)	H—N(CH ₃)C ₆ H ₅		74(3)
H—C ₆ H ₅		103	H—NF ₂		76(3)
H—CH ₂ C ₆ H ₅		85(1)	H—N ₃		85



	75	$\text{H}-\text{NO}$		< 49
	74	$\text{H}-\text{O}$	101.3(5)	102.3(5)
		$\text{H}-\text{OH}$	118.0(2)	119.2(2)
		$\text{H}-\text{OCH}_3$		104.4(10)
		$\text{H}-\text{OCH}_2\text{CH}_3$		104.2
	95.5(10)	$\text{H}-\text{OC}(\text{CH}_3)_3$		105(1)
	92.5(10)	$\text{H}-\text{OCH}_2\text{C}(\text{CH}_3)_3$		102.3(15)
	97(3)	$\text{H}-\text{OC}_6\text{H}_5$		88(5)
97(5)		$\text{H}-\text{ONO}$		78.3(5)
	104	$\text{H}-\text{ONO}_2$		101.2(5)
88(2)	90(2)	$\text{H}-\text{OOH}$	88.5(20)	89.5(20)
	101	$\text{H}-\text{OOCCH}_3$		112(4)
	99.0	$\text{H}-\text{OOCCH}_2\text{CH}_3$		110(4)
89(3)	90(3)	$\text{H}-\text{OOCCH}_2\text{CH}_2\text{CH}_3$		103(4)
	94(2)	$\text{H}-\text{SH}$	90(1)	91(1)
	95(2)	$\text{H}-\text{SCH}_3$		ca 88
	101(2)	$\text{H}-\text{SiH}_3$		94(3)
	101(2)	$\text{H}-\text{Si}(\text{CH}_3)_3$		90(3)
105(3)	106(3)	$\text{H}-\text{SiCl}_3$		91.3(14)
	104(1)	$\dot{\text{C}}\text{H}_2-\text{H}$		106
	106.7(11)	$\dot{\text{C}}\text{H}-\text{H}$		106
	99.5(1)	$\dot{\text{C}}-\text{H}$		81
	103.1(15)	$\dot{\text{C}}\text{H}_2\text{CH}_2-\text{H}$		39
	104(2)	$\dot{\text{O}}\text{CH}_2-\text{H}$		22
	103(2)	$\dot{\text{C}}\text{O}-\text{H}$		19
	103(2)	$\dot{\text{C}}\text{HCH}-\text{H}$		43
127(5)	129(5)	$\text{H}-\dot{\text{O}}$		102
	ca 93	$\text{H}-\text{O}\dot{\text{O}}$		47
	90(2)	$\text{H}-\text{O}\dot{\text{C}}\text{H}_2$		31
	87(2)	$\text{H}-\text{OO}\dot{\text{C}}$		31
	95(2)	$\dot{\text{C}}\text{H}-\text{H}$		ca 125
	99(1)	$\dot{\text{C}}\text{OCH}_2-\text{H}$		43.5
	98.3(18)			

TABLE 3.5 Bond Strengths (*continued*)

Bond	D_0° , kcal · mol ⁻¹	ΔH_f° , kcal · mol ⁻¹	Bond	D_0° , kcal · mol ⁻¹	ΔH_f° , kcal · mol ⁻¹
Hydrogen (<i>continued</i>)			Nitrogen		
$\text{CH}_2\text{CO—H}$		36	N—N	225.07(1)	225.96(1)
		40	F ₂ N—NF ₂	20(1)	21(1)
		47.5	H ₂ N—NH ₂		71(2)
		24	H ₂ N—NHCH ₃		65
C ⁺ —H		85	H ₂ N—N(CH ₃) ₂		63
CH ₃ ⁺ —H		30	H ₂ N—NHC ₆ H ₅		51
CH ₃ CH ₂ ⁺ —H		29	HN—N ₂		9(1)
CH ₂ CH ₃ ⁺ —H		79	ON—N	113.5(10)	114.9(10)
H—H ⁺		62	ON—NO ₂	8.4(2)	9.5(2)
Iodine			O ₂ N—NO ₂	12.7(5)	13.7(5)
I—Br	41.9(1)	42.5(1)	NN—O		40
I—CH ₃	54(3)	55.5(30)	ON—O		73
I—CH ₂ CH ₃		53.5	HN=NH		109(10)
I—CH(CH ₃) ₂		53	HN=O		115
I—C(CH ₃) ₂		49.5	N≡N		226
I—CH ₂ CF ₃		56(1)	N—N ⁺		200
I—CF ₂ CH ₃		52(1)	N—NO ⁺		155
			NN—O ⁺		56
			ON ⁺ —O		56
			Osmium		
			O ₃ Os—O		72(5)
			Oxygen		
			HO—CH ₃	88.5(30)	90(3)
			HO—(CH=CH ₂)		87

I—CF ₂ CF ₃		51(1)	HO—CH ₂ CH=CH ₂		109
I—C ₃ F ₇		50(1)	HO—C ₆ H ₅		103
I—(CH=CHCH ₃)		41	HO—CH ₂ C ₆ H ₅		77
I—CH ₃ ⁺		62	HO—CHO		96(3)
I—C ₆ H ₅		64(1)	HO—COCH ₃		108(5)
I—C ₆ F ₃		66	HO—COCH ₂ CH ₃		43
I—Cl	49.7(1)	50.5(1)	HO—Cl		60(3)
I—COCH ₃		52.5	HO—I		56(3)
I—CN		73(1)	HO—NCH ₃		50
I—F	66.4(10)	67(1)	HO—OC(CH ₃) ₃		46(2)
I ⁺ —H		70	O—O	117.97(10)	119.11
I—I	35.60(1)	36.15	HO—OH	49.5(5)	51.1(5)
I—I ⁺		61	CF ₃ O—OCF ₃		46
I—NO		17(1)	CH ₃ O—OCH ₃		37.6(2)
I—NO ₂		18(1)	C ₂ H ₅ O—OC ₂ H ₅		38
			C ₃ H ₇ O—OC ₃ H ₇		37
Lead			O—OF	110.7	
			O—O ₂ ClF		58
CH ₃ —Pb(CH ₃) ₃		49.4(10)	FO—OF		62(20)
			O=PBr ₃		119(5)
Lithium			O=PCl ₃		122(5)
			O=PF ₃		130(5)
Li—H	58		O—O ⁺		168
			HO—CH ₃ ⁺		67
Mercury			Phosphorus		
Hg—Br	16.4(10)	17.4(10)	P—Br		63.7
CH ₃ —HgCH ₃		57.5	P—Cl		78.5
C ₂ H ₅ —HgC ₂ H ₅		43.7(10)	P—F		117
C ₃ H ₇ —HgC ₃ H ₇		47.1	P—H		79(1)
(CH ₃) ₂ CH—HgCH(CH ₃) ₂		40.7	P—O	141.5(10)	142.3(10)
C ₆ H ₅ —HgC ₆ H ₅		68	P—P	115(2)	116(2)
			P=S	82	

TABLE 3.5 Bond Strengths (continued)

Bond	D_0° , kcal · mol ⁻¹	ΔH_{f298}° , kcal · mol ⁻¹	Bond	D_0° , kcal · mol ⁻¹	ΔH_{f298}° , kcal · mol ⁻¹				
Ruthenium			Sulfur						
O—RuO ₃	104		S—Cl O ₂ S—F S—N S—O OS—O O ₂ S—O S—S HS—SH S—Te HS ⁺ —H HS—H ⁺ OS—O ⁺	16 115 123.6(20) 130.8(20) 81.9(10) 101.5(15) 60	61 83.2(10) 102.5(15) 65(5) 104 161 155				
Selenium									
Se—Cl	81(23) 65	58 68							
Se—F									
Se—O									
Se—Se									
Silicon									
Si—Br	69(14)	135				Tin			
Si—Cl	76(12)					BrSn—Br Br ₃ Sn—Br C ₂ H ₅ Sn—(C ₂ H ₅) ₃ Sn—Cl Sn—H Sn—I Sn—O Sn—S	78 65 ca 57 76 61.0(7) 65 130(5) 111(5)	78 65 ca 57 76 61.0(7) 65 131(5) 112(5)	
Si—F	74(6)								Xenon
Si—H			56	Xe—F					31(1)
Si—I									
Si—N									
Si—O									
Si—S									
Si—Se	134(6)		42 81(4) 81 88(7)						
Si—Si	122(9)								
H ₃ Si—SiH ₃									
(CH ₃) ₃ Si—Si(CH ₃) ₃									
(C ₆ H ₅) ₃ Si—Si(C ₆ H ₅) ₃									
Si—Te									

Sodium			Zinc		
Na—H	47	91(3)	Zn—H	19.6(5)	ca 48
Na—K	14.3		C ₂ H ₅ Zn—C ₂ H ₅		
Na—Na	17.3				
Na—OH					

BOND AND GROUP DIPOLE MOMENTS

All bonds between equal atoms are given zero values. Because of their symmetry, methane and ethane molecules are nonpolar. The principle of bond moments thus requires that the CH_3 group moment equal one H—C moment. Hence the substitution of any aliphatic H by CH_3 does not alter the dipole moment, and all saturated hydrocarbons have zero moments as long as the tetrahedral angles are maintained.

The group moment always includes the C—X bond. When the group is attached to an aromatic system, the moment contains the contributions through resonance of those polar structures postulated as arising through charge shifts around the ring.

All values for bond and group dipole moments in Tables 3.6 and 3.7 were obtained in benzene solution.

TABLE 3.6 Bond Dipole Moments

Bond	Moment, D*	Bond	Moment, D*
H—C		Se—C	0.7
Aliphatic	0.3	Si—C	1.2
Aromatic	0.0	Si—H	1.0
C—C	0.0	Si—N	1.55
C \equiv C	0.0	H—Sb	-0.08
C—O		G—As	-0.10
Ether, aliphatic	0.74	H—P	0.36
Alcohol, aliphatic	0.7	H—I	0.38
C=O		H—Br	0.78
Aliphatic	2.4	H—Cl	1.08
Aromatic	2.65	H—F	1.94
O—H	1.51	C—Te	0.6
C—S	0.9	N—F	0.17
C=S	2.0	P—I	0.3
S—H	0.65	P—Br	0.36
S—O	(0.2)	P—Cl	0.81
S=O		As—I	0.78
Aliphatic	2.8	As—Br	1.27
Aromatic	3.3	As—Cl	1.64
C—N, aliphatic	0.45	As—F	2.03
C=N	1.4	Sb—I	0.8
C \equiv N (nitrile)	3.6	Sb—Br	1.9
NC (isonitrile)	3.0	Sb—Cl	2.6
N—H	1.31	S—Cl	0.7
N—O	0.3	Cl—O	0.7
N=O	2.0	I—Br	1.2
N: lone pair on $sp^3\text{N}$	1.0	I—Cl	1
C—P, aliphatic	0.8	Br—Cl	0.57
P—O	(0.3)	Br—F	1.3
P=O	2.7	Cl—F	0.88
P—S	0.5	Li—C	1.4
P=S	2.9	K—Cl	10.6
B—C, aliphatic	0.7	K—F	7.3
B—O	0.25		

TABLE 3.6 Bond Dipole Moments (*continued*)

Bond	Moment, D*	Bond	Moment, D*
Cs—Cl	10.5	Dative (coordination) bonds (<i>continued</i>)	
Cs—F	7.9		
Dative (coordination) bonds		P → O	2.9
N → B	2.6	S → O	3.0
O → B	3.6	As → O	4.2
S → B	3.8	Se → O	3.1
P → B	4.4	Te → O	2.3
N → O	4.3	P → S	3.1
		P → Se	3.2
		Sb → S	4.5

*To convert debye units D into coulomb-meters, multiply by 3.33564×10^{-30} .

TABLE 3.7 Group Dipole Moments

Group	Moment, D*	
	Aromatic C—X	Aliphatic C—X
C—CH ₃	0.37	0.0
C—C ₂ H ₅	0.37	0.0
C—C(CH ₃) ₃	0.5	0.0
C—CH=CH ₂	< 0.4	0.6
C—C≡CH	0.7	0.9
C—F	1.47	1.79
C—Cl	1.59	1.87
C—Br	1.57	1.82
C—I	1.40	1.65
C—CH ₂ F	1.77(g)	
C—CF ₃	2.54	2.32
C—CH ₂ Cl	1.85	1.95
C—CHCl ₂	2.04	1.94
C—CCl ₃	2.11	1.57
C—CH ₂ Br	1.86	1.96
C—C≡N	4.05	3.4
C—NC	3.5	3.5
C—CH ₂ CN	1.86	2.0
C—C=O	2.65	2.4
C—CHO	2.96	2.49
C—COOH	1.64	1.63
C—CO—CH ₃	2.96	2.75
C—CO—OCH ₃	1.83	1.75
C—CO—OC ₂ H ₅	1.9	1.8
C—OH	1.6	1.7
C—OCH ₃	1.28	1.28
C—OCF ₃	2.36	

TABLE 3.7 Group Dipole Moments (*continued*)

Group	Moment, D*	
	Aromatic C—X	Aliphatic C—X
C—OCOCH ₃	1.69	
C—OC ₆ H ₅	1.16	1.16
C—CH ₂ OH	1.68	1.68
C—NH ₂	1.53	1.46
C—NHCH ₃	1.71	
C—N(CH ₃) ₂	1.58	0.86
C—NHCOCH ₃	3.69	
C—N(C ₆ H ₅) ₂	(0.3)	−0.3
C—NCO	2.32	2.8
C—N ₃	1.44	
C—NO	3.09	
C—NO ₂	4.01	2.70
C—CH ₂ NO ₂	3.3	3.4
C—SH	1.22	1.55
C—SCH ₃	1.34	1.40
C—SCF ₃	2.50	
C—SCN	3.59	3.6
C—NCS	2.9	3.3
C—SC ₆ H ₅	1.51	1.5
C—SF ₅	3.4	
C—SOCF ₃	3.88	
(C—) ₂ SO ₂	5.05	4.53
(C—) ₂ SO ₂ CH ₃	4.73	
(C—) ₂ SO ₂ CF ₃	4.32	
C—SeH	1.08	
C—SeCH ₃	1.31	1.32
C—Si(CH ₃) ₃	0.44	0.4

*To convert debye units D into coulomb-meters, multiply by 3.33564×10^{-30} .

SECTION 4

PHYSICAL PROPERTIES

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SOLUBILITIES

TABLE 4.1 Solubility of Gases in Water

Explanation of the column headings

α , Volume of gas in milliliters (mL). The column or line entry headed “ α ” gives the volume of gas (in milliliters) at standard conditions (0°C and 760 mm or 101.325 kN·m⁻²) dissolved in 1 mL of water at the temperature stated (in degrees Celsius) and when the pressure of the gas without the water vapor is 760 mm.

A, Volume of gas in milliliters (mL). The line entry “A” indicates the same quantity as “ α ” except that the gas itself is at the uniform pressure of 760 mm when in equilibrium with water.

I, Volume of gas in milliliters (mL). The column headed “I” gives the volume of the gas (in milliliters) dissolved in 1 mL of water when the pressure of the gas plus that of the water vapor is 760 mm.

q, Weight of the gas in grams (g). The column headed “q” gives the weight of gas (in grams) dissolved in 100 g of water when the pressure of the gas plus that of the water vapor is 760 mm

Temp. °C	Acetylene		Air*		Ammonia		Bromine	
	α	q	$\alpha(\times 10^3)$	% oxygen in air	α	q	α	q
0	1.73	0.200	29.18	34.91	1130	89.5	60.5	42.9
1	1.68	0.194	28.42	34.87	—	—	—	—
2	1.63	0.188	27.69	34.82	—	—	54.1	38.3
3	1.58	0.182	26.99	34.78	—	—	—	—
4	1.53	0.176	26.32	34.74	1047	79.6	48.3	34.2
5	1.49	0.171	25.68	34.69	—	—	—	—
6	1.45	0.167	25.06	34.65	—	—	43.3	30.6
7	1.41	0.162	24.47	34.60	—	—	—	—
8	1.37	0.157	23.90	34.56	947	72.0	38.9	27.5
9	1.34	0.154	23.36	34.52	—	—	—	—
10	1.31	0.150	22.84	34.47	870	68.4	35.1	24.8
11	1.27	0.146	22.34	34.43	—	—	—	—
12	1.24	0.142	21.87	34.38	857	65.1	31.5	22.2
13	1.21	0.138	21.41	34.34	837	63.6	—	—
14	1.18	0.135	20.97	34.30	—	—	28.4	20.0
15	1.15	0.131	20.55	34.25	770	—	—	—
16	1.13	0.129	20.14	34.21	775	58.7	25.7	18.0
17	1.10	0.125	19.75	34.17	—	—	—	—
18	1.08	0.123	19.38	34.12	—	—	23.4	16.4
19	1.05	0.119	19.02	34.08	—	—	—	—
20	1.03	0.117	18.68	34.03	680	52.9	21.3	14.9
21	1.01	0.115	18.34	33.99	—	—	—	—
22	0.99	0.112	18.01	33.95	—	—	19.4	13.5
23	0.97	0.110	17.69	33.90	—	—	—	—
24	0.95	0.107	17.38	33.86	639	48.2	17.7	12.3
25	0.93	0.105	17.08	33.82	—	—	—	—
26	0.91	0.102	16.79	33.77	—	—	16.3	11.3
27	0.89	0.100	16.50	33.73	—	—	—	—
28	0.87	0.098	16.21	33.68	586	44.0	15.0	10.3
29	0.85	0.095	15.92	33.64	—	—	—	—
30	0.84	0.094	15.64	33.60	530	41.0	13.8	9.5
35	—	—	—	—	—	—	—	—
40	—	—	14.18	—	400	31.6	9.4	6.3
45	—	—	—	—	—	—	—	—
50	—	—	12.97	—	290	23.5	6.5	4.1
60	—	—	12.16	—	200	16.8	4.9	2.9
70	—	—	—	—	—	11.1	3.8	1.9
80	—	—	11.26	—	—	6.5	3.0	1.2
90	—	—	—	—	—	3.0	—	—
100	—	—	11.05	—	—	0.0	—	—

*Free from NH₃ and CO₂; total pressure of air + water vapor is 760 mm.

TABLE 4.1 Solubility of Gases in Water (*continued*)

Temp. °C	Carbon dioxide		Carbon monoxide		Chlorine		Ethane		Ethylene		Hydrogen	
	α	q	α	q	l	q	α	q	α	q	α	q
0	1.713	0.334 6	0.035 37	0.004 397	—	—	0.098 74	0.013 17	0.226	0.028 1	0.021 48	0.000 192 2
1	1.646	0.321 3	0.034 55	0.004 293	—	—	0.094 76	0.012 63	0.219	0.027 2	0.021 26	0.000 190 1
2	1.584	0.309 1	0.033 75	0.004 191	—	—	0.090 93	0.012 12	0.211	0.026 2	0.021 05	0.000 188 1
3	1.527	0.297 8	0.032 97	0.004 092	—	—	0.087 25	0.011 62	0.204	0.025 3	0.020 84	0.000 186 2
4	1.473	0.287 1	0.032 22	0.003 996	—	—	0.083 72	0.011 14	0.197	0.024 4	0.020 64	0.000 184 3
5	1.424	0.277 4	0.031 49	0.003 903	—	—	0.080 33	0.010 69	0.191	0.023 7	0.020 44	0.000 182 4
6	1.377	0.268 1	0.030 78	0.003 813	—	—	0.077 09	0.010 25	0.184	0.022 8	0.020 25	0.000 180 6
7	1.331	0.258 9	0.030 09	0.003 725	—	—	0.074 00	0.009 83	0.178	0.022 0	0.020 07	0.000 178 9
8	1.282	0.249 2	0.029 42	0.003 640	—	—	0.071 06	0.009 43	0.173	0.021 4	0.019 89	0.000 177 2
9	1.237	0.240 3	0.028 78	0.003 559	—	—	0.068 26	0.009 06	0.167	0.020 7	0.019 72	0.000 175 6
10	1.194	0.231 8	0.028 16	0.003 479	3.148	0.997 2	0.065 61	0.008 70	0.162	0.020 0	0.019 55	0.000 174 0
11	1.154	0.223 9	0.027 57	0.003 405	3.047	0.965 4	0.063 28	0.008 38	0.157	0.019 4	0.019 40	0.000 172 5
12	1.117	0.216 5	0.027 01	0.003 332	2.950	0.934 6	0.061 06	0.008 08	0.152	0.018 8	0.019 25	0.000 171 0
13	1.083	0.209 8	0.026 46	0.003 261	2.856	0.905 0	0.058 94	0.007 80	0.148	0.018 3	0.019 11	0.000 169 6
14	1.050	0.203 2	0.025 93	0.003 194	2.767	0.876 8	0.056 94	0.007 53	0.143	0.017 6	0.018 97	0.000 168 2
15	1.019	0.197 0	0.025 43	0.003 130	2.680	0.849 5	0.055 04	0.007 27	0.139	0.017 1	0.018 83	0.000 166 8
16	0.985	0.190 3	0.024 94	0.003 066	2.597	0.823 2	0.053 26	0.007 03	0.136	0.016 7	0.018 69	0.000 165 4
17	0.956	0.184 5	0.024 48	0.003 007	2.517	0.797 9	0.051 59	0.006 80	0.132	0.016 2	0.018 56	0.000 164 1
18	0.928	0.178 9	0.024 02	0.002 947	2.440	0.773 8	0.050 03	0.006 59	0.129	0.015 8	0.018 44	0.000 162 8
19	0.902	0.173 7	0.023 60	0.002 891	2.368	0.751 0	0.048 58	0.006 39	0.125	0.015 3	0.018 31	0.000 161 6
20	0.878	0.168 8	0.023 19	0.002 838	2.299	0.729 3	0.047 24	0.006 20	0.122	0.014 9	0.018 19	0.000 160 3
21	0.854	0.164 0	0.022 81	0.002 789	2.238	0.710 0	0.045 89	0.006 02	0.119	0.014 6	0.018 05	0.000 158 8
22	0.829	0.159 0	0.022 44	0.002 739	2.180	0.691 8	0.044 59	0.005 84	0.116	0.014 2	0.017 92	0.000 157 5
23	0.804	0.154 0	0.022 08	0.002 691	2.123	0.673 9	0.043 35	0.005 67	0.114	0.013 9	0.017 79	0.000 156 1
24	0.781	0.149 3	0.021 74	0.002 646	2.070	0.657 2	0.042 17	0.005 51	0.111	0.013 5	0.017 66	0.000 154 8

TABLE 4.1 Solubility of Gases in Water (*continued*)

Temp. °C	Carbon dioxide		Carbon monoxide		Chlorine		Ethane		Ethylene		Hydrogen	
	α	q	α	q	l	q	α	q	α	q	α	q
25	0.759	0.144 9	0.021 42	0.002 603	2.019	0.641 3	0.041 04	0.005 35	0.108	0.013 1	0.017 54	0.000 153 5
26	0.738	0.140 6	0.021 10	0.002 560	1.970	0.625 9	0.039 97	0.005 20	0.106	0.012 9	0.017 42	0.000 152 2
27	0.718	0.136 6	0.020 80	0.002 519	1.923	0.611 2	0.038 95	0.005 06	0.104	0.012 6	0.017 31	0.000 150 9
28	0.699	0.132 7	0.020 51	0.002 479	1.880	0.597 5	0.037 99	0.004 93	0.102	0.012 3	0.017 20	0.000 149 6
29	0.682	0.129 2	0.020 24	0.002 442	1.839	0.584 7	0.037 09	0.004 80	0.100	0.012 1	0.017 09	0.000 148 4
30	0.665	0.125 7	0.019 98	0.002 405	1.799	0.572 3	0.036 24	0.004 68	0.098	0.011 8	0.016 99	0.000 147 4
35	0.592	0.110 5	0.018 77	0.002 231	1.602	0.510 4	0.032 30	0.004 12	—	—	0.016 66	0.000 142 5
40	0.530	0.097 3	0.017 75	0.002 075	1.438	0.459 0	0.029 15	0.003 66	—	—	0.016 44	0.000 138 4
45	0.479	0.086 0	0.016 90	0.001 933	1.322	0.422 8	0.026 60	0.003 27	—	—	0.016 24	0.000 134 1
50	0.436	0.076 1	0.016 15	0.001 797	1.225	0.392 5	0.024 59	0.002 94	—	—	0.016 08	0.000 128 7
60	0.359	0.057 6	0.014 88	0.001 522	1.023	0.329 5	0.021 77	0.002 39	—	—	0.016 00	0.000 117 8
70	—	—	0.014 40	0.001 276	0.862	0.279 3	0.019 48	0.001 85	—	—	0.016 0	0.000 102
80	—	—	0.014 30	0.000 980	0.683	0.222 7	0.018 26	0.001 34	—	—	0.016 0	0.000 079
90	—	—	0.014 2	0.000 57	0.39	0.127	0.017 6	0.000 8	—	—	0.016 0	0.000 046
100	—	—	0.014 1	0.000 00	0.00	0.000	0.017 2	0.000 0	—	—	0.016 0	0.000 000

TABLE 4.1 Solubility of Gases in Water (*continued*)

Temp. °C	Hydrogen sulfide		Methane		Nitric oxide		Nitrogen*		Oxygen		Sulfur dioxide	
	α	q	α	q	α	q	α	q	α	q	l	q
0	4.670	0.706 6	0.055 63	0.003 959	0.073 81	0.009 833	0.023 54	0.002 942	0.048 89	0.006 945	79.789	22.83
1	4.522	0.683 9	0.054 01	0.003 842	0.071 84	0.009 564	0.022 97	0.002 869	0.047 58	0.006 756	77.210	22.09
2	4.379	0.661 9	0.052 44	0.003 728	0.069 93	0.009 305	0.022 41	0.002 798	0.046 33	0.006 574	74.691	21.37
3	4.241	0.640 7	0.050 93	0.003 619	0.068 09	0.009 057	0.021 87	0.002 730	0.045 12	0.006 400	72.230	20.66
4	4.107	0.620 1	0.049 46	0.003 513	0.066 32	0.008 816	0.021 35	0.002 663	0.043 97	0.006 232	69.828	19.98
5	3.977	0.600 1	0.048 05	0.003 410	0.064 61	0.008 584	0.020 86	0.002 600	0.042 87	0.006 072	67.485	19.31
6	3.852	0.580 9	0.046 69	0.003 312	0.062 98	0.008 361	0.020 37	0.002 537	0.041 80	0.005 918	65.200	18.65
7	3.732	0.562 4	0.045 39	0.003 217	0.061 40	0.008 147	0.019 90	0.002 477	0.040 80	0.005 773	62.973	18.02
8	3.616	0.544 6	0.044 13	0.003 127	0.059 90	0.007 943	0.019 45	0.002 419	0.039 83	0.005 632	60.805	17.40
9	3.505	0.527 6	0.042 92	0.003 039	0.058 46	0.007 747	0.019 02	0.002 365	0.038 91	0.005 498	58.697	16.80
10	3.399	0.511 2	0.041 77	0.002 955	0.057 09	0.007 560	0.018 61	0.002 312	0.038 02	0.005 368	56.647	16.21
11	3.300	0.496 0	0.040 72	0.002 879	0.055 87	0.007 393	0.018 23	0.002 263	0.037 18	0.005 246	54.655	15.64
12	3.206	0.481 4	0.039 70	0.002 805	0.05470	0.007 233	0.017 86	0.002 216	0.036 37	0.005 128	52.723	15.09
13	3.115	0.467 4	0.038 72	0.002 733	0.053 57	0.007 078	0.017 50	0.002 170	0.035 59	0.005 014	50.849	14.56
14	3.028	0.454 0	0.037 79	0.002 665	0.052 50	0.006 930	0.017 17	0.002 126	0.034 86	0.004 906	49.033	14.04
15	2.945	0.441 1	0.036 90	0.002 599	0.051 47	0.006 788	0.016 85	0.002 085	0.034 15	0.004 802	47.276	13.54
16	2.865	0.428 7	0.036 06	0.002 538	0.050 49	0.006 652	0.016 54	0.002 045	0.033 48	0.004 703	45.578	13.05
17	2.789	0.416 9	0.035 25	0.002 478	0.049 56	0.006 524	0.016 25	0.002 006	0.032 83	0.004 606	43.939	12.59
18	2.717	0.405 6	0.034 48	0.002 422	0.048 68	0.006 400	0.014 97	0.001 970	0.032 20	0.004 514	42.360	12.14
19	2.647	0.394 8	0.033 76	0.002 369	0.047 85	0.006 283	0.015 70	0.001 935	0.031 61	0.004 426	40.838	11.70

TABLE 4.1 Solubility of Gases in Water (*continued*)

Temp. °C	Hydrogen sulfide		Methane		Nitric oxide		Nitrogen*		Oxygen		Sulfur dioxide	
	α	q	α	q	α	q	α	q	l	q	α	q
20	2.582	0.384 6	0.033 08	0.002 319	0.047 06	0.006 173	0.015 45	0.001 901	0.031 02	0.004 339	39.374	11.28
21	2.517	0.374 5	0.032 43	0.002 270	0.046 25	0.006 059	0.015 22	0.001 869	0.030 44	0.004 252	37.970	10.88
22	2.456	0.364 8	0.031 80	0.002 222	0.045 45	0.005 947	0.014 98	0.001 838	0.029 88	0.004 169	36.617	10.50
23	2.396	0.355 4	0.031 19	0.002 177	0.044 69	0.005 838	0.014 75	0.001 809	0.029 34	0.004 087	35.302	10.12
24	2.338	0.346 3	0.030 61	0.002 133	0.043 95	0.005 733	0.014 54	0.001 780	0.028 81	0.004 007	34.026	9.76
25	2.282	0.337 5	0.030 06	0.002 091	0.043 23	0.005 630	0.014 34	0.001 751	0.028 31	0.003 931	32.786	9.41
26	2.229	0.329 0	0.029 52	0.002 050	0.042 54	0.005 530	0.014 13	0.001 724	0.027 83	0.003 857	31.584	9.06
27	2.177	0.320 8	0.029 01	0.002 011	0.041 88	0.005 435	0.013 94	0.001 698	0.027 36	0.003 787	30.422	8.73
28	2.128	0.313 0	0.028 52	0.001 974	0.041 24	0.005 342	0.013 76	0.001 672	0.026 91	0.003 718	29.314	8.42
29	2.081	0.305 5	0.028 06	0.001 938	0.040 63	0.005 252	0.013 58	0.001 647	0.026 49	0.003 651	28.210	8.10
30	2.037	0.298 3	0.027 62	0.001 904	0.040 04	0.005 165	0.013 42	0.001 624	0.026 08	0.003 588	27.161	7.80
35	1.831	0.264 8	0.025 46	0.001 733	0.037 34	0.004 757	0.012 56	0.001 501	0.024 40	0.003 315	22.489	6.47
40	1.660	0.236 1	0.023 69	0.001 586	0.035 07	0.004 394	0.011 84	0.001 391	0.023 06	0.003 082	18.766	5.41
45	1.516	0.211 0	0.022 38	0.001 466	0.033 11	0.004 059	0.011 30	0.001 300	0.021 87	0.002 858	—	—
50	1.392	0.188 3	0.021 34	0.001 359	0.031 52	0.003 758	0.010 88	0.001 216	0.020 90	0.002 657	—	—
60	1.190	0.148 0	0.019 54	0.001 144	0.029 54	0.003 237	0.010 23	0.001 052	0.019 46	0.002 274	—	—
70	1.022	0.1101	0.018 25	0.000 926	0.028 10	0.002 668	0.009 77	0.000 851	0.018 33	0.001 856	—	—
80	0.917	0.076 5	0.017 70	0.000 695	0.027 00	0.001 984	0.009 58	0.000 660	0.017 61	0.001 381	—	—
90	0.84	0.041	0.017 35	0.000 40	0.026 5	0.001 13	0.009 5	0.000 38	0.017 2	0.000 79	—	—
100	0.81	0.000	0.017 0	0.000 00	0.026 3	0.000 00	0.009 5	0.000 00	0.017 0	0.000 00	—	—

*Atmospheric nitrogen containing 98.815% N₂ by volume + 1.185% inert gases.

TABLE 4.1 Solubility of Gases in Water (*continued*)

Substance		0°	10°	20°	30°	40°	60°	80°
Argon	α	0.052 8	0.041 3	0.033 7	0.028 8	0.025 1	0.020 9	0.018 4
Helium	A	0.009 8	0.009 11	0.008 6	0.008 39	0.008 41	0.009 02	0.0009 42 ^{70°}
Hydrogen bromide	l	612	582		533 ^{25°}		469 ^{50°}	406 ^{75°}
Hydrogen chloride	α	512	475	442	412	385	339	
Krypton	α	0.110 5	0.081 0	0.062 6	0.051 1	0.043 3	0.035 7	
Neon	A		0.011 7 ^{9°}	0.010 6	0.010 0	0.009 48 ^{42°}		0.009 84 ^{73°}
Nitrous oxide	A		0.88	0.63				
Ozone	$\text{g} \cdot \text{L}^{-1}$	0.039 4	0.029 9 ^{12°}	0.021 0 ^{19°}	0.0139 ^{27°}	0.004 2	0	
Radon	α	0.510	0.326	0.222	0.162	0.126	0.085	
Xenon	α	0.242	0.174	0.123	0.098	0.082		

VAPOR PRESSURES

TABLE 4.2 Vapor Pressure of Mercury

Temp. °C	mm of Hg	Temp. °C	mm of Hg	Temp. °C	mm of Hg
0	0.000 185	78	0.078 89	158	3.873
2	0.000 228	80	0.088 80	160	4.189
4	0.000 276	82	0.100 0		
6	0.000 335	84	0.112 4	162	4.528
8	0.000 406	86	0.126 1	164	4.890
10	0.000 490	88	0.141 3	166	5.277
		90	0.1582	168	5.689
12	0.000 588			170	6.128
14	0.000 706	92	0.1769		
16	0.000 846	94	0.1976	172	6.596
18	0.001 009	96	0.2202	174	7.095
20	0.001 201	98	0.2453	176	7.626
		100	0.2729	178	8.193
22	0.001 426			180	8.796
24	0.001 691	102	0.3032		
26	0.002 000	104	0.3366	182	9.436
28	0.002 359	106	0.3731	184	10.116
30	0.002 777	108	0.4132	186	10.839
		110	0.4572	188	11.607
32	0.003 261	112	0.5052	190	12.423
34	0.003 823	114	0.5576		
36	0.004 471	116	0.6150	192	13.287
38	0.005 219	118	0.6776	194	14.203
40	0.006 079	120	0.7457	196	15.173
				198	16.200
42	0.007 067	122	0.8198	200	17.287
44	0.008 200	124	0.9004		
46	0.009 497	126	0.9882		
48	0.010 98	128	1.084	202	18.437
50	0.012 67	130	1.186	204	19.652
				206	20.936
52	0.014 59	132	1.298	208	22.292
54	0.016 77	134	1.419	210	23.723
56	0.019 25	136	1.551		
58	0.022 06	138	1.692	212	25.233
60	0.025 24	140	1.845	214	26.826
				216	28.504
62	0.028 83	142	2.010	218	30.271
64	0.032 87	144	2.188	220	32.133
66	0.037 40	146	2.379		
68	0.042 51	148	2.585		
70	0.048 25	150	2.807	222	34.092
				224	36.153
72	0.054 69	152	3.046	226	38.318
74	0.061 89	154	3.303	228	40.595
76	0.069 93	156	3.578	230	42.989

TABLE 4.2 Vapor Pressure of Mercury (*continued*)

Temp. °C	mm of Hg	Temp. °C	mm of Hg	Temp. °C	mm of Hg
232	45.503	302	257.78	372	994.34
234	48.141	304	269.17	374	1028.9
236	50.909	306	280.98	376	1064.4
238	53.812	308	293.21	378	1100.9
240	56.855	310	305.89	380	1138.4
242	60.044	312	319.02	382	1177.0
244	63.384	314	332.62	384	1216.6
246	66.882	316	346.70	386	1257.3
248	70.543	318	361.26	388	1299.1
250	74.375	320	376.33	390	1341.9
252	78.381	322	391.92	392	1386.1
254	82.568	324	408.04	394	1431.3
256	86.944	326	424.71	396	1477.7
258	91.518	328	441.94	398	1525.2
260	96.296	330	459.74	400	1574.1
262	101.28	332	478.13	430	2464
264	106.48	334	497.12	460	3715
266	111.91	336	516.74	490	5420
268	117.57	338	537.00		
270	123.47	340	557.90	520	7691
				550	10650
272	129.62	342	579.45	600	22.87 atm
274	136.02	344	601.69	650	35.49 atm
276	142.69	346	624.64	700	52.51 atm
278	149.64	348	648.30		
280	156.87	350	672.69	750	74.86 atm
				800	103.31 atm
282	164.39	352	697.83	850	138.42 atm
284	172.21	354	723.73	900*	180.92 atm
286	180.34	356	750.43	950	226.58 atm
288	188.79	358	777.92		
290	197.57	360	806.23	1000	290.5 atm
				1050	358.1 atm
292	206.70	362	835.38	1100	437.3 atm
294	216.17	364	865.36	1150	521.3 atm
296	226.00	366	896.23	1200	616.8 atm
298	236.21	368	928.02	1250	721.4 atm
300	246.80	370	960.66	1300	835.9 atm

*Critical point.

TABLE 4.3 Vapor Pressure of Water for Temperatures from -10 to 120°C

The values in the table are for water in contact with its own vapor. Where the water is in contact with air at a temperature t in degrees Celsius, the following correction must be added: Correction (when $t \leq 40^{\circ}\text{C}$) = $p(0.775 - 0.000\,313\,t)/100$; correction (when $t > 50^{\circ}\text{C}$) = $p(0.0652 - 0.000\,087\,5\,t)/100$.

$t, ^{\circ}\text{C}$	p, mmHg	$t, ^{\circ}\text{C}$	p, mmHg	$t, ^{\circ}\text{C}$	p, mmHg	$t, ^{\circ}\text{C}$	p, mmHg
-10.0	2.149	11.5	10.176	22.2	20.070	30.8	33.312
-9.5	2.236	12.0	10.518	22.4	20.316	31.0	33.695
-9.0	2.326	12.5	10.870	22.6	20.565	31.2	34.082
-8.5	2.418	13.0	11.231	22.8	20.815	31.4	34.471
-8.0	2.514	13.5	11.604	23.0	21.068	31.6	34.864
-7.5	2.613	14.0	11.987	23.2	21.324	31.8	35.261
-7.0	2.715	14.5	12.382	23.4	21.583	32.0	35.663
-6.5	2.822	15.0	12.788	23.6	21.845	32.2	36.068
-6.0	2.931	15.2	12.953	23.8	22.110	32.4	36.477
-5.5	3.046	15.4	13.121	24.0	22.387	32.6	36.891
-5.0	3.163	15.6	13.290	24.2	22.648	32.8	37.308
-4.5	3.284	15.8	13.461	24.4	22.922	33.0	37.729
-4.0	3.410	16.0	13.634	24.6	23.198	33.2	38.155
-3.5	3.540	16.2	13.809	24.8	23.476	33.4	38.584
-3.0	3.673	16.4	13.987	25.0	23.756	33.6	39.018
-2.5	3.813	16.6	14.166	25.2	24.039	33.8	39.457
-2.0	3.956	16.8	13.347	25.4	24.326	34.0	39.898
-1.5	4.105	17.0	14.530	25.6	24.617	34.2	40.344
-1.0	4.258	17.2	14.715	25.8	24.912	34.4	40.796
-0.5	4.416	17.4	14.903	26.0	25.209	34.6	41.251
0.0	4.579	17.6	15.092	26.2	25.509	34.8	41.710
0.5	4.750	17.8	15.284	26.4	25.812	35.0	42.175
1.0	4.926	18.0	15.477	26.6	26.117	35.2	42.644
1.5	5.107	18.2	15.673	26.8	26.426	35.4	43.117
2.0	5.294	18.4	15.871	27.0	26.739	35.6	43.595
2.5	5.486	18.6	16.071	27.2	27.055	35.8	44.078
3.0	5.685	18.8	16.272	27.4	27.374	36.0	44.563
3.5	5.889	19.0	16.477	27.6	27.696	36.2	45.054
4.0	6.101	19.2	16.685	27.8	28.021	36.4	45.549
4.5	6.318	19.4	16.894	28.0	28.349	36.6	46.050
5.0	6.543	19.6	17.105	28.2	28.680	36.8	46.556
5.5	6.775	19.8	17.319	28.4	29.015	37.0	47.067
6.0	7.013	20.0	17.535	28.6	29.354	37.2	47.582
6.5	7.259	20.2	17.753	28.8	29.697	37.4	48.102
7.0	7.513	20.4	17.974	29.0	30.043	37.6	48.627
7.5	7.775	20.6	18.197	29.2	30.392	37.8	49.157
8.0	8.045	20.8	18.422	29.4	30.745	38.0	49.692
8.5	8.323	21.0	18.650	29.6	31.102	38.2	50.231
9.0	8.609	21.2	18.880	29.8	31.461	38.4	50.774
9.5	8.905	21.4	19.113	30.0	31.824	38.6	51.323
10.0	9.209	21.6	19.349	30.2	32.191	38.8	51.879
10.5	9.521	21.8	19.587	30.4	32.561	39.0	52.442
11.0	9.844	22.0	19.827	30.6	32.934	39.2	53.009

TABLE 4.3 Vapor Pressure of Water for Temperatures from -10 to 120°C (*continued*)

$t, ^{\circ}\text{C}$	p, mmHg	$t, ^{\circ}\text{C}$	p, mmHg	$t, ^{\circ}\text{C}$	p, mmHg	$t, ^{\circ}\text{C}$	p, mmHg
39.4	54.580	58.5	139.34	78.5	334.2	96.4	667.31
39.6	54.156	59.0	142.60	79.0	341.0	96.6	672.20
39.8	54.737	59.5	145.99	79.5	348.1	96.8	677.12
40.0	55.324	60.0	149.38	80.0	355.1	97.0	682.07
40.5	56.81	60.5	152.91	80.5	362.4	97.2	687.04
41.0	58.34	61.0	156.43	81.0	369.7	97.4	692.05
41.5	59.90	61.5	160.10	81.5	377.3	97.6	697.10
42.0	61.50	62.0	163.27	82.0	384.9	97.8	702.17
42.5	63.13	62.5	167.58	82.5	392.8	98.0	707.27
43.0	64.80	63.0	171.38	83.0	400.6	98.2	712.40
43.5	66.51	63.5	175.35	83.5	408.7	98.4	717.56
44.0	68.26	64.0	179.31	84.0	416.8	98.6	722.75
44.5	70.05	64.5	183.43	84.5	425.2	98.8	727.98
45.0	71.88	65.0	187.54	85.0	433.6	99.0	733.24
45.5	73.74	65.5	191.82	85.5	442.3	99.2	738.53
46.0	75.65	66.0	196.09	86.0	450.9	99.4	743.85
46.5	77.61	66.5	200.53	86.5	459.8	99.6	749.20
47.0	79.60	67.0	204.96	87.0	468.7	99.8	754.58
47.5	81.64	67.5	209.57	87.5	477.9	100.0	760.00
48.0	83.71	68.0	214.17	88.0	487.1	101.0	787.57
48.5	85.85	68.5	218.95	88.5	496.6	102.0	815.86
49.0	88.02	69.0	223.73	89.0	506.1	103.0	845.12
49.5	90.24	69.5	228.72	89.5	515.9	104.0	875.06
50.0	92.51	70.0	233.7	90.0	525.76	105.0	906.07
50.5	94.86	70.5	238.8	90.5	535.83	106.0	937.92
51.0	97.20	71.0	243.9	91.0	546.05	107.0	970.60
51.5	99.65	71.5	249.3	91.5	556.44	108.0	1004.42
52.0	102.09	72.0	254.6	92.0	566.99	109.0	1038.92
52.5	104.65	72.5	260.2	92.5	577.71	110.0	1074.56
53.0	107.20	73.0	265.7	93.0	588.60	111.0	1111.20
53.5	109.86	73.5	271.5	93.5	599.66	112.0	1148.74
54.0	112.51	74.0	277.2	94.0	610.90	1130	1187.42
54.5	115.28	74.5	283.2	94.5	622.31	114.0	1227.25
55.0	118.04	75.0	289.1	95.0	633.90	115.0	1267.98
55.5	120.92	75.5	295.3	95.2	638.59	116.0	1309.94
56.0	123.80	76.0	301.4	95.4	643.30	117.0	1352.95
56.5	126.81	76.5	307.7	95.6	648.05	118.0	1397.18
57.0	129.82	77.0	314.1	95.8	652.82	119.0	1442.63
57.5	132.95	77.5	320.7	96.0	657.62	120.0	1489.14
58.0	136.08	78.0	327.3	96.2	662.45		

TABLE 4.4 Vapor Pressure of Deuterium Oxide

<i>t</i> , °C	<i>p</i> , mmHg	<i>t</i> , °C	<i>p</i> , mmHg	<i>t</i> , °C	<i>p</i> , mmHg
0	3.65	20	15.2	80	331.6
1	3.93	30	28.0	90	495.5
2	4.29	40	49.3	100	722.2
3	4.65	50	83.6	101.43	760.0
3.8	5.05	60	136.6		
10	7.79	70	216.1		

BOILING POINTS

TABLE 4.5A Boiling Points for Common Organic Solvents

Arranged in order of increasing boiling point

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
Ethylene oxide	10.6	Oxirane	Benzene	80.1	
Chloroethane	12.3	Ethyl chloride	Cyclohexane	80.7	
Furan	31.4		Propyl formate	80.9	
Methyl formate	31.5		Acetonitrile	81.6	
Diethyl ether	34.6	Ethyl ether	2-Propanol	82.4	Isopropyl alcohol
Propylene oxide	34.5		1,1-Dimethylethanol	82.4	<i>t</i> -Butanol
Pentane	36.1		Cyclohexene	83.0	
Bromoethane	38.4	Ethyl bromide	Diisopropyl amine	83.5	
Dichloromethane	39.8	Methylene chloride	1,2-Dichloroethane	83.7	
Dimethoxyethane	42.3	DME, glyme	Thiophene	84.2	
Carbon disulfide	46.3		Trichloroethylene	87.2	
1-Isopropoxy-2-propanol	47.9		Isopropyl acetate	88.2	
Ethyl formate	54.2		1-Bromo-2-methylpropane	91.5	Isobutyl bromide
Acetone	56.2	Dimethyl ketone	2,5-Dimethylfuran	93–94	
Methyl acetate	56.3		Ethyl chloroformate	94.0	
1,1-Dichloroethane	57.3		Allyl alcohol	96.6	
Dichloroethylene	60.6		1,2-Dichloropropane	96.8	
Chloroform	61.2		1-Propanol	97.2	<i>n</i> -Propyl alcohol
Methanol	64.7		Heptane	98.4	
Tetrahydrofuran	66.0	THF	1-Chloro-3-methylbutane	99.0	
Diisopropyl ether	68.0	Isopropyl ether	Ethyl propanoate	99.1	Ethyl propionate
Hexane	68.7		2-Butanol	99.6	<i>sec</i> -Butanol
1-Chloro-2-methylpropane	68.9	Isobutyl chloride	Formic acid	100.8	
1,1,1-Trichloroethane	74.0		Methylcyclohexane	100.9	
1,3-Dioxolane	74–75		1,4-Dioxane	101.2	
Carbon tetrachloride	76.7		Nitromethane	101.2	
Ethyl acetate	77.1		Propyl acetate	101.5	
1-Chlorobutane	77.9	Butyl chloride	2-Pentanone	101.7	Methyl propyl ketone
Ethanol	78.3		3-Pentanone	102.0	Diethyl ketone
2-Butanone	79.6	Methyl ethyl ketone	2-Methyl-2-butanol	102.0	<i>t</i> -Pentanol
2-Methyltetrahydrofuran	80.0		1,1-Diethoxyethane	102.7	

TABLE 4.5A Boiling Points for Common Organic Solvents (*continued*)

Arranged in order of increasing boiling point

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
Butyl formate	106.6		4-Heptanone	143.7	Dipropyl ketone
2-Methyl-1-propanol	107.9	Isobutanol	<i>o</i> -Xylene	144.4	1,2-Dimethylbenzene
Toluene	110.6	Methylbenzene	2-Methoxyethyl acetate	144.5	
<i>sec</i> -Butyl acetate	112.3		1,1,2, 2-Tetrachloroethane	146.3	
1,1,2-Trichloroethane	113.5		3-Heptanone	147.8	Ethyl butyl ketone
Nitroethane	114.1		Tribromomethane	149.6	Bromoform
Pyridine	115.2		Nonane	150.8	
3-Pentanol	115.6		2-Heptanone	151	Methyl pentyl ketone
4-Methyl-2-pentanone	115.7	Methyl isobutyl ketone	Isopropylbenzene	152.4	Cumene
1-Chloro-2, 3-epoxypropane	116.1	Epichlorohydrin	<i>N,N</i> -Dimethylformamide	153.0	DMF
1-Butanol	117.7		Methoxybenzene	153.8	Anisole
Acetic acid	117.9		Ethyl lactate	154.5	
Isobutyl acetate	118.0		Cyclohexanone	155.7	
2-Pentanol	119.3	<i>sec</i> -Pentanol	Bromobenzene	156.2	
1-Bromo-3-methylbutane	119.7	Isopentyl bromide	1,2,3-Trichloropropane	156.9	
1-Methoxy-2-propanol	120.1		1-Hexanol	157.5	
2-Nitropropane	120.3	Nitroisopropane	Propylbenzene	159.2	
Tetrachloroethylene	121.1		Cyclohexanol	161.1	
Ethyl butanoate	121.6	Ethyl butyrate	Bis(2-methoxyethyl) ether	160	Diglyme
3-Hexanone	123	Ethyl propyl ketone	Isopentyl propanoate	160.2	Isopentyl propionate
2,4-Dimethyl-3-pentanone	124	Diisopropyl ketone	2-Heptanol	160.4	
2-Methoxyethanol	124.6		Pentachloroethane	160.5	
Octane	125.7		2-Furaldehyde	161.8	Furfural
Butyl acetate	126.1		2,6-Dimethyl-4-heptanone	168.1	Diisobutyl ketone
Diethyl carbonate	126.8		4-Hydroxy-4-methyl-2-pentanone	169.2	
2-Hexanone	127.2	Methyl butyl ketone	2-Furanmethanol	170.0	2-Hydroxy methylfuran
1-Chloro-2-propanol	127.4		Ethoxybenzene	170	Phenetole
2-Chloroethanol	128.6		2-Butoxyethanol	170.2	Butyl cellosolve
1-Nitropropane	131.2		Diisopentyl ether	173.4	
Chlorobenzene	131.7		Decane	174.2	
1,2-Dibromoethane	131.7		1,3-Dichloro-2-propanol	174.3	
4-Methyl-2-pentanol	131.7		Cyclohexyl acetate	174–175	
3-Methyl-1-butanol	132.0		1-Heptanol	175.8	
Cyclohexylamine	134.8	Aminocyclohexane	Furfuryl acetate	175–177	
2-Ethoxyethanol	134.8		4-Isopropyl-1-methylbenzene	177.1	<i>p</i> -Cymene
Ethylbenzene	136.2				
1-Pentanol	138				
<i>p</i> -Xylene	138.4	1,4-Dimethylbenzene			
<i>m</i> -Xylene	139.1	1,3-Dimethylbenzene			
Acetic anhydride	140.0				
2,4-Pentanedione	140.6	Acetylacetone			
Isopentyl acetate	142				
Dibutyl ether	142.4				

TABLE 4.5A Boiling Points for Common Organic Solvents (*continued*)*Arranged in order of increasing boiling point*

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
Isopentyl butanoate	178.6	Isopentyl butyrate	<i>o</i> -Chloroaniline	208.8	1-Amino-2-chlorobenzene
Bis(2-chloroethyl) ether	178.8	Dichloro diethyl ether	Nitrobenzene	210.8	
2-Octanol	179		Ethyl benzoate	212.4	
1,2-Dichlorobenzene	180.4	<i>o</i> -Dichlorobenzene	Isophorone	215.2	3,5, 5-Trimethylcyclohex-2-en-1-one
Ethyl acetoacetate	180.8				
Phenol	181.8	Hydroxybenzene	Naphthalene	217.7	
2-Ethyl-1-hexanol	184.3		2-(2-Ethoxyethoxy) ethyl acetate	218.5	
Aniline	184.4	Aminobenzene	Acetamide	221.2	
Benzyl ethyl ether	185.0		Methyl salicylate	223.0	
Diethyl oxalate	185.4		Diethyl maleate	225.3	
1,2-Propanediol	188	Propylene glycol	1,4-Butanediol	230	
Bis(2-ethoxyethyl) ether	188.4		Propyl benzoate	231.2	
Dimethylsulfoxide	189.0	DMSO	1-Decanol	230.2	
1,2-Ethanediol diacetate	190.2	Diacetoxyethane	Phenylacetonitrile	233.5	Cyano-methylbenzene
Benzonitrile	191.0	Cyanobenzene	Quinoline	237	
2,5-Hexanedione	191.4		Tributyl borate	238.5	
2-(2-Methoxyethoxy) ethanol	194.1		Propylene carbonate	240	
<i>N,N</i> -Dimethylaniline	194.2	Dimethyl-aminobenzene	2-Phenoxyethanol	240	
1-Octanol	195.2		Bis(2-hydroxyethyl) ether	245	Diethylene glycol
1,2-Ethanediol	197.3	Ethylene glycol	Dibutyl oxalate	245.5	
Diethyl malonate	199.3		Butyl benzoate	250	
Methyl benzoate	199.5		1,2,3-Propanetriol triacetate	258–259	Glycerol triacetate
<i>o</i> -Toluidine	200.4	1-Amino-2-methylbenzene	1-Chloronaphthalene	259.3	
<i>p</i> -Toluidine	200.6	1-Amino-4-methylbenzene	Isopentyl benzoate	262	
2-(2-Ethoxyethoxy) ethanol	202		<i>trans</i> -Ethyl cinnamate	271.0	
Acetophenone	202.1	Methyl phenyl-ketone	Bis (2-(2-methoxy-ethoxy)-ethyl) ether	275.3	Triglyme
1,2-Dibutoxyethane	203.6		1-Methoxy-2-nitrobenzene	277	
1,2-Phenylethanol	203.9	Phenethyl alcohol	Isopentyl salicylate	277–278	
<i>m</i> -Toluidine	203.4	1-Amino-3-methylbenzene	1-Bromonaphthalene	281.1	
Benzyl alcohol	205.5	Hydroxy-methylbenzene	Dimethyl <i>o</i> -phthalate	283.7	1,2-Bis(carbo-methoxy) benzene
Camphor	207	1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-one	2,2'-(Ethylenedioxy) bisethanol	285	
1,3-Butanediol	207.5		Glycerol	290	
1,2,3,4-Tetrahydronaphthalene	207.6	Tetralin	Diethyl <i>o</i> -phthalate	295	
γ -Valerolactone	207–208		Benzyl benzoate	323.5	
			Dibutyl <i>o</i> -phthalate	340.0	
			Dibutyl decanedioate	344–345	

TABLE 4.5B Boiling Points for Common Organic Solvents

Arranged alphabetically by solvent name

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
Acetamide	221.2		Chlorobenzene	131.7	
Acetic acid	117.9		1-Chlorobutane	77.9	Butyl chloride
Acetic anhydride	140.0		1-Chloro-2,3-epoxypropane	116.1	Epichlorohydrin
Acetone	56.2	Dimethyl ketone	1-Chloro-2-propanol	127.4	
Acetonitrile	81.6		Chloroethane	12.3	Ethyl chloride
Acetophenone	202.1	Methyl phenyl ketone	2-Chloroethanol	128.6	
Allyl alcohol	96.6		Chloroform	61.2	
Aniline	184.4	Aminobenzene	1-Chloro-3-methylbutane	99.0	
Benzene	80.1		1-Chloro-2-methylpropane	68.9	Isobutyl chloride
Benzonitrile	191.0	Cyanobenzene	1-Chloronaphthalene	259.3	
Benzyl alcohol	205.5	Hydroxy-methylbenzene	Cyclohexane	80.7	
Benzyl benzoate	323.5		Cyclohexanol	161.1	
Benzyl ethyl ether	185.0		Cyclohexanone	155.7	
Bis(2-(2-methoxyethoxy)-ethyl) ether	275.3	Triglyme	Cyclohexene	83.0	
Bis(2-chloroethyl) ether	178.8	Dichloro diethyl ether	Cyclohexyl acetate	174–175	
Bis(2-ethoxyethyl) ether	188.4		Cyclohexylamine	134.8	Aminocyclohexane
Bis(2-hydroxyethyl) ether	245	Diethylene glycol	Decane	174.2	
Bis(2-methoxyethyl) ether	160	Diglyme	1-Decanol	230.2	
Bromobenzene	156.2		1,2-Dibromoethane	131.7	
Bromoethane	38.4	Ethyl bromide	1,2-Dibutoxyethane	203.6	
1-Bromo-2-methylpropane	91.5	Isobutyl bromide	Dibutyl decanedioate	344–345	
1-Bromo-3-methylbutane	119.7	Isopentyl bromide	Dibutyl ether	142.4	
1-Bromonaphthalene	281.1		Dibutyl <i>o</i> -phthalate	340.0	
1,3-Butanediol	207.5		Dibutyl oxalate	245.5	
1,4-Butanediol	230		1,2-Dichlorobenzene	180.4	<i>o</i> -Dichlorobenzene
1-Butanol	117.7		Dichloroethylene	60.6	
2-Butanol	99.6	<i>sec</i> -Butanol	Dichloromethane	39.8	Methylene chloride
2-Butanone	79.6	Methyl ethyl ketone	1,1-Dichloroethane	57.3	
2-Butoxyethanol	170.2	Butyl cellosolve	1,2-Dichloroethane	83.7	
Butyl acetate	126.1		1,2-Dichloropropane	96.8	
<i>sec</i> -Butyl acetate	112.3		1,3-Dichloro-2-propanol	174.3	
Butyl benzoate	250		1,1-Diethoxyethane	102.7	
Butyl formate	106.6		Diethyl carbonate	126.8	
Camphor	207	1,7,7-Trimethylbicyclo [2.2.1] heptan-2-one	Diethyl ether	34.6	Ethyl ether
			Diethyl maleate	225.3	
			Diethyl malonate	199.3	
			Diethyl <i>o</i> -phthalate	295	
			Diethyl oxalate	185.4	
			Diisopentyl ether	173.4	
			Diisopropyl amine	83.5	
			Diisopropyl ether	68.0	Isopropyl ether
			Dimethoxyethane	42.3	DME, glyme
Carbon disulfide	46.3				
Carbon tetrachloride	76.7				
<i>o</i> -Chloroaniline	208.8	1-Amino-2-chlorobenzene			

TABLE 4.5B Boiling Points for Common Organic Solvents (*continued*)*Arranged alphabetically by solvent name*

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
<i>N,N</i> -Dimethylaniline	194.2	Dimethyl-aminobenzene	2-Heptanone	151	Methyl pentyl ketone
1,1-Dimethylethanol	82.4	<i>t</i> -Butanol	3-Heptanone	147.8	Ethyl butyl ketone
<i>N,N</i> -Dimethyl-formamide	153.0	DMF	4-Heptanone	143.7	Dipropyl ketone
2,5-Dimethylfuran	93–94		Hexane	68.7	
2,6-Dimethyl-4-heptanone	168.1	Diisobutyl ketone	2,5-Hexanedione	191.4	
2,4-Dimethyl-3-pentanone	124	Diisopropyl ketone	1-Hexanol	157.5	
Dimethyl <i>o</i> -phthalate	283.7	1,2-Bis(carbo-methoxy)benzene	2-Hexanone	127.2	Methyl butyl ketone
Dimethylsulfoxide	189.0	DMSO	3-Hexanone	123	Ethyl propyl ketone
1,4-Dioxane	101.2		4-Hydroxy-4-methyl-2-pentanone	169.2	
1,3-Dioxolane	74–75		Isobutyl acetate	118.0	
1,2-Ethanediol	197.3	Ethylene glycol	Isopentyl acetate	142	
1,2-Ethanediol diacetate	190.2	Diacetoxyethane	Isopentyl benzoate	262	
Ethoxybenzene	170	Phenetole	Isopentyl butanoate	178.6	Isopentyl butyrate
2-Ethoxyethanol	134.8		Isopentyl propanoate	160.2	Isopentyl propionate
2-(2-Ethoxyethoxy) ethanol	202		Isopentyl salicylate	277–278	
2-(2-Ethoxyethoxy) ethyl acetate	218.5		Isophorone	215.2	3,5,5-Trimethylcyclohex-2-en-1-one
Ethyl acetate	77.1		Isopropyl acetate	88.2	
Ethyl acetoacetate	180.8		Isopropylbenzene	152.4	Cumene
Ethyl benzoate	212.4		1-Isopropoxy-2-propanol	47.9	
Ethyl butanoate	121.6	Ethyl butyrate	4-Isopropyl-1-methylbenzene	177.1	<i>p</i> -Cymene
Ethyl chloroformate	94.0		Methanol	64.7	
<i>trans</i> -Ethyl cinnamate	271.0		Methoxybenzene	153.8	Anisole
Ethyl formate	54.2		Methyl acetate	56.3	
Ethyl lactate	154.5		Methyl benzoate	199.5	
Ethyl propanoate	99.1	Ethyl propionate	Methyl formate	31.5	
Ethylbenzene	136.2		Methyl salicylate	223.0	
Ethylene oxide	10.6	Oxirane	Methylcyclohexane	100.9	
2,2'-(Ethylenedioxy) bisethanol	285		1-Methoxy-2-nitrobenzene	277	
2-Ethyl-1-hexanol	184.3		1-Methoxy-2-propanol	120.1	
Formic acid	100.8		2-(2-Methoxyethoxy) ethanol	194.1	
2-Furaldehyde	161.8	Furfural	2-Methoxyethanol	124.6	
Furan	31.4		2-Methoxyethyl acetate	144.5	
2-Furanmethanol	170.0	2-Hydroxy-methylfuran	2-Methyl-1-propanol	107.9	Isobutanol
Furfuryl acetate	175–177		2-Methyl-2-butanol	102.0	<i>t</i> -Pentanol
Glycerol	290		2-Methyltetrahydrofuran	80.0	
Heptane	98.4		3-Methyl-1-butanol	132.0	
1-Heptanol	175.8		4-Methyl-2-pentanol	131.7	
2-Heptanol	160.4		4-Methyl-2-pentanone	115.7	Methyl isobutyl ketone

TABLE 4.5B Boiling Points for Common Organic Solvents (*continued*)*Arranged alphabetically by solvent name*

Compound name	bp (°C)	Other name	Compound name	bp (°C)	Other name
Naphthalene	217.7		Propyl formate	80.9	
Nitrobenzene	210.8		Propylbenzene	159.2	
Nitroethane	114.1		Pyridine	115.2	
Nitromethane	101.2		Quinoline	237	
1-Nitropropane	131.2		1,1,2,2-Tetra- chloroethane	146.3	
2-Nitropropane	120.3	Nitroisopropane	Tetrachloroethylene	121.1	
Nonane	150.8		Tetrahydrofuran	66.0	THF
Octane	125.7		Thiophene	84.2	
1-Octanol	195.2		Toluene	110.6	Methylbenzene
2-Octanol	179		<i>o</i> -Toluidine	200.4	1-Amino- 2-methylbenzene
Pentachloroethane	160.5		<i>m</i> -Toluidine	203.4	1-Amino- 3-methylbenzene
Pentane	36.1		<i>p</i> -Toluidine	200.6	1-Amino- 4-methylbenzene
2,4-Pentanedione	140.6	Acetylacetone	Tribromomethane	149.6	Bromoform
1-Pentanol	138		Tributyl borate	238.5	
2-Pentanol	119.3	<i>sec</i> -Pentanol	1,1,1-Trichloroethane	74.0	
3-Pentanol	115.6		1,1,2-Trichloroethane	113.5	
2-Pentanone	101.7	Methyl propyl ketone	Trichloroethylene	87.2	
3-Pentanone	102.0	Diethyl ketone	1,2,3,4-Tetrahy- dronaphthalene	207.6	Tetralin
Phenol	181.8	Hydroxybenzene	1,2,3-Trichloro propane	156.9	
2-Phenoxyethanol	240		γ -Valerolactone	207– 208	
Phenylacetone	233.5	Cyano- methylbenzene	<i>o</i> -Xylene	144.4	1,2-Dimethyl- benzene
1-Phenylethanol	203.9	Phenethyl alcohol	<i>m</i> -Xylene	139.1	1,3-Dimethyl- benzene
1,2-Propanediol	188	Propylene glycol	<i>p</i> -Xylene	138.4	1,4-Dimethyl- benzene
1,2,3-Propanetriol triacetate	258– 259	Glycerol triacetate			
1-Propanol	97.2	<i>n</i> -Propyl alcohol			
2-Propanol	82.4	Isopropyl alcohol			
Propylene carbonate	240				
Propylene oxide	34.5				
Propyl acetate	101.5				
Propyl benzoate	231.2				

TABLE 4.5C Boiling Points for Common Organic Solvents*Arranged by compound type in order of increasing boiling point*

	Compound name	(°C)	Other name
acid	Formic acid	100.8	
acid	Acetic acid	117.9	
alcohol	1-Isopropoxy-2-propanol	47.9	
alcohol	Methanol	64.7	
alcohol	Ethanol	78.3	
alcohol	2-Propanol	82.4	Isopropyl alcohol
alcohol	1,1-Dimethylethanol	82.4	<i>t</i> -Butanol
alcohol	Allyl alcohol	96.6	

TABLE 4.5C Boiling Points for Common Organic Solvents (*continued*)*Arranged by compound type in order of increasing boiling point*

	Compound name	(°C)	Other name
alcohol	1-Propanol	97.2	<i>n</i> -Propyl alcohol
alcohol	2-Butanol	99.6	<i>sec</i> -Butanol
alcohol	2-Methyl-2-butanol	102.0	<i>t</i> -Pentanol
alcohol	2-Methyl-1-propanol	107.9	Isobutanol
alcohol	3-Pentanol	115.6	
alcohol	1-Butanol	117.7	
alcohol	2-Pentanol	119.3	<i>sec</i> -Pentanol
alcohol	1-Methoxy-2-propanol	120.1	
alcohol	2-Methoxyethanol	124.6	
alcohol	1-Chloro-2-propanol	127.4	
alcohol	2-Chloroethanol	128.6	
alcohol	4-Methyl-2-pentanol	131.7	
alcohol	3-Methyl-1-butanol	132.0	
alcohol	2-Ethoxyethanol	134.8	
alcohol	1-Pentanol	138	
alcohol	1-Hexanol	157.5	
alcohol	Cyclohexanol	161.1	
alcohol	2-Heptanol	160.4	
alcohol	4-Hydroxy-4-methyl-2-pentanone	169.2	
alcohol	2-Furanmethanol	170.0	2-Hydroxymethylfuran
alcohol	2-Butoxyethanol	170.2	Butyl cellosolve
alcohol	1,3-Dichloro-2-propanol	174.3	
alcohol	1-Heptanol	175.8	
alcohol	2-Octanol	179	
alcohol	Phenol	181.8	Hydroxybenzene
alcohol	2-Ethyl-1-hexanol	184.3	
alcohol	1,2-Propanediol	188	Propylene glycol
alcohol	2-(2-Methoxyethoxy) ethanol	194.1	
alcohol	1-Octanol	195.2	
alcohol	1,2-Ethanediol	197.3	Ethylene glycol
alcohol	2-(2-Ethoxyethoxy) ethanol	202	
alcohol	1-Phenylethanol	203.9	Phenethyl alcohol
alcohol	Benzyl alcohol	205.5	Hydroxymethylbenzene
alcohol	1,3-Butanediol	207.5	
alcohol	Methyl salicylate	223.0	
alcohol	1,4-Butanediol	230	
alcohol	1-Decanol	230.2	
alcohol	2-Phenoxyethanol	240	
alcohol	Bis(2-hydroxyethyl) ether	245	Diethylene glycol
alcohol	Isopentyl salicylate	277–278	
alcohol	2,2'-(Ethylenedioxy)bisethanol	285	
alcohol	Glycerol	290	
aldehyde	2-Furaldehyde	161.8	Furfural
amide	<i>N,N</i> -Dimethylformamide	153.0	DMF
amide	Acetamide	221.2	
amine	Diisopropylamine	83.5	
amine	Pyridine	115.2	

TABLE 4.5C Boiling Points for Common Organic Solvents (*continued*)*Arranged by compound type in order of increasing boiling point*

	Compound name	(°C)	Other name
amine	Cyclohexylamine	134.8	Aminocyclohexane
amine	Aniline	184.4	Aminobenzene
amine	<i>N,N</i> -Dimethylaniline	194.2	Dimethylaminobenzene
amine	<i>o</i> -Toluidine	200.4	1-Amino-2-methylbenzene
amine	<i>p</i> -Toluidine	200.6	1-Amino-4-methylbenzene
amine	<i>m</i> -Toluidine	203.4	1-Amino-3-methylbenzene
amine	<i>o</i> -Chloroaniline	208.8	1-Amino-2-chlorobenzene
amine	Quinoline	237	
anhydride	Acetic anhydride	140.0	
bromide	Bromoethane	38.4	Ethyl bromide
bromide	1-Bromo-2-methylpropane	91.5	Isobutyl bromide
bromide	1-Bromo-3-methylbutane	119.7	Isopentyl bromide
bromide	1,2-Dibromoethane	131.7	
bromide	Tribromomethane	149.6	Bromoform
bromide	Bromobenzene	156.2	
bromide	1-Bromonaphthalene	281.1	
chloride	Chloroethane	12.3	Ethyl chloride
chloride	Dichloromethane	39.8	Methylene chloride
chloride	1,1-Dichloroethane	57.3	
chloride	Dichloroethylene	60.6	
chloride	Chloroform	61.2	
chloride	1-Chloro-2-methylpropane	68.9	Isobutyl chloride
chloride	1,1,1-Trichloroethane	74.0	
chloride	Carbon tetrachloride	76.7	
chloride	1-Chlorobutane	77.9	Butyl chloride
chloride	1,2-Dichloroethane	83.7	
chloride	Trichloroethylene	87.2	
chloride	1,2-Dichloropropane	96.8	
chloride	1-Chloro-3-methylbutane	99.0	
chloride	1,1,2-Trichloroethane	113.5	
chloride	1-Chloro-2,3-epoxypropane	116.1	Epichlorohydrin
chloride	Tetrachloroethylene	121.1	
chloride	1-Chloro-2-propanol	127.4	
chloride	2-Chloroethanol	128.6	
chloride	Chlorobenzene	131.7	
chloride	1,1,2,2-Tetrachloroethane	146.3	
chloride	1,2,3-Trichloropropane	156.9	
chloride	Pentachloroethane	160.5	
chloride	1,3-Dichloro-2-propanol	174.3	
chloride	Bis(2-chloroethyl) ether	178.8	Dichloro diethyl ether
chloride	1,2-Dichlorobenzene	180.4	<i>o</i> -Dichlorobenzene
chloride	<i>o</i> -Chloroaniline	208.8	1-Amino-2-chlorobenzene
chloride	1-Chloronaphthalene	259.3	
ester	Methyl formate	31.5	
ester	Ethyl formate	54.2	

TABLE 4.5C Boiling Points for Common Organic Solvents (*continued*)*Arranged by compound type in order of increasing boiling point*

	Compound name	(°C)	Other name
ester	Methyl acetate	56.3	
ester	Ethyl acetate	77.1	
ester	Propyl formate	80.9	
ester	Isopropyl acetate	88.2	
ester	Methyl chloroformate	94.0	
ester	Ethyl propanoate	99.1	Ethyl propionate
ester	Propyl acetate	101.5	
ester	Butyl formate	106.6	
ester	<i>sec</i> -Butyl acetate	112.3	
ester	Isobutyl acetate	118.0	
ester	Ethyl butanoate	121.6	Ethyl butyrate
ester	Butyl acetate	126.1	
ester	Diethyl carbonate	126.8	
ester	Isopentyl acetate	142	
ester	2-Methoxyethyl acetate	144.5	
ester	Ethyl lactate	154.5	
ester	Isopentyl propanoate	160.2	Isopentyl propionate
ester	Cyclohexyl acetate	174–175	
ester	Furfuryl acetate	175–177	
ester	Isopentyl butanoate	178.6	Isopentyl butyrate
ester	Ethyl acetoacetate	180.8	
ester	Diethyl oxalate	185.4	
ester	1,2-Ethanediol diacetate	190.2	Diacetoxyethane
ester	Diethyl malonate	199.3	
ester	Methyl benzoate	199.5	
ester	γ -Valerolactone	207–208	
ester	Ethyl benzoate	212.4	
ester	2-(2-Ethoxyethoxy)ethyl acetate	218.5	
ester	Methyl salicylate	223.0	
ester	Diethyl maleate	225.3	
ester	Propyl benzoate	231.2	
ester	Propylene carbonate	240	
ester	Dibutyl oxalate	245.5	
ester	Butyl benzoate	250	
ester	1,2,3-Propanetriol triacetate	258–259	Glycerol triacetate
ester	Isopentyl benzoate	262	
ester	<i>trans</i> -Ethyl cinnamate	271.0	
ester	Isopentyl salicylate	277–278	
ester	Dimethyl <i>o</i> -phthalate	283.7	1,2-Bis(carbomethoxy) benzene
ester	Diethyl <i>o</i> -phthalate	295	
ester	Benzyl benzoate	323.5	
ester	Dibutyl <i>o</i> -phthalate	340.0	
ester	Dibutyl decanedioate	344–345	
ether	Ethylene oxide	10.6	Oxirane
ether	Furan	31.4	

TABLE 4.5C Boiling Points for Common Organic Solvents (*continued*)*Arranged by compound type in order of increasing boiling point*

	Compound name	(°C)	Other name
ether	Diethyl ether	34.6	Ethyl ether
ether	Propylene oxide	34.5	
ether	Dimethoxyethane	42.3	DME, glyme
ether	1-Isopropoxy-2-propanol	47.9	
ether	Tetrahydrofuran	66.0	THF
ether	Diisopropyl ether	68.0	Isopropyl ether
ether	1,3-Dioxolane	74–75	
ether	2-Methyltetrahydrofuran	80.0	
ether	2,5-Dimethylfuran	93–94	
ether	1,4-Dioxane	101.2	
ether	1,1-Diethoxyethane	102.7	
ether	1-Chloro-2,3-epoxypropane	116.1	Epichlorohydrin
ether	1-Methoxy-2-propanol	120.1	
ether	2-Methoxyethanol	124.6	
ether	2-Ethoxyethanol	134.8	
ether	Dibutyl ether	142.4	
ether	2-Methoxyethyl acetate	144.5	
ether	Methoxybenzene	153.8	Anisole
ether	Bis(2-methoxyethyl) ether	160	Diglyme
ether	2-Furanmethanol	170.0	2-Hydroxymethylfuran
ether	Ethoxybenzene	170	Phenetole
ether	2-Butoxyethanol	170.2	Butyl cellosolve
ether	Diisopentyl ether	173.4	
ether	Bis(2-chloroethyl) ether	178.8	Dichloro diethyl ether
ether	Benzyl ethyl ether	185.0	
ether	Bis(2-ethoxyethyl)ether	188.4	
ether	2-(2Methoxyethoxy)ethanol	194.1	
ether	2-(2-Ethoxyethoxy) ethanol	202	
ether	1,2 Dibutoxyethane	203.6	
ether	2-(2-Ethoxyethoxy)ethyl acetate	218.5	
ether	2-Phenoxyethanol	240	
ether	Bis(2-hydroxyethyl) ether	245	Diethylene glycol
ether	Bis(2-(2-methoxyethoxy)-ethyl) ether	275.3	Triglyme
ether	1-Methoxy-2-nitrobenzene	277	
ether	2,2'-(Ethylenedioxy) bisethanol	285	
hydrocarbon	Pentane	36.1	
hydrocarbon	Hexane	68.7	
hydrocarbon	Benzene	80.1	
hydrocarbon	Cyclohexane	80.7	
hydrocarbon	Cyclohexene	83.0	
hydrocarbon	Heptane	98.4	
hydrocarbon	Methylcyclohexane	100.9	
hydrocarbon	Toluene	110.6	Methylbenzene
hydrocarbon	Octane	125.7	
hydrocarbon	Ethylbenzene	136.2	
hydrocarbon	<i>p</i> -Xylene	138.4	1,4-Dimethylbenzene
hydrocarbon	<i>m</i> -Xylene	139.1	1,3-Dimethylbenzene

TABLE 4.5C Boiling Points for Common Organic Solvents (*continued*)*Arranged by compound type in order of increasing boiling point*

	Compound name	(°C)	Other name
hydrocarbon	<i>o</i> -Xylene	144.4	1,2-Dimethylbenzene
hydrocarbon	Nonane	150.8	
hydrocarbon	Isopropylbenzene	152.4	Cumene
hydrocarbon	Propylbenzene	159.2	
hydrocarbon	Decane	174.2	
hydrocarbon	4-Isopropyl-1-methylbenzene	177.1	<i>p</i> -Cymene
hydrocarbon	1,2,3,4-Tetrahydronaphthalene	207.6	Tetralin
hydrocarbon	Naphthalene	217.7	
ketone	Acetone	56.2	Dimethyl ketone
ketone	2-Butanone	79.6	Methyl ethyl ketone
ketone	2-Pentanone	101.7	Methyl propyl ketone
ketone	3-Pentanone	102.0	Diethyl ketone
ketone	4-Methyl-2-pentanone	115.7	Methyl isobutyl ketone
ketone	3-Hexanone	123	Ethyl propyl ketone
ketone	2,4-Dimethyl-3-pentanone	124	Diisopropyl ketone
ketone	2-Hexanone	127.2	Methyl butyl ketone
ketone	2,4-Pentanedione	140.6	Acetylacetone
ketone	4-Heptanone	143.7	Dipropyl ketone
ketone	3-Heptanone	147.8	Ethyl butyl ketone
ketone	2-Heptanone	151	Methyl pentyl ketone
ketone	Cyclohexanone	155.7	
ketone	2,6-Dimethyl-4-heptanone	168.1	Diisobutyl ketone
ketone	4-Hydroxy-4-methyl-2-pentanone	169.2	
ketone	2,5-Hexanedione	191.4	
ketone	Acetophenone	202.1	Methyl phenyl ketone
ketone	Camphor	207	1,7,7-Trimethylbicyclo- [2.2.1] heptan-2-one
ketone	Isophorone	215.2	3,5,5-Trimethylcyclo- hex-2-en-1-one
miscellaneous	Carbon disulfide	46.3	
miscellaneous	Tributyl borate	238.5	
nitrile	Acetonitrile	81.6	
nitrile	Benzonitrile	191.0	Cyanobenzene
nitrile	Phenylacetoneitrile	233.5	Cyanomethylbenzene
nitro compound	Nitromethane	101.2	
nitro compound	Nitroethane	114.1	
nitro compound	2-Nitropropane	120.3	Nitroisopropane
nitro compound	1-Nitropropane	131.2	
nitro compound	Nitrobenzene	210.8	
nitro compound	1-Methoxy-2-nitrobenzene	277	
sulfide	Thiophene	84.2	
sulfoxide	Dimethylsulfoxide	189.0	DMSO

TABLE 4.6 Molecular Elevation of the Boiling Point*Ebullioscopic constants*

Molecular weights can be determined with the relation

$$M = K_b \frac{1000 w_2}{w_1 \Delta T_b}$$

where ΔT_b is the elevation of the boiling point brought about by the addition of w_2 grams of solute to w_1 grams of solvent and K_b is the ebullioscopic constant. In the column headed "Barometric correction" is given the number of degrees for each millimeter of difference between the barometric reading and 760 mmHg to be subtracted from K_b if the pressure is lower, or added if higher, than 760 mm. In general, the effect is within experimental error if the pressure is within 10 mm of 760 mm.

Compound	Barometric correction	K_b
Acetic acid	0.000 8	3.07
Acetic anhydride		3.53
Acetone	0.000 4	1.71
Acetonitrile		1.30
Acetophenone		5.65
Aniline	0.000 9	3.52
Benzene	0.000 7	2.53
Benzonitrile		3.87
Bromobenzene	0.001 6	6.26
Bromoethane		2.53
2-Butanone		2.28
cis-2-Butene-1,4-diol		2.86
D-(+)-Camphor	0.001 5	5.611
Carbon disulfide	0.000 6	2.34
Carbon tetrachloride	0.001 3	5.03
Chlorobenzene	0.001 1	4.15
Chloroethane		1.95
Chloroform	0.000 9	3.63
Cyclohexane	0.000 7	2.79
1,2-Dibromoethane	0.001 6	6.608
1,1-Dichloroethane		3.13
1,2-Dichloroethane		3.44
Dichloromethane		2.60
Diethyl ether	0.000 5	2.02
Diethyl sulfide		3.23
Dimethoxymethane		2.125
N,N-Dimethylacetamide		3.22
Dimethyl sulfide		1.85
1,4-Dioxane		3.270
Ethanol	0.000 3	1.22
Ethoxybenzene		5.0
Ethyl acetate	0.000 7	2.77
Formic acid		2.4
Glycerol		6.52
Heptane	0.000 8	3.43
Hexane		2.75
2-Hydroxybenzaldehyde		4.96

TABLE 4.6 Molecular Elevation of the Boiling Point (*continued*)

Compound	Barometric correction	K_b
Iodoethane		5.16
Iodomethane		4.19
4-Isopropyl-1-methylbenzene		5.52
Methanol	0.000 2	0.83
Methoxybenzene		4.502
Methyl acetate	0.000 5	2.15
2-Methyl-2-butanol		2.255
3-Methyl-1-butanol		2.65
3-Methylbutyl acetate		4.83
Methyl formate		1.649
2-Methyl-1-propanol		2.166
2-Methyl-2-propanol		1.745
Naphthalene	0.001 4	5.80
Nitrobenzene		5.24
Nitroethane		2.60
Nitromethane		1.86
Octane		4.02
Pentyl acetate		4.83
Phenol	0.000 9	3.60
Piperidine		2.84
1-Propanol		1.59
Propionic acid		3.51
Propionitrile		1.87
Pyridine		2.710
Quinoline		5.84
1,1,2,2-Tetrachloroethylene		5.50
1,2,3,4-Tetrahydronaphthalene		5.582
Toluene	0.000 8	3.33
<i>p</i> -Toluidine		4.14
Trichloroethylene		4.43
1,1,2-Trichloro-1,2,2-trifluoroethane		5.75
Triethylamine		3.45
Water	0.000 1	0.512

Distillation is an important historical method for the separation of liquids. A mixture or solution of two liquids is heated until the vapor pressure of the lower boiling compound reaches the pressure of the surroundings. This may be ambient pressure or a lowered pressure caused by application of a vacuum. In either event, vaporization occurs, the vapors are condensed on a cold surface, and the condensed liquid is collected. If the boiling points of the two liquids are sufficiently different given the pressure and efficiency of the apparatus, separation may be achieved. A zeotrope is a mixture that can be separated by distillation.

In contrast, certain mixtures of two (binary) or three (ternary) components form constant boiling mixtures that cannot be separated by distillation. In such cases, each component contributes a fixed amount and the boiling point of the mixture is characteristic of the components. Such a system is called an azeotrope. The boiling point of an azeotrope may be higher or lower than that of the individual components. Common binary azeotropes are listed in Table 4.7 and ternary azeotropes are listed in Table 4.8.

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures

A zeotrope is a mixture that can be separated by distillation.

A. Binary azeotropes containing water

System	BP of azeotrope, °C	Composition, wt %	
		Water	Other component
Inorganic acids			
Hydrogen bromide	126	52.5	47.5
Hydrogen chloride	108.58	79.78	20.22
Hydrogen fluoride	111.35	64.4	35.6
Hydrogen iodide	127	43	57
Hydrogen peroxide	zeotrope		
Nitric acid	120.7	32.6	67.4
Perchloric acid	203	28.4	71.6
Organic acids			
Formic acid	107.2	22.6	77.4
Acetic acid	zeotrope		
Propionic acid	99.9	82.3	17.7
Isobutyric acid	99.3	79	21
Butyric acid	99.4	81.6	18.4
Pentanoic acid	99.8	89	11
Isopentanoic acid	99.5	81.6	18.4
Perfluorobutyric acid	97	71	29
Crotonic acid	99.9	97.8	2.2
Alcohols			
Ethanol	78.17	4	96
Allyl alcohol	88.9	27.7	72.3
1-Propanol	71.7	71.7	28.3
2-Propanol	80.3	12.6	87.4
1-Butanol	92.7	42.5	57.5
2-Butanol	87.0	26.8	73.2
2-Methyl-2-propanol	79.9	11.7	88.3
1-Pentanol	95.8	54.4	45.6
2-Pentanol	91.7	36.5	63.5
3-Pentanol	91.7	36.0	64.0
2,2-Dimethyl-2-propanol	87.35	27.5	72.5
1-Hexanol	97.8	67.2	32.8
1-Octanol	99.4	90	10
Cyclopentanol	96.25	58	42
1-Heptanol	98.7	83	17
Phenol	99.52	90.8	9.2
2-Methoxyphenol	99.5	87.5	12.5

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

System	BP of azeotrope, °C	Composition, wt %	
		Water	Other component
Alcohols (continued)			
1-Phenylphenol	99.95	98.75	1.25
Benzyl alcohol	99.9	91	9
2,3-Dimethyl-2, 3-butanediol	zeotrope		
Furfuryl alcohol	98.5	80	20
Aldehydes			
Propionaldehyde	47.5	2	98
Butyraldehyde	68	6	94
Pentanal	83	19	81
Paraldehyde	90	28.5	71.5
Furaldehyde	97.5	65	35
Amines			
N-Methylbutylamine	82.7	15	85
Furfurylamine	99	74	26
Piperidine	92.8	35	65
Pyridine	93.6	41.3	58.7
2-Methylpyridine	93.5	48	52
3-Methylpyridine	97	60	40
4-Methylpyridine	97.35	62.8	37.2
2,6-Dimethylpyridine	96.02	51.8	48.2
Dibutylamine	97	50.5	49.5
Diethylamine	99.8	92.8	7.2
Triallylamine	95	38	62
Tributylamine	99.65	79.7	20.3
Aniline	98.6	80.8	19.2
N-Ethylaniline	99.2	83.9	16.1
1-Methyl-2-(2-pyridyl) pyrrolidine	99.85	97.5	2.5
Halogenated hydrocarbons			
Chloroform	56.1	2.8	97.2
Carbon tetrachloride	42.6	2.8	97.2
Trichloroethylene	73.4	17	83
Tetrachloroethylene	88.5	17.2	82.8
1,2-Dichloroethane	72	8.3	91.7
1-Chloropropane	44	2.2	97.8
1,2-Dichloropropane	78	12	88
Chlorobenzene	90.2	28.4	71.6

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Water	Other component
Esters			
Ethyl formate	52.6	5	95
Isopropyl formate	65.0	3	97
Propyl formate	71.6	2.3	97.7
Isobutyl formate	80.4	7.8	92.2
Butyl formate	83.8	14.5	85.5
Isopentyl formate	90.2	21	79
Pentyl formate	91.6	28.4	71.6
Benzyl formate	99.2	80	20
Ethyl acetate	70.38	8.47	91.53
Allyl acetate	83	14.7	85.3
Isopropyl acetate	76.6	10.6	89.4
Propyl acetate	87.4	16.5	83.5
Isobutyl acetate	82.4	14	86
Butyl acetate	90.2	28.7	71.3
Isopentyl acetate	93.8	36.3	63.7
Pentyl acetate	95.2	41	59
Hexyl acetate	97.4	61	39
Phenyl acetate	98.9	75.1	24.9
Benzyl acetate	99.6	87.5	12.5
Methyl propionate	71.4	3.9	96.1
Ethyl propionate	81.2	10	90
Isopropyl propionate	85.2	19.9	80.1
Propyl propionate	88.9	23	77
Isobutyl propionate	92.75	52.2	47.8
Isopentyl propionate	96.55	48.5	51.5
Methyl butyrate	82.7	11.5	88.5
Ethyl butyrate	87.9	21.5	78.5
Propyl butyrate	94.1	36.4	63.6
Isobutyl butyrate	96.3	46	54
Butyl butyrate	97.2	53	47
Isopentyl butyrate	98.05	63.5	36.5
Methyl isobutyrate	77.7	6.8	93.2
Ethyl isobutyrate	85.2	15.2	84.8
Propyl isobutyrate	92.2	30.8	69.2
Isobutyl isobutyrate	95.5	39.4	60.6
Isopentyl isobutyrate	97.4	56.0	44.0
Methyl isopentanoate	87.2	19.2	80.8
Ethyl isopentanoate	92.2	30.2	69.8
Propyl isopentanoate	96.2	45.2	54.8
Isobutyl isopentanoate	97.4	55.8	44.2
Isopentyl isopentanoate	98.8	74.1	25.9

TABLE 4.7 Binary Azeotropic (Constant-Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Water	Other component
Esters (<i>continued</i>)			
Ethyl pentanoate	94.5	40	60
Ethyl hexanoate	97.2	54	46
Methyl benzoate	99.08	79.2	20.8
Ethyl benzoate	99.4	84.0	16.0
Propyl benzoate	99.7	90.9	9.1
Butyl benzoate	99.9	94	6
Isopentyl benzoate	99.9	95.6	4.4
Ethyl phenylacetate	99.7	91.3	8.7
Methyl cinnamate	99.9	95.5	4.5
Methyl phthalate	99.95	97.5	2.5
Diethyl <i>o</i> -phthalate	99.98	98.0	2.0
Ethyl chloroacetate	95.2	45.1	54.9
Butyl chloroacetate	98.12	75.5	24.5
Methyl acrylate	71	7.2	92.8
Isobutyl carbonate	98.6	74	26
Ethyl crotonate	93.5	38	62
Methyl lactate	99	80	20
1,2-Ethanediol diacetate	99.7	84.6	15.4
Ethyl nitrate	74.35	22	78
Propyl nitrate	84.8	20	80
Isobutyl nitrate	89.0	25	75
Methyl sulfate	98.6	73	27
Ethers			
Ethyl vinyl ether	34.6	1.5	98.5
Diethyl ether	34.2	1.3	98.7
Ethyl propyl ether	59.5	4	96
Diisopropyl ether	62.2	4.5	95.5
Butyl ethyl ether	76.6	11.9	88.1
Diisobutyl ether	88.6	23	77
Dibutyl ether	92.9	33	67
Diisopentyl ether	97.4	54	46
1,1-Diethoxyethane	82.6	14.5	85.5
Diphenyl ether	99.33	96.75	3.25
Methoxybenzene	95.5	40.5	59.5
Hydrocarbons			
Pentane	34.6	1.4	98.6
Hexane	61.6	5.6	94.4
Heptane	79.2	12.9	87.1
2,2,4-Trimethylpentane	78.8	11.1	88.9

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Water	Other component
Hydrocarbons (<i>continued</i>)			
Nonane	94.8	82	18
Undecane	98.85	96.0	4.0
Dodecane	99.45	98	2
Acrolein	52.4	2.6	97.4
Cyclohexene	70.8	8.93	91.07
Cyclohexane	69.5	8.4	91.6
1-Octene	88.0	28.7	71.3
Benzene	69.25	8.83	91.17
Toluene	84.1	13.5	86.5
Ethylbenzene	92.0	33.0	67.0
<i>m</i> -Xylene	92	35.8	64.2
Isopropylbenzene	95	43.8	56.2
Naphthalene	98.8	84	16
Ketones			
Acetone	zeotrope		
2-Butanone	73.5	11	89
2-Pentanone	83.3	19.5	80.5
Cyclopentanone	94.6	42.4	57.6
4-Methyl-2-pentanone	87.9	24.3	75.7
2-Heptanone	95	48	52
3-Heptanone	94.6	42.2	57.8
4-Heptanone	94.3	40.5	59.5
4-Hydroxy-4-methyl-2-pentanone	98.8	87.3	12.7
4-Methyl-3-penten-2-one	91.8	34.8	65.2
Nitriles			
Acetonitrile	76.5	16.3	83.7
Isobutyronitrile	82.5	23	77
Butyronitrile	88.7	32.5	67.5
Acrylonitrile	70.6	14.3	85.7
Miscellaneous			
Hydrazine	120	32.3	67.7
Acetamide	zeotrope		
Nitromethane	83.59	23.6	76.4
Nitroethane	87.22	28.5	71.5
2,5-Dimethylfuran	77.0	11.7	88.3
Trioxane	91.4	30	70
Carbon disulfide	42.6	2.8	97.2

TABLE 4.7 Binary Azeotropic (Constant-Boiling) Mixtures (*continued*)**B. Binary azeotropes containing organic acids**

System	BP of azeotrope, °C	Composition, wt %	
		Acid	Other component
Formic acid			
2-Methylbutane	27.2	4	96
Pentane	34.2	20	80
Hexane	60.6	28	72
Methylcyclopentane	63.3	29	71
Cyclohexane	70.7	70	30
Methylcyclohexane	80.2	46.5	53.5
Heptane	78.2	56.5	43.5
Octane	90.5	63	37
Benzene	71.05	31	69
Toluene	85.8	50	50
<i>o</i> -Xylene	95.5	74	26
<i>m</i> -Xylene	92.8	71.8	28.2
Styrene	97.8	73	27
Iodomethane	42.1	6	94
Chloroform	59.15	15	85
Carbon tetrachloride	66.65	18.5	81.5
Trichloroethylene	74.1	25	75
Tetrachloroethylene	88.2	50	50
Bromoethane	38.2	3	97
1,2-Dibromoethane	94.7	51.5	48.5
1,2-Dichloroethane	77.4	14	86
1-Bromopropane	64.7	27	73
2-Bromopropane	77.4	14	86
1-Chloropropane	45.6	8	92
2-Chloropropane	34.7	1.5	98.5
1-Chloro-2-methylpropane	63.0	19	81
Bromobenzene	98.1	68	32
Chlorobenzene	93.7	59	41
Fluorobenzene	73.0	27	73
<i>o</i> -Chlorotoluene	100.2	83	17
Pyridine	127.43	61.4	38.6
2-Methylpyridine	158.0	25	75
2-Pentanone	105.3	32	68
3-Pentanone	105.4	33	67
Nitromethane	97.07	45.5	54.5
Diethyl sulfide	82.2	35	65
Diisopropyl sulfide	93.5	62	38
Dipropyl sulfide	98.0	83	17
Carbon disulfide	42.55	17	83

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Acid	Other component
Acetic acid			
Hexane	68.3	6.0	94.0
Heptane	91.7	23	67
Octane	105.7	53.7	46.3
Nonane	112.9	69	31
Decane	116.75	79.5	20.5
Undecane	117.9	95	5
Cyclohexane	78.8	9.6	90.4
Methylcyclohexane	96.3	31	69
Benzene	80.05	2.0	98.0
Toluene	100.6	28.1	71.9
<i>o</i> -Xylene	116.6	78	22
<i>m</i> -Xylene	115.35	72.5	27.5
<i>p</i> -Xylene	115.25	72	28
Ethylbenzene	114.65	66	34
Styrene	116.8	85.7	14.3
Isopropylbenzene	116.0	84	16
Triethylamine	163	67	33
Nitromethane	101.2	96	4
Nitroethane	112.4	30	70
Pyridine	138.1	51.1	48.9
2-Methylpyridine	144.1	40.4	59.6
3-Methylpyridine	152.5	30.4	69.6
4-Methylpyridine	154.3	30.3	69.7
2,6-Dimethylpyridine	148.1	22.9	77.1
Carbon tetrachloride	76	98.46	1.54
Trichloroethylene	86.5	96.2	3.8
Tetrachloroethylene	107.4	61.5	38.5
1,2-Dibromoethane	114.4	55	45
2-Iodopropane	88.3	9	91
1-Bromobutane	97.6	18	82
1-Bromo-2-methylpropane	90.2	12	88
Chlorobenzene	114.7	58.5	41.5
Trichloronitromethane	107.65	80.5	19.5
1,4-Dioxane	119.5	77	23
Diisopropyl sulfide	111.5	48	52
Propanoic (Propionic) acid			
Heptane	97.8	2	98
Octane	120.9	21.5	78.5

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Acid	Other component
Acetic acid (<i>continued</i>)			
Nonane	134.3	54.0	46.0
Decane	139.8	80.5	19.5
<i>o</i> -Xylene	135.4	43	57
<i>p</i> -Xylene	132.5	34	66
1,3,5-Trimethylbenzene	139.3	77	23
Isopropylbenzene	139.0	65	35
Propylbenzene	139.5	75	25
Camphene	138.0	65	35
α -Pinene	136.4	58.5	41.5
Methoxybenzene	140.8	96	4
Pyridine	148.6	67.2	32.8
2-Methylpyridine	154.5	55.0	45.0
1,2-Dibromoethane	127.8	17.5	82.5
1-Iodo-2-methylpropane	119.5	9	91
Chlorobenzene	128.9	18	82
Dipropyl sulfide	136.5	45	55
Butyric (butanoic) acid			
Undecane	162.4	84.4	15.5
<i>o</i> -Xylene	143.0	10	90
<i>m</i> -Xylene	138.5	6	94
<i>p</i> -Xylene	137.8	5.5	94.5
Ethylbenzene	135.8	4	96
Styrene	143.5	15	85
1,2,4-Trimethylbenzene	159.5	45	55
1,3,5-Trimethylbenzene	158.0	38	62
Isopropylbenzene	149.5	20	80
Propylbenzene	154.5	28	72
Butylbenzene	162.5	75	25
Naphthalene	zeotrope		
Indene	163.7	84	16
Camphene	152.3	2.8	97.2
Methoxybenzene	152.9	12	88
Pyridine	163.2	92.0	8.0
2-Furaldehyde	159.4	42.5	57.5
1,2-Dibromoethane	131.1	3.5	96.5
1-Iodobutane	129.8	2.5	97.5
Chlorobenzene	131.75	2.8	97.2
1,4-Dichlorobenzene	162.0	57	43
<i>o</i> -Bromotoluene	163.0	72	28
<i>m</i> -Bromotoluene	163.6	79.5	20.5
<i>p</i> -Bromotoluene	161.5	75	25
α -Chlorotoluene	160.8	65	35
Ethyl bromoacetate	157.4	84	16
Propyl chloroacetate	160.5	40	60

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt%	
		Acid	Other component
Isobutyric (2-methylpropanoic) acid			
2,7-Dimethyloctane	148.6	48	52
<i>o</i> -Xylene	141.0	22	78
<i>m</i> -Xylene	139.9	15	85
<i>p</i> -Xylene	136.4	13	87
Styrene	142.0	27	73
1,2,4-Trimethylbenzene	152.3	63	37
Isopropylbenzene	146.8	35	65
Propylbenzene	149.3	49	51
Camphene	148.1	45	55
D-Limonene	152.5	78	22
Methoxybenzene	149.0	42	58
Ethyl bromoacetate	153.0	40	60
Ethyl 2-oxopropionate	153.0	60	40
1,2-Dibromoethane	130.5	6.5	93.5
1-Iodobutane	128.8	7	93
1-Bromohexane	148.0	35	65
Bromobenzene	148.6	35	65
Chlorobenzene	131.5	8	92
<i>o</i> -Bromotoluene	153.9	85	15
α -Chlorotoluene	153.5	80	20
Diisopentyl ether	154.2	93	7
Ethyl bromoacetate	153.0	40	60

C. Binary azeotropes containing alcohol

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
Methanol			
Pentane	30.9	7	93
Cyclopentane	38.8	14	86
Cyclohexane	53.9	36.4	63.6
Methylcyclohexane	59.2	54	46
Heptane	59.1	51.5	48.5
Octane	62.8	67.5	32.5
Nonane	64.1	83.4	16.6
Benzene	57.5	39.1	60.9
Fluorobenzene	59.7	32	68
Toluene	63.5	72.5	27.5
Bromomethane	3.55	99.55	0.45
Iodomethane	37.8	95.5	4.5

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (continued)

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
Methanol (<i>continued</i>)			
Bromodichloromethane	63.8	60	40
Chloroform	53.4	87.4	12.6
Carbon tetrachloride	55.7	79.44	20.56
Bromoethane	34.9	5.3	94.7
1,2-Dichloroethane	61.0	32	68
Trichloroethylene	59.3	38	62
1-Bromopropane	54.5	21	79
2-Bromopropane	48.6	15.0	85.0
1-Chloropropane	40.5	9.5	90.5
2-Chloropropane	33.4	6	94
2-Iodopropane	61.0	38	62
1-Chlorobutane	57.0	27	73
Isobutyl formate	64.6	95	5
Methyl acetate	53.5	19	81
Methyl acrylate	62.5	54	46
Methyl nitrate	52.5	73	27
Acetone	55.5	12.1	87.9
1,4-Dioxane	zeotrope		
Dipropyl ether	63.8	72	28
Methyl <i>tert</i> -butyl ether	51.3	14.3	85.7
Diethyl sulfide	61.2	62	38
Carbon disulfide	39.8	71	29
Thiophene	59.7	16.4	83.6
Nitromethane	64.4	9.1	90.9
Ethanol			
Pentane	34.3	5	95
Cyclopentane	44.7	7.5	92.5
Hexane	58.7	21	79
Cyclohexane	64.8	29.2	70.8
Heptane	70.9	49	51
Octane	77.0	78	22
Benzene	67.9	31.7	68.3
Fluorobenzene	70.0	75	25
Toluene	76.7	68	32
Bromodichloromethane	75.5	72	28
Iodomethane	41.2	96.8	3.2
Chloroform	59.3	93	7
Trichloronitromethane	77.5	34	66
Carbon tetrachloride	65.0	84.2	15.8
1,2-Dichloroethane	70.5	37	63
3-Chloro-1-propene	44	5	95

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
Ethanol (<i>continued</i>)			
1-Bromopropane	62.8	20.5	79.5
2-Bromopropane	55.6	10.5	89.5
1-Chloropropane	45.0	6	94
2-Chloropropane	35.6	2.8	97.2
1-Iodopropane	75.4	44	56
2-Iodopropane	71.5	27	73
1-Bromobutane	75.0	43	57
1-Chlorobutane	65.7	20.3	79.7
2-Butanone	74.8	40	60
1,1-Diethoxyethane	78.0	76	24
Dipropyl ether	74.5	44	56
Acetonitrile	72.5	44	56
Acrylonitrile	70.8	41	59
Nitromethane	76.1	29	71
Carbon disulfide	42.6	91	9
Diethyl sulfide	72.6	56	44
1-Propanol			
Hexane	65.7	4	96
Cyclohexane	74.7	18.5	81.5
Methylcyclohexane	87.0	34.7	65.3
Heptane	84.6	34.7	65.3
Octane	93.9	70	30
Benzene	77.1	16.9	83.1
Toluene	92.5	51.2	48.8
<i>o</i> -Xylene	zeotrope		
<i>m</i> -Xylene	97.1	94	6
<i>p</i> -Xylene	96.9	92.2	7.8
Styrene	97.0	8	92
Propyl formate	80.7	3	97
Butyl formate	95.5	64	36
Propyl acetate	94.7	51	49
Ethyl propionate	93.4	48	52
Methyl butyrate	94.4	49	51
Dipropyl ether	85.7	30	70
1,1-Diethoxyethane	92.4	37	63
1,4-Dioxane	95.3	55	45
Chloroform	zeotrope		
Carbon tetrachloride	73.4	92.1	7.9
Trichloronitromethane	94.1	58.5	41.5
Iodoethane	70	93	7
1,2-Dichloroethane	80.7	19	81

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
1-Propanol (<i>continued</i>)			
Tetrachloroethylene	94.0	52	48
1-Bromopropane	69.7	9	91
1-Chlorobutane	74.8	18	82
Chlorobenzene	96.5	80	20
Fluorobenzene	80.2	18	82
Nitromethane	89.1	48.4	51.6
1-Nitropropane	97.0	8.8	91.2
Carbon disulfide	45.7	94.5	5.5
2-Propanol			
Pentane	35.5	6	94
Hexane	62.7	23	77
Cyclohexane	69.4	32	68
Heptane	76.4	50.5	49.5
Octane	81.6	84	16
Benzene	71.7	33.7	66.3
Fluorobenzene	74.5	30	70
Toluene	80.6	69	31
Chloroform	60.8	4.2	95.8
Trichloronitromethane	81.9	35	65
Carbon tetrachloride	69.0	18	82
1,2-Dichloroethane	74.7	43.5	56.5
Iodoethane	67.1	15	85
3-Bromo-1-propene	66.5	20	80
1-Chloropropane	46.4	2.8	97.2
1-Bromopropane	66.8	20.5	79.5
2-Bromopropane	57.8	12	88
1-Iodopropane	79.8	42	58
2-Iodopropane	76.0	32	68
1-Chlorobutane	70.8	23	77
Ethyl acetate	75.3	25	75
Isopropyl acetate	81.3	60	40
Methyl propionate	76.4	37	63
Acrylonitrile	71.7	56	44
Butylamine	74.7	60	40
2-Butanone	77.5	32	68
1,1-Diethoxyethane	81.3	63	37
Ethyl propyl ether	62.0	10	90
Diisopropyl ether	66.2	14.1	85.9

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
1-Butanol			
Cyclohexane	79.8	9.5	90.5
Cyclohexene	82.0	5	95
Hexane	68.2	3.2	96.8
Methylcyclohexane	95.3	20	80
Heptane	93.9	18	82
Octane	108.5	45.2	54.8
Nonane	115.9	71.5	28.5
Toluene	105.5	27.8	72.2
<i>o</i> -Xylene	116.8	75	25
<i>m</i> -Xylene	116.5	71.5	28.5
<i>p</i> -Xylene	115.7	68	32
Ethylbenzene	115.9	65.1	34.9
Butyl formate	105.8	23.6	76.4
Isopentyl formate	115.9	69	31
Butyl acetate	117.2	47	53
Isobutyl acetate	114.5	50	50
Ethyl butyrate	115.7	64	36
Ethyl isobutyrate	109.2	17	83
Methyl isopentanoate	113.5	40	60
Ethyl borate	113.0	52	48
Ethyl carbonate	116.5	63	37
Isobutyl nitrate	112.8	45	55
Dibutyl ether	117.8	82.5	17.5
Diisobutyl ether	113.5	48	52
1,1-Diethoxyethane	101.0	13	87
Carbon tetrachloride	76.6	97.6	2.4
Tetrachloroethylene	110.0	68	32
2-Bromo-2-methylpropane	90.2	7	93
2-Iodo-2-methylpropane	110.5	30	70
Chlorobenzene	115.3	56	44
Paraldehyde	115.8	52	48
Hexaldehyde	116.8	77.1	22.9
Ethylenediamine	124.7	35.7	64.3
Pyridine	118.6	69	31
1-Nitropropane	115.3	32.2	67.8
Butyronitrile	113.0	50	50
Diisopropyl sulfide	112.0	45	55
2-Methyl-2-propanol			
Cyclohexene	80.5	14.2	85.8
Cyclohexane	78.3	14	86

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Water	Other component
2-Methyl-2-propanol (<i>continued</i>)			
Methylcyclopentane	71.0	5	95
Hexane	68.3	2.5	97.5
Methylcyclohexane	92.6	32	68
Heptane	90.8	27	73
2,5-Dimethylhexane	98.7	42	58
1,3-Dimethylcyclohexane	102.2	56	44
2,2,4-Trimethylpentane	92.0	27	73
Benzene	79.3	7.4	92.6
Chlorobenzene	107.1	63	37
Fluorobenzene	84.0	9	91
Toluene	101.2	45	55
Ethylbenzene	107.2	80	20
<i>p</i> -Xylene	107.1	88.6	11.4
Butyl formate	103.0	40	60
Isobutyl formate	97.4	12	88
Propyl acetate	101.0	17	83
Isobutyl acetate	107.6	92	8
Methyl butyrate	101.3	25	75
Ethyl isobutyrate	105.5	52	48
Methyl chloroacetate	107.6	12	88
Dipropyl ether	89.5	10	90
Isobutyl vinyl ether	82.7	6.2	93.8
1,1-Diethoxyethane	98.2	20	80
2-Pentanone	101.8	19	81
3-Pentanone	107.7	20	80
1,2-Dichloroethane	83.5	6.5	93.5
1-Bromobutane	95.0	21	79
1-Chlorobutane	77.7	4	96
2-Bromo-2-methylpropane	88.8	12	88
2-Iodo-2-methylpropane	104.0	36	64
1-Nitropropane	105.3	15.2	84.8
Isobutyl nitrate	105.6	36	64
Diisopropyl sulfide	105.8	73	27
3-Methyl-1-butanol			
Heptane	97.7	7	93
Octane	117.0	30	70
Toluene	109.7	10	90
Ethylbenzene	125.7	49	51
Isopropylbenzene	131.6	94	6
Camphene	130.9	24	76

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
3-Methyl-1-butanol (<i>continued</i>)			
Bromobenzene	131.7	85	15
<i>o</i> -Fluorotoluene	112.1	14.0	86.0
Butyl acetate	125.9	16.5	83.5
Paraldehyde	123.5	22.0	78.0
Dibutyl ether	129.8	65	35
Cyclohexanol			
<i>o</i> -Xylene	143.0	14	86
<i>m</i> -Xylene	138.9	5	95
Propylbenzene	153.8	40	60
Indene	160.0	75	25
Camphene	151.9	41	59
Cineole	160.6	92	8
Allyl alcohol			
Methylcyclohexane	85.0	42	58
Hexane	65.5	4.5	95.5
Cyclohexane	74.0	58	42
2,5-Dimethylhexane	89.3	50	50
Octane	93.4	68	32
Benzene	76.75	17.36	82.64
Toluene	92.4	50	50
Propyl acetate	94.2	53	47
Methyl butyrate	93.8	55	45
1,2-Dichloroethane	79.9	18	82
3-Iodo-1-propene	89.4	28	72
Chlorobenzene	96.2	85	15
Diethyl sulfide	85.1	45	55
Phenol			
2,7-Dimethyloctane	159.5	6	94
Decane	168.0	35	65
Tridecane	180.6	83.1	16.9
Butylbenzene	175.0	46	54
1,2,4-Trimethylbenzene	166.0	25	75
1,3,5-Trimethylbenzene	163.5	21	79
Indene	177.8	47	53
Camphene	156.1	22	78
Benzaldehyde	175.6	51.0	49.0

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
Phenol (<i>continued</i>)			
1-Octanol	195.4	13	87
2-Octanol	184.5	50	50
Dipentyl ether	180.2	78	22
Diisopentyl ether	172.2	15	85
2-Methylpyridine	185.5	75.4	24.6
3-Methylpyridine	188.9	71.2	29.8
4-Methylpyridine	190.0	67.5	32.5
2,4-Dimethylpyridine	193.4	57.0	43.0
2,6-Dimethylpyridine	185.5	72.5	27.5
2,4,6-Trimethylpyridine	195.2	52.3	47.7
Aniline	185.8	41.9	58.1
Ethylene diacetate	195.5	39.2	60.8
Iodobenzene	177.7	53	47
Benzyl alcohol			
Naphthalene	204.1	60	40
D-Limonene	176.4	11	89
1,3,5-Triethylbenzene	203.2	57	43
<i>o</i> -Cresol	zeotrope		
<i>m</i> -Cresol	207.1	61	39
<i>p</i> -Cresol	206.8	62	38
<i>N</i> -Methylaniline	195.8	30	70
<i>N,N</i> -Dimethylaniline	193.9	6.5	93.5
<i>N</i> -Ethylaniline	202.8	50	50
<i>N, N</i> -Diethylaniline	204.2	72	28
Iodobenzene	187.8	12	88
Nitrobenzene	204.0	58	42
<i>o</i> -Bromotoluene	181.3	7	93
Borneol	205.1	85.8	14.2
2-Ethoxyethanol			
Methylcyclohexane	98.6	15	85
Heptane	96.5	14	86
Octane	116.0	38	62
Toluene	110.2	10.8	89.2
Ethylbenzene	127.8	48	52
<i>p</i> -Xylene	128.6	50	50
Styrene	130.0	55	45
Propylbenzene	134.6	80	20
Isopropylbenzene	133.2	67	33
Camphene	131.0	65	35
Propyl butyrate	133.5	72	28

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
2-Butoxyethanol			
Dipentene	164.0	53	47
1,3,5-Trimethylbenzene	162.0	32	68
Butylbenzene	169.6	73.4	26.6
Camphene	154.5	30	70
<i>o</i> -Cresol	191.6	15	85
Phenetole	167.1	52	48
Cineole	168.9	58.5	41.5
Benzaldehyde	171.0	91	9
Diisobutyl sulfide	163.8	42	58
1,2-Ethanediol			
Heptane	97.9	3	97
Decane	161.0	23	77
Tridecane	188.0	55	45
Toluene	110.1	2.3	97.7
Styrene	139.5	16.5	83.5
Stilbene	196.8	87	13
<i>m</i> -Xylene	135.1	6.55	93.45
<i>p</i> -Xylene	134.5	6.4	93.6
1,3,5-Trimethylbenzene	156	13	87
Propylbenzene	152	19	81
Isopropylbenzene	147.0	18	82
Naphthalene	183.9	51	49
1-Methylnaphthalene	190.3	60.0	40.0
2-Methylnaphthalene	189.1	57.2	42.8
Anthracene	197	98.3	1.7
Indene	168.4	26	74
Acenaphthene	194.65	74.2	25.8
Fluorene	196.0	82	18
Camphene	152.5	20	80
Camphor	186.2	40	60
Biphenyl	192.3	66.5	33.5
Diphenylmethane	193.3	68.5	31.5
Benzyl alcohol	193.1	56	44
2-Phenylethanol	194.4	69	31
<i>o</i> -Cresol	189.6	27	73
<i>m</i> -Cresol	195.2	60	40
3,4-Dimethylphenol	197.2	89	11
Menthol	188.6	51.5	48.5
Ethyl benzoate	186.1	46.5	53.5
<i>o</i> -Bromotoluene	166.8	25	75
Dibutyl ether	139.5	6.4	93.6

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Alcohol	Other component
1,2-Ethanediol (<i>continued</i>)			
Methoxybenzene	150.5	10.5	89.5
Diphenyl ether	193.1	60	40
Benzyl phenyl ether	195.5	87	13
Acetophenone	185.7	52	48
2,4-Dimethylaniline	188.6	47	53
<i>N,N</i> -Dimethylaniline	175.9	33.5	66.5
<i>m</i> -Toluidine	188.6	42	58
2,4,6-Trimethylpyridine	170.5	9.7	90.3
Quinoline	196.4	79.5	20.5
Tetrachloroethylene	119.1	94	6
1,2-Dibromoethane	129.8	4	96
Chlorobenzene	130.1	94.4	5.6
α -Chlorotoluene	167.0	30	70
Nitrobenzene	185.9	59	41
<i>o</i> -Nitrotoluene	188.5	48.5	51.5
1,2-Ethanediol monoacetate			
Indene	180.0	20	80
1-Octanol	189.5	71	29
Phenol	197.5	65	35
<i>o</i> -Cresol	199.5	51	49
<i>m</i> -Cresol	206.5	31	69
<i>p</i> -Cresol	206.0	33	67
Dipentyl ether	180.8	42	58
Diisopentyl ether	170.2	28	72
<i>m</i> -Bromotoluene	182.0	32	68
<i>D. Binary azeotropes containing ketones</i>			
System	BP of azeotrope, °C	Composition, wt %	
		Ketone	Other component
Acetone			
Cyclopentane	41.0	36	64
Pentane	32.5	20	80
Cyclohexane	53.0	67.5	32.5
Hexane	49.8	59	41

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Ketone	Other component
Acetone (<i>continued</i>)			
Heptane	55.9	89.5	10.5
Diethylamine	51.4	38.2	61.8
Methyl acetate	55.8	48.3	51.7
Diisopropyl ether	54.2	61	39
Chloroform	64.4	78.1	21.9
Carbon tetrachloride	56.1	11.5	88.5
Carbon disulfide	39.3	67	33
Ethylene sulfide	51.5	57	43
2-Butanone			
Cyclohexane	71.8	40	60
Hexane	64.2	28.6	71.4
Heptane	77.0	70	30
2,5-Dimethylhexane	79.0	95	5
Benzene	78.33	44	56
2-Methyl-2-propanol	78.7	69	31
Butylamine	74.0	35	65
Ethyl acetate	77.1	11.8	88.2
Methyl propionate	79.0	60	40
Butyl nitrite	76.7	30	70
1-Chlorobutane	77.0	38	62
Fluorobenzene	79.3	75	25

E. Miscellaneous binary azeotropes

System	BP of azeotrope, °C	Composition, wt %	
		Solvent	Other component
Solvent: acetamide			
Dipentene	169.2	18	82
Biphenyl	213.0	50.5	49.5
Diphenylmethane	215.2	56.5	43.5
1,2-Diphenylethane	218.2	68	32
<i>o</i> -Xylene	142.6	11	89
<i>m</i> -Xylene	138.4	10	90
<i>p</i> -Xylene	137.8	8	92
Styrene	144	12	88
4-Isopropyl-1-methylbenzene	170.5	19	81

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Solvent	Other component
Solvent: acetamide (<i>continued</i>)			
Naphthalene	199.6	27	73
1-Methylnaphthalene	209.8	43.8	56.2
2-Methylnaphthalene	208.3	40	60
Indene	177.2	17.5	82.5
Acenaphthene	217.1	64.2	35.8
Camphene	155.5	12	88
Camphor	199.8	23	77
Benzaldehyde	178.6	6.5	93.5
3,4-Dimethylphenol	221.1	96	4
2-Methoxy-4-(2-propenyl)-phenol	220.8	88	12
<i>N</i> -Methylaniline	193.8	14	86
<i>N</i> -Ethylaniline	199.0	18	82
<i>N,N</i> -Diethylaniline	198.1	24	76
Diphenyl ether	214.6	52	48
Safrole	208.8	32	68
Tetrachloroethylene	120.5	97.4	2.6
Solvent: aniline			
Nonane	149.2	13.5	86.5
Decane	167.3	36	64
Undecane	175.3	57.5	42.5
Dodecane	180.4	71.5	28.5
Tridecane	182.9	86.2	13.8
Tetradecane	183.9	95.2	4.8
Butylbenzene	177.8	46	54
1,2,4-Trimethylbenzene	168.6	13.5	86.5
1,3,5-Trimethylbenzene	164.3	12.0	88.0
Indene	179.8	41.5	58.5
1-Octanol	183.9	83	17
<i>o</i> -Cresol	191.3	8	92
Dipentyl ether	177.5	55	45
Diisopentyl ether	169.3	28	72
Hexachloroethane	176.8	66	34
Solvent: pyridine			
Heptane	95.6	25.3	74.7
Octane	109.5	56.1	43.9
Nonane	115.1	89.9	10.1
Toluene	110.1	22.2	77.8
Phenol	183.1	13.1	86.9
Piperidine	106.1	8	92

TABLE 4.7 Binary Azeotropic (Constant Boiling) Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %	
		Solvent	Other component
Solvent: thiophene			
Methylcyclopentane	71.5	14	86
Cyclohexane	77.9	41.2	58.8
Hexane	68.5	11.2	88.8
Heptane	83.1	83.2	16.8
2,3-Dimethylpentane	80.9	64	36
2,4-Dimethylpentane	76.6	42.7	57.3
Solvent: benzene			
Methylcyclopentane	71.7	16	84
Cyclohexene	78.9	64.7	35.3
Cyclohexane	77.6	51.9	48.1
Hexane	68.5	4.7	95.3
Heptane	80.1	99.3	0.7
2,2-Dimethylpentane	75.9	46.3	53.7
2,3-Dimethylpentane	79.4	78.8	21.2
2,4-Dimethylpentane	75.2	48.3	51.7
2,2,4-Trimethylpentane	80.1	97.7	2.3
Solvent: bis(2-hydroxyethyl) ether			
Biphenyl	232.7	48	52
Diphenylmethane	236.0	52	48
1,3,5-Trimethylbenzene	210.0	22	78
Naphthalene	212.6	22	78
1-Methylnaphthalene	277.0	45	55
2-Methylnaphthalene	225.5	39	61
Acenaphthene	239.6	62	38
Fluorene	243.0	80	20
Benzyl acetate	214.9	7	93
Bornyl acetate	223.0	18	82
Ethyl fumarate	217.1	10	90
Dimethyl <i>o</i> -phthalate	245.4	96.3	3.7
Methyl salicylate	220.6	15	85
2-Hydroxy-1-isopropyl-4-methylbenzene	232.3	13	87
1,2-Dihydroxybenzene	259.5	46	54
Safrole	225.5	33	67
Isosafrole	233.5	46	54
Benzyl phenyl ether	241.5	80	20
Nitrobenzene	210.0	10	90
<i>m</i> -Nitrotoluene	224.2	25	75
<i>o</i> -Nitrophenol	216.0	10.5	89.5
Quinoline	233.6	29	71
<i>p</i> -Dibromobenzene	212.9	13	87

TABLE 4.8 Ternary Azeotropic Mixtures
A. Ternary azeotropes containing water and alcohols

System	BP of azeotrope, °C	Composition, wt %		
		Water	Alcohol	Other component
Methanol				
Chloroform	52.3	1.3	8.2	90.5
2-Methyl-1,3-butadiene	30.2	0.6	5.4	94.0
Methyl chloroacetate	67.9	6.3	81.2	13.5
Ethanol				
Acetonitrile	72.9	1	55	44
Acrylonitrile	69.5	8.7	20.3	71.0
Benzene	64.9	7.4	18.5	74.1
Butylamine	81.8	7.5	42.5	50.0
Butyl methyl ether	62	6.3	8.6	85.1
Carbon disulfide	41.3	1.6	5.0	93.4
Carbon tetrachloride	62	4.5	10.0	85.5
Chloroform	55.3	2.3	3.5	94.2
Crotonaldehyde	78.0	4.8	87.9	7.3
Cyclohexane	62.6	4.8	19.7	75.5
1,2-Dichloroethane	66.7	5	17	78
1,1-Diethoxyethane	77.8	11.4	27.6	61.0
Diethoxymethane	73.2	12.1	18.4	69.5
Ethyl acetate	70.2	9.0	8.4	82.6
Heptane	68.8	6.1	33.0	60.9
Hexane	56.0	3	12	85
Toluene	74.4	12	37	51
Trichloroethylene	67.0	5.5	16.1	78.4
Triethylamine	74.7	9	13	78
1-Propanol				
Benzene	67	7.6	10.1	82.3
Carbon tetrachloride	65.4	5	11	84
Cyclohexane	66.6	8.5	10.0	81.5
1,1-Dipropoxyethane	87.6	27.4	51.6	21.0
Dipropoxymethane	86.4	8.0	44.8	47.2
Dipropyl ether	74.8	11.7	20.2	68.1
3-Pentanone	81.2	20	20	60
Propyl acetate	82.5	17.0	10.0	73.0
Propyl formate	70.8	13	5	82
Tetrachloroethylene	81.2	12.5	20.7	66.8
2-Propanol				
Benzene	66.5	7.5	18.7	73.8
Butylamine	83	12.5	40.5	47.0

TABLE 4.8 Ternary Azeotropic Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt %		
		Water	Alcohol	Other component
2-Propanol (<i>continued</i>)				
Cyclohexane	64.3	7.5	18.5	74.0
Toluene	76.3	13.1	38.2	48.7
Trichloroethylene	69.4	7	20	73
1-Butanol				
Butyl acetate	89.4	37.3	27.4	35.3
Butyl formate	83.6	21.3	10.0	68.7
Dibutyl ether	90.6	29.9	34.6	35.5
Heptane	78.1	41.4	7.6	51.0
Hexane	61.5	19.2	2.9	77.9
Nonane	90.0	69.9	18.3	11.8
Octane	86.1	60.0	14.6	25.4
2-Butanol				
Carbon tetrachloride	65	4.05	4.95	91.00
Cyclohexane	69.7	8.9	10.8	80.3
Isooctane	76.3	9	19	72
2-Methyl-1-propanol				
Isobutyl acetate	86.8	30.4	23.1	46.5
Isobutyl formate	80.2	17.3	6.7	76.0
Toluene	81.3	17.9	16.4	65.7
2-Methyl-2-propanol				
Benzene	67.3	8.1	21.4	70.5
Carbon tetrachloride	64.7	3.1	11.9	85.0
Cyclohexane	65.0	8	21	71
3-Methyl-1-butanol				
Isopentyl acetate	93.6	44.8	31.2	24.0
Isopentyl formate	89.8	32.4	19.6	48.0
Allyl alcohol				
Benzene	68.2	8.6	9.2	82.2
Carbon tetrachloride	65.2	5	11	84
Cyclohexane	66.2	8	11	81
Hexane	59.7	8.5	5.1	86.4

TABLE 4.8 Ternary Azeotropic Mixtures (*continued*)**B. Other ternary azeotropes**

System	BP of azeotrope, °C	Composition, wt %	System	BP of azeotrope, °C	Composition, wt %
Water	32.5	0.4	Water	71.4	7.9
Acetone		7.6	Nitromethane		29.7
2-Methyl-1,3-butadiene		92.0	Heptane		62.4
Water	66	8.2	Water	80.7	17.4
Acetonitrile		23.3	Nitromethane		58.3
Benzene		68.5	Nonane		24.3
Water	67	6.4	Water	77.4	12.4
Acetonitrile		20.5	Nitromethane		44.3
Trichloroethylene		73.1	Octane		43.3
Water	68.6	3.5	Water	33.1	2.1
Acetonitrile		9.6	Nitromethane		6.5
Triethylamine		86.9	Pentane		91.4
Water	63.6	5	Water	82.8	20.6
2-Butanone		35	Nitromethane		73.3
Cyclohexane		60	Undecane		6.1
Water	55.0	4	Water	93.5	40.5
Butyraldehyde		21	Pyridine		54.5
Hexane		75	Dodecane		5.0
Water	107.6	21.3	Water	93.1	38.5
Formic acid		76.3	Pyridine		51.0
Isopentanoic acid		2.4	Undecane		10.5
Water	107.0	15.5	Water	92.3	35.5
Formic acid		66.8	Pyridine		45.5
Isobutyric acid		17.7	Decane		19.0

Water	107.6	19.5
Formic acid		75.9
Butyric acid		4.6
Water	107.2	18.6
Formic acid		71.9
Propionic acid		9.5
Water	105	11.0
Hydrogen bromide		10.4
Chlorobenzene		78.6
Water	96.9	20.2
Hydrogen chloride		5.3
Chlorobenzene		74.5
Water	107.3	64.8
Hydrogen chloride		15.8
Phenol		19.4
Water	116.1	54
Hydrogen fluoride		10
Fluorosilic acid		36
Water	75.1	11.5
Nitroethane		75.1
Heptane		64.0
Water	59.5	8.4
Nitroethane		9.3
Hexane		82.3
Water	82.4	19.1
Nitromethane		68.1
Decane		12.8
Water	83.1	21.5
Nitromethane		75.3
Dodecane		3.2

Water	90.5	30.5
Pyridine		37.0
Nonane		32.5
Water	86.7	22.4
Pyridine		25.5
Octane		52.0
Water	78.6	14.0
Pyridine		15.5
Heptane		70.5
Acetic acid	134.4	23
Pyridine		55
Acetic anhydride		22
Acetic acid	134.1	31.4
Pyridine		38.2
Decane		30.4
Acetic acid	129.1	13.5
Pyridine		25.2
Ethylbenzene		61.3
Acetic acid	98.5	3.4
Pyridine		10.6
Heptane		86.0
Acetic acid	128.0	20.7
Pyridine		29.4
Nonane		49.9
Acetic acid	115.7	10.4
Pyridine		20.1
Octane		69.5
Acetic acid	132.2	17.7
Pyridine		30.5
<i>o</i> -Xylene		51.8

TABLE 4.8 Ternary Azeotropic Mixtures (*continued*)

System	BP of azeotrope, °C	Composition, wt%	System	BP of azeotrope, °C	Composition, wt%
Acetic acid	129.2	10.2	Methanol	47.4	14.6
Pyridine		22.5	Methyl acetate		36.8
<i>p</i> -Xylene		67.3	Hexane		48.6
Acetic acid	163.0	75.0	Ethanol	63.2	10.4
2,6-Dimethylpyridine		13.8	Acetone		24.3
Undecane		11.2	Chloroform		65.3
Acetic acid	147.0	12.6	Ethanol	70.1	8
2,6-Dimethylpyridine		74.3	Acetonitrile		34
Decane		13.1	Triethylamine		58
Acetic acid	141.3	19.9	Ethanol	64.7	29.6
2-Methylpyridine		46.8	Benzene		12.8
Decane		33.3	Cyclohexane		57.6
Acetic acid	135.0	12.8	Ethanol	57.3	9.5
2-Methylpyridine		38.4	Chloroform		56.1
Nonane		48.8	Hexane		34.4
Acetic acid	121.3	3.6	1-Propanol	73.8	15.5
2-Methylpyridine		24.8	Benzene		30.4
Octane		71.6	Cyclohexane		54.2
Acetic acid	77.2	7.6	2-Propanol	69.1	31.1
Benzene		34.4	Benzene		15.0
Cyclohexane		58.0	Cyclohexane		53.9
Acetic acid	132	15	1-Butanol	77.4	4
2-Methyl-1-butanol		54	Benzene		48
Isopentyl acetate		31	Cyclohexane		48
Propionic acid	149.3	29.5	1-Butanol	108.7	11.9
2-Methylpyridine		32.0	Pyridine		20.7
Decane		38.5	Toluene		76.4

Propionic acid	140.1	16.5	1,2-Ethanediol	185.0	8.7
2-Methylpyridine		21.5	Phenol		74.6
Nonane		42.0	2,6-Dimethylpyridine		16.7
Propionic acid	123.7	4.5	1,2-Ethanediol	185.1	5.9
2-Methylpyridine		10.5	Phenol		79.1
Octane		85.0	2-Methylpyridine		15.0
Propionic acid	153.4	43.0	1,2-Ethanediol	186.4	15.9
2-Methylpyridine		40.0	Phenol		67.7
Undecane		17.0	3-Methylpyridine		16.4
Propionic acid	147.1	55.5	1,2-Ethanediol	188.6	29.5
Pyridine		26.4	Phenol		54.8
Undecane		18.1	2,4,6-Trimethylpyridine		15.7
Methanol	57.5	23	Acetone	60.8	3.6
Acetone		30	Chloroform		68.8
Chloroform		47	Hexane		27.6
Methanol	47	14.6	Acetone	49.7	51.1
Acetone		30.8	Methyl acetate		5.6
Hexane		59.6	Hexane		43.3
Methanol	53.7	17.4	Chloroform	62.0	79.7
Acetone		5.8	Ethyl formate		5.3
Methyl acetate		76.8	2-Bromopropane		15.7
Methanol	50.8	17.8	1,4-Dioxane	101.8	44.3
Methyl acetate		48.6	2-Methyl-1-propanol		26.7
Cyclohexane		33.6	Toluene		29.0

FREEZING POINTS

Crystalline organic compounds typically have a characteristic melting point. In some cases, a compound may have more than one arrangement in the crystal and such polymorphs will exhibit differences in melting behavior. For the most part, however, the melting point of a compound is characteristic and invariant for a pure sample. When contaminated by a second substance, however, the melting (or freezing) point is typically lowered.

A classical test used to determine if two samples that have the same melting point are identical is to intimately mix them and record the melting point of the mixture. If the melting point of the blend is identical to that of each individual compound prior to mixing, the two substances are judged to be identical. When the two compounds are not the same, the melting point of the mixture is typically lowered and broadened.

The melting or freezing point depression can be used to determine an approximate molecular weight for a given substance. The cryoscopic constant K_f gives the depression of the melting point ΔT (in degrees Celsius) produced when 1 mol of solute is dissolved in 1000 g of a solvent. It is applicable only to dilute solutions for which the number of moles of solute is negligible in comparison with the number of moles of solvent. Because camphor is conveniently available and has a large K_f value, it is often used in this application. A known amount of the substance whose molecular weight is to be determined (the solute) is mixed with a larger amount of camphor (the solvent). Melting the mixture permits intimate mixing. The lowering or depression of the freezing point is then used to calculate the molecular weight from the following equation

$$M_2 = \frac{1000w_2K_f}{w_1\Delta T}$$

where M_2 is the molecular weight to be determined of the solute, w_1 is the exact weight of the solvent, w_2 is the exact weight of the added compound of unknown molecular mass, ΔT is the change in temperature, and K_f is the cryoscopic constant given in the Table 4.9A.

In Table 4.9A, a range of compounds and their cryoscopic constants are recorded. All of the same data are included in Table 4.9B but they are rearranged in order of increasing melting point at the left and decreasing K_f at the right.

TABLE 4.9A Molecular Lowering of the Melting of Freezing Point

Compound	K_f	MP	Compound	K_f	MP
Acetamide	4.04	80.1	Camphene	31.08	51–52
Acetic acid	3.90	16.63	Camphorquinone	45.7	199
Acetone	2.40	–95.35	D-(+)-Camphor	39.7	178.8
Ammonia	0.957	–77.75	Carbon tetrachloride	29.8	–22.9
Aniline	5.87	–5.98	<i>o</i> -Cresol	5.60	30.9
Antimony(III) chloride	17.95	73.4	<i>p</i> -Cresol	6.96	34.8
Benzene	5.12	5.53	Cyclohexane	20.0	6.5
Benzonitrile	5.34	–12.75	Cyclohexanol	39.3	25.2
Benzophenone	9.8	48.1	Cyclohexylcyclohexane	14.52	3–4
Bicyclohexane	14.52	3–4	Cyclopentadecanone	21.3	64–66
Biphenyl	8.0	68.8	Z-Decahydronaphthalene	19.47	–43.0
Borneol	35.8	204	<i>E</i> -Decahydronaphthalene	20.81	–30.4
Bornylamine	40.6	163	Dibenz[<i>de,kl</i>]anthracene	25.7	273–274
Butanedinitrile	18.26	57.9	Dibenzyl ether	6.27	3.5

TABLE 4.9A Molecular Lowering of the Melting of Freezing Point (*continued*)

Compound	K_f	MP	Compound	K_f	MP
1,2-Dibromoethane	12.5	10.0	Nitrobenzene	6.852	5.8
Diethyl ether	1.79	−116.3	Octadecanoic acid	4.50	70
1,2-Dimethoxybenzene	6.38	22.5	2-Oxohexa-		
<i>N, N</i> -Dimethylacetamide	4.46	−20.0	methyleneimine	7.30	69.2
2,2-Dimethyl-1-propanol	11.0	52–54	Phenol	7.40	40.9
Dimethyl sulfoxide	4.07	18.5	Pyridine	4.75	−41.6
1,4-Dioxane	4.63	11.7	Quinoline	1.95	−14.9
Diphenylamine	8.60	53–54	Succinonitrile	18.26	46–48
Diphenyl ether	7.88	26.9	Sulfuric acid	1.86	10.38
1,2-Ethanediamine	2.43	8.5	1,1,2,2,-Tetrabro-		
Ethoxybenzene	7.15	−29.5	moethane	21.7	0.0
Formamide	3.85	2.6	1,1,2,2,-Tetrachloro1,2-	37.7	26.0
Formic acid	2.77	8.5	difluoroethane		
Glycerol	3.3–3.7	18.18	Tetramethylene sulfone	64.1	27.6
Hexamethylphos-			<i>p</i> -Toluidine	5.372	43.8
phoramide	6.93	7.2	Tribromomethane	14.4	8.1
<i>N</i> -Methylacetamide	6.65	30.6	1,3,3-Trimethyl-2-	6.7	1–2
2-Methyl-2-butanol	10.4	−9.0	oxabicyclo[2.2.2]octane		
Methylcyclohexane	14.13	−126.6	Triphenylmethane	12.45	93.4
Methyl Z-9-octadecenoate	3.4	19.9	Water	1.86	0.000
2-Methyl -2-propanol	8.37	25.8	<i>p</i> -Xylene	4.3	13.3
Naphthalene	6.94	80.2			

The same data are presented in Table 4.9B but the information is rearranged at the left in order of increasing melting point and at the right in order of decreasing K_f .

TABLE 4.9B Molecular Lowering of the Melting of Freezing Point

Compound	K_f	MP	Compound	K_f	MP
Methylcyclohexane	14.13	−126.6	Tetramethylene sulfone	64.1	27.6
Diethyl ether	1.79	−116.3	Camphorquinone	45.7	199
Acetone	2.4	−95.35	Bornylamine	40.6	163
Ammonia	0.957	−77.75	D-(+)-Camphor	39.7	178.8
Z-Decahydronaphthalene	19.47	−43	Cyclohexanol	39.3	25.2
Pyridine	4.75	−41.6	1,1,2,2-Tetrachloro-1,2-	37.7	26
<i>E</i> -Decahydronaphthalene	20.81	−30.4	difluoroethane		
Ethoxybenzene	7.15	−29.5	Borneol	35.8	204
Carbon tetrachloride	29.8	−22.9	Camphene	31.08	51–52
<i>N, N</i> -Dimethylacetamide	4.46	−20	Carbon tetrachloride	29.8	−22.9
Quinoline	1.95	−14.9	Dibenz[<i>de,kl</i>]anthracene	25.7	273–274
Benzonitrile	5.34	−12.75	1,1,2,2-Tetrabromoethane	21.7	0
2-Methyl-2-butanol	10.4	−9	Cyclopentadecanone	21.3	64–66
Aniline	5.87	−5.98	<i>E</i> -Decahydronaphthalene	20.81	−30.4
1,1,2,2-Tetrabromoethane	21.7	0	Cyclohexane	20	6.5
Water	1.86	0	Z-Decahydronaphthalene	19.47	−43
1,3,3-Trimethyl-2-	6.7	1–2	Succinonitrile	18.26	46–48
oxabicyclo[2.2.2]octane			Butanedinitrile	18.26	57.9

TABLE 4.9B Molecular Lowering of the Melting of Freezing Point (*continued*)

Compound	K_f	MP	Compound	K_f	MP
Formamide	3.85	2.6	Antimony(III) chloride	17.95	73.4
Bicyclohexane	14.52	3–4	Bicyclohexane	14.52	3–4
Dibenzyl ether	6.27	3.5	Cyclohexylcyclohexane	14.52	6.5
Benzene	5.12	5.53	Tri bromomethane	14.4	8.1
Nitrobenzene	6.852	5.8	Methylcyclohexane	14.13	–126.6
Cyclohexane	20	6.5	1,2-Dibromoethane	12.5	10
Cyclohexylcyclohexane	14.52	6.5	Triphenylmethane	12.45	93.4
Hexamethyl- phosphoramide	6.93	7.2	2,2-Dimethyl-1-propanol	11	52–54
Tribromomethane	14.4	8.1	2-Methyl-2-butanol	10.4	–9
1,2-Ethanediamine	2.43	8.5	Benzophenone	9.8	48.1
Formic acid	2.77	8.5	Diphenylamine	8.6	53–54
1,2-Dibromoethane	12.5	10	2-Methyl-2-propanol	8.37	25.8
Sulfuric acid	1.86	10.38	Biphenyl	8	68.8
1,4-Dioxane	4.63	11.7	Diphenyl ether	7.88	26.9
<i>p</i> -Xylene	4.3	13.3	Phenol	7.4	40.9
Acetic acid	3.9	16.63	2-Oxo hexamethylene imine	7.3	69.2
Glycerol	3.3–3.7	18.18	Ethoxybenzene	7.15	–29.5
Dimethyl sulfoxide	4.07	18.5	<i>p</i> -Cresol	6.96	34.8
Methyl Z-9-octadecenoate	3.4	19.9	Naphthalene	6.94	80.2
1,2-Dimethoxybenzene	6.38	22.5	Hexamethylphosphoramide	6.93	7.2
Cyclohexanol	39.3	25.2	Nitrobenzene	6.852	5.8
2-Methyl-2-propanol	8.37	25.8	1,3,3-Trimethyl-2- oxabicyclo[2.2.2]octane	6.7	1–2
1,1,2,2-Tetrachloro-1,2- difluoroethane	37.7	26	<i>N</i> -Methylacetamide	6.65	30.6
Diphenyl ether	7.88	26.9	1,2-Dimethoxybenzene	6.38	22.5
Tetramethylene sulfone	64.1	27.6	Dibenzyl ether	6.27	3.5
<i>N</i> -Methylacetamide	6.65	30.6	Aniline	5.87	–5.98
<i>o</i> -Cresol	5.6	30.9	<i>o</i> -Cresol	5.6	30.9
<i>p</i> -Cresol	6.96	34.8	<i>p</i> -Toluidine	5.372	43.8
Phenol	7.4	40.9	Benzonitrile	5.34	–12.75
<i>p</i> -Toluidine	5.372	43.8	Benzene	5.12	5.53
Succinonitrile	18.26	46–48	Pyridine	4.75	–41.6
Benzophenone	9.8	48.1	1,4-Dioxane	4.63	11.7
Camphene	31.08	51–52	Octadecanoic acid	4.5	70
2,2-Dimethyl-1-propanol	11	52–54	<i>N, N</i> -Dimethylacetamide	4.46	–20
Diphenylamine	8.6	53–54	<i>p</i> -Xylene	4.3	13.3
Butanedinitrile	18.26	57.9	Dimethyl sulfoxide	4.07	18.5
Cyclopentadecanone	21.3	64–66	Acetamide	4.04	80.1
Biphenyl	8	68.8	Acetic acid	3.9	16.63
2-Oxo hexamethylene imine	7.3	69.2	Formamide	3.85	2.6
Octadecanoic acid	4.5	70	Glycerol	3.3–3.7	18.18
Antimony(III) chloride	17.95	73.4	Methyl Z-9-octadecenoate	3.4	19.9
Acetamide	4.04	80.1	Formic acid	2.77	8.5
Naphthalene	6.94	80.2	1,2-Ethanediamine	2.43	8.5
Triphenylmethane	12.45	93.4	Acetone	2.4	–95.35
Bornylamine	40.6	163	Quinoline	1.95	–14.9
D-(+)-Camphor	39.7	178.8	Water	1.86	0
Camphorquinone	45.7	199	Sulfuric acid	1.86	10.38
Borneol	35.8	204	Diethyl ether	1.79	–116.3
Dibenz[<i>de,kl</i>] anthracene	25.7	273–274	Ammonia	0.957	–77.75

VISCOSITY, DIELECTRIC CONSTANT, DIPOLE MOMENT, SURFACE TENSION, AND REFRACTIVE INDEX

Several additional physical properties are summarized in Table 4.10. These are viscosity, dielectric constant, dipole moment, and surface tension for selected common organic compounds.

Viscosity

Viscosity may be thought of as a fluid's resistance to flow or internal friction. It is characterized by the property called viscosity, which is designated η (eta). A fluid passing through a tube will flow more freely if its viscosity is low and more slowly if it is more viscous. Viscosity is given in Table 4.10 in units of milliNewton-second-meter⁻² or mN·s·m⁻². In fluid mechanics, the unit "poise" is equal to a force of 1 dyne·cm⁻² for two fluids passing each other at a rate of 1 cm·s⁻¹. Viscosity is typically greater at lower temperatures; temperatures (in °C) are given in parentheses in the table.

Dielectric Constant

The dielectric constant (or relative permittivity) is usually expressed using the symbol ϵ . The dielectric ϵ is defined as the ratio of electric fields E_0/E for a vacuum and a substance placed between the plates of a capacitor. The dielectric constant of a vacuum is 1 and substances that can orient to greater or lesser extents in the applied field will have higher dielectric constants. The dielectric constant of heptane at 20°C is ~1.9. Acetonitrile, CH₃C≡N:, has a dielectric constant at 20°C of 37.5. The dielectric constant for water is near 80.

The choice of a solvent for a particular reaction will usually depend on more than one variable. These include the liquid temperature range, the dielectric constant, and whether or not the solvent is reactive in the chemical reaction. The most important consideration in the latter context is often the presence of an easily transferred proton. Certain solvents, such as acetone, are considered aprotic but may transfer a proton under basic conditions. Thus the designations given below are general and approximate. They are intended to guide the reader to the more detailed information contained in the full tables.

Common Solvents Listed in Order of Increasing Dielectric Constant (Ascending Polarity)

Aprotic Solvents		Protic Solvents
Dielectric constants < 15	Dielectric constants > 15	Dielectric range 6–80
carbon disulfide	acetone	acetic acid
carbon tetrachloride	benzonitrile	trifluoroacetic acid
tetrachloroethylene	hexamethylphosphoramide	phenols
1,2-dichloroethylene	<i>N</i> -methylpyrrolidone	butanols
chlorobenzene	nitrobenzene	propanols
dichloromethane	nitromethane	ethanol
chloroform	<i>N,N</i> -dimethylformamide (DMF)	2,2,2-trifluoroethanol
1,4-dioxane	acetonitrile	methanol
diphenyl ether	dimethyl sulfoxide (DMSO)	various glycols
diethyl ether		water

Aprotic Solvents		Protic Solvents
Dielectric constants < 15	Dielectric constants > 15	Dielectric range 6–80
tetrahydrofuran (THF) 1,2-dimethoxyethane (DME) ethyl acetate butyl acetate <i>N,N</i> -dimethylaniline pyridine		

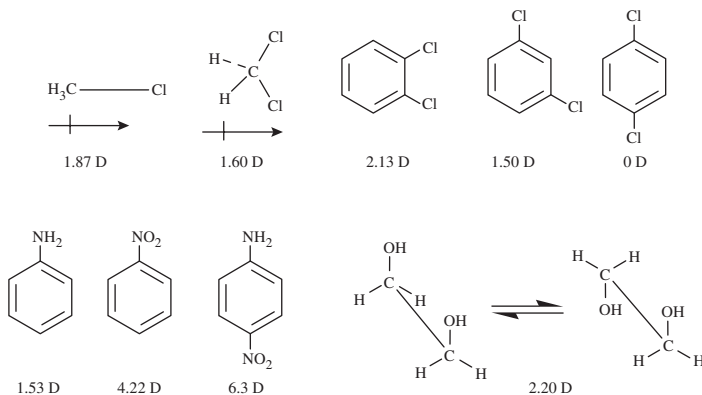
Dipole Moment

The dipole moment of a molecule is the vectorial sum of the individual dipoles within it. Bond dipoles are usually represented using the symbol μ and are expressed in units of Debye. The dipoles result from charge separation. The carbon–carbon bond in ethane, $\text{H}_3\text{C}-\text{CH}_3$ is symmetrical and not expected to have a dipole moment. The carbon–oxygen bond of methanol (CH_3OH), on the other hand, links two elements of differing electronegativity and is expected to have a significant molecular dipole. Methanol's molecular dipole is ~ 1.7 whereas, for ethane, it is 0.

Experimentally, the molecular dipole can be measured. Individual bond dipoles cannot be measured but they have been inferred from experimental data for a variety of compounds. Estimates of the molecular dipole can be made by vector addition of individual moments. Such estimates (calculations) are indicative but may differ significantly from the measured values. The latter are recorded in Table 4.10.

Four examples of dipole moments are instructive. First, the dipoles for chloromethane and dichloromethane are 1.87 D and 1.60 D, respectively. Although two chlorine–carbon bonds are present in the latter, the dipole is not along either but rather bisects the angle between them. This is illustrated schematically using the stylized arrow with its positive end in the form of a cross. The orientation question is shown clearly in the rigid dichlorobenzene framework. The dipole is 2.13 D for the *ortho*-isomer and 0 D when the dipoles exactly oppose each other.

The orientation of dipoles can be assessed by comparing otherwise identical molecules. For example, amino is electron releasing and nitro is electron withdrawing. The molecular dipoles (1.53 D for aniline and 4.22 D for nitrobenzene) add to give an overall molecular dipole of 6.3 D for 4-nitroaniline. The importance of two polar C–O bonds should be large



if they are added and small if they oppose. The dynamics of the system must be taken into account for structures such as 1,2-dihydroxyethane (ethylene glycol), which is illustrated in the eclipsed and staggered conformers.

Surface Tension

The surface tension is the force that acts on the surface of a liquid that tends to minimize the surface area of the liquid. Surface tension is also sometimes referred to as interfacial force or interfacial tension. The property of surface tension is temperature dependent. For the majority of compounds the dependence of the surface tension γ on the temperature can be given as

$$\gamma = a - bt$$

where a and b are constants and t is the temperature in $^{\circ}\text{C}$.

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances

States:	[g], gas	Solvents:	[B], benzene,	C_6H_6
	[lq], liquid		[C], carbon tetrachloride,	CCl_4
			[D], 1,4-dioxane,	$\text{C}_4\text{H}_8\text{O}_2$
			[H], hexane,	C_6H_{14}
			[cH], cyclohexane,	C_6H_{12}

The temperature in degrees Celsius at which the viscosity, dielectric constant, dipole moment, and surface tension of a substance were measured is shown in this table in parentheses after the value. The solvent used or the physical state of the substance are also shown in parentheses after the temperature in square brackets, for example, [g] or [b]

Alternate names for entries are listed in Table 1-14 at the bottom of each double page.

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				a	b
Acetaldehyde	0.280 (0) 0.256 (10) 0.22 (20)	21.8(10) 21.1 (21)	2.71 [g]	23.90	0.1360
Acetaldoxime	1.415 (20)	3 (23)	0.830 (20) [lq] 0.90 (25) [B]	30.1 (35)	
Acetamide	1.32 (105) 1.06 (120)	59.2 (83) 60.6 (94)	3.90 (25) [B] 2.44 (30) [B]	47.66	0.102 1
Acetanilide	2.22 (120) 1.90 (130)	3.65 (25) [B]	46.21	0.091 2	
Acetic acid	1.232 (20) 0.796 (50)	6.15 (20) 6.29 (40)	1.76[g] 1.92 (20) [B]	29.58	0.009 4

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Acetic anhydride	0.907 (20) 0.699 (40)	23.3 (0) 21.2 (20)	2.8 [g] 3.15 (20) [B]	35.52	0.143 6
Acetone [lq]	0.391 (0) 0.318 (20)	20.7 (25) 17.6 (56)	2.77 (22) [B]	26.26	0.112
[g]	0.009 33 (100) 0.012 8 (225)	1.015 9 (100)	2.87		
Acetonitrile	0.397 (10) 0.329 (30)	37.5 (20) 26.6 (82)	3.97 [g] 3.47 (20) [B]	29.58	0.117 8
Acetophenone	2.015 (15) 1.511 (30)	17.39 (25) 8.64 (202)	2.96 (30) [B]	41.92	0.115 4
Acetyl bromide		16.2 (20)	2.45 (20) [B]		
Acetyl chloride [lq]		16.9 (2) 15.8 (22)	2.47 (20) [B]	26.7 (15)	
[g]		1.0217 (20)	2.71		
Acetylene [g]	0.010 2 (30) 0.012 6 (101)	1.001 34 (0)	0	3.42	0.193 5 [lq]
Acrylic acid	1.3 (20) 1.16 (25)			28.1 (30)	
Acrylonitrile	0.35 (20) 0.34 (25)	33.0 (20)	3.91 [g] 3.54 (25) [B]	29.58	0.117 8
Allyl acetate	0.207 (30)			28.73	0.118 6
Allylamine	0.375 (25)		1.3 (25) [B]	27.49	0.128 7
Allyl isothiocyanate		17.2 (18)	3.2 (20) [B]	36.76	0.107 4
2-Aminoethanol	30.85 (15) 19.35 (25)	37.72 (25)	2.59 (25) [D]	51.11	0.111 7
Aniline	5.30 (15) 4.40 (20) 3.18 (30)	6.89 (20) 5.93 (70)	1.53 (20) [B]	44.83	0.108 5
Benzaldehyde	1.321 (25)	19.7 (0) 17.8 (20) 3.8 (20)	2.77 (20) [lq] 1.2 (25) [B]	40.72	0.109 0
Benzaldehyde oxime (mp 30) (mp 128)			1.5 (25) [B]		
Benzene	0.649 (20) 0.566 (30) 0.395 (60)	2.292 (15) 2.274 (25) 1.002 8 [g]	0	28.88 (20)	27.56 (30)
Benzamide			3.42 (25) [B]	47.26	0.070 5
Benzenesulfonyl chloride			4.50 (20) [B]	45.48	0.111 7
Benzenethiol	1.239 (20) 1.144 (25)	4.38 (25)	1.13 (25) [lq] 1.19 (20) [B]	41.41	0.120 2

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Benzonitrile	1.447 (15) 1.111 (30)	26.5 (20) 24.0 (40)	4.40 [g] 3.9 (20) [B]	41.69	0.115 9
Benzophenone	4.79 (55) 1.38 (120)	14.60 (18) 11.4 (50)	3.09 (50) [lq] 2.98 (25) [B]	46.31	0.112 8
Benzoyl bromide	1.956 (20) 1.798 (25)	21.33 (20) 20.74 (25)	3.40 (20) [B]	45.85	0.139 7
Benzoyl chloride		29 (0) 23 (20)	3.16 (25) [B]	41.34	0.108 4
Benzyl acetate	1.399 (45)	5.1 (21)	1.80 (25) [B]		
Benzyl alcohol	5.58 (20) 4.65 (30) 3.01 (45)	13.0 (20) 9.5 (70)	1.67 (25) [B]	38.25	0.138 1
Benzylamine	1.59 (25)	5.5 (1) 4.6 (21)	1.15 (20) [lq] 1.38 (25) [B]	42.33	0.121 3
Benzyl benzoate	8.51 (25)	4.9 (20)	2.06 (30) [B]	48.07	0.106 5
Benzyl butyl <i>o</i> -phthalate	65 (20)				
Benzyl chloride	1.400 (20) 1.290 (25)	7.0 (13)	1.83 (20) [B]	39.92	0.122 7
Benzylethylamine		4.3 (20)			
Benzyl ethyl ether		3.9 (20)		32.83 (20)	29.97 (40)
Biphenyl		2.53 (75)	0	41.52	0.093 1
Bis(2-ethoxyethyl)ether			1.92 (25) [B]	29.74	0.117 6
Bis(2-hydroxyethyl)ether	38.0 (20) 30.0 (25)	31.69 (20)	2.31 (20) [B]	46.97	0.088 0
1,2-Bis(methoxyethoxy)-ethane	3.76 (20)				
Bis(2-methoxyethyl) ether	1.99 (20)		1.97 (25) [B]	32.47	0.116 4
DL-Bornyl acetate	0.981 (25)	4.6 (21)	1.89 (22)		
3-Bromoaniline	6.81(20) 3.70 (40)	13.0 (19)	2.67 (20) [B]		
4-Bromoaniline	1.81 (80)	7.06 (30)	2.88 (25) [B]		
Bromobenzene	1.196 (15) 0.985 (30)	5.40 (25)	1.70 [g] 1.50 (20) [lq]	38.14	0.116 0
1-Bromobutane	0.633 (20) 0.597 (25)	7.88 (−10) 7.07 (20)	2.17 [g] 2.04 (20) [lq]	28.71	0.112 6
DL-2-Bromobutane	1.434 (20)	8.64 (25)	2.22 [g] 2.14 (25) [lq] 2.15 (20) [B]	27.48	0.110 7
1-Bromo-2-chlorobenzene		6.80 (20)			
1-Bromo-3-chlorobenzene		4.58 (20)	1.52 (22) [B]		
1-Bromo-4-chlorobenzene			0.1 (25) [B]	40.03	0.100 2

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Bromochloro- methane	0.670 (20)	7.79	1.66 (25) [B]	33.32 (20)	
Bromocyclo- hexane	2.0 (25)	11 (−65) 7.9 (25)	1.08 (25) [lq] 2.3 (25) [B]	36.13	0.111 7
1-Bromodecane		4.75 (1) 4.44 (25)	2.08 (20) [lq] 1.90 (25) [lq]	31.26	0.085 6
Bromodichloro- methane			1.31 (25) [B]	35.11	0.129 4
1-Bromododecane		4.07 (25)	2.01 (25) [lq] 1.89 (25) [B]	32.58	0.088 2
Bromoethane	0.397 (20) 0.348 (30)	13.6 (−60) 9.39 (20)	2.03 [g] 2.04 (20) [lq]	26.52	0.115 9
1-Bromo-2- ethoxyethane				31.98	0.112 9
1-Bromo-2- ethoxypentane		6.45 (25)	2.32 (25) [B]		
2-Bromo-2- ethoxypentane		6.40 (25)	2.07 (25) [B]		
3-Bromo-3- ethoxypentane		8.24 (25)	2.15 (25) [B]		
Bromoethylene		4.78 (25)	1.42 [g]		
Bromoform	2.152 (15) 1.741 (30)	4.39 (20)	1.00 [g] 0.92 (25) [lq]	48.14	0.130 8
1-Bromoheptane		5.33 (25) 4.48 (90)	2.17 [g] 2.02 (20) [lq]	30.74	0.098 2
2-Bromoheptane		6.46 (22)	2.08 (20) [B]		
3-Bromoheptane		6.93 (22)	2.06 (20) [B]		
4-Bromoheptane		6.81 (22)	2.06 (20) [B]		
1-Bromohexa- decane		3.71 (25)	1.98 (20) [lq] 1.96 (25) [C]	33.37	0.086 1
1-Bromohexane		6.30 (1) 5.82 (25)	2.06 (20) [lq]	29.81	0.096 7
Bromomethane		9.82 (0) 1.006 8 (100) [g]	1.79 [g]	26.52	0.115 9
1-Bromo-3- methylbutane		8.04 (−56) 6.05 (20)	1.95 (20) [B]	28.10	0.099 6
2-Bromo-3- methylbutyric acid		6.5 (20)			
1-Bromo-2- methylpropane	0.643 (20) 0.518 (40) 3.26 (90)	7.70 (0) 7.2 (25)	1.92 (25) [lq] 1.99 (20) [B]	26.96	0.105 9
1-Bromonaph- thalene	5.99 (15) 3.20 (40)	5.83 (25) 5.12 (20)	1.29 (25) [lq]	46.44	0.101 8
1-Bromononane		5.42 (−20) 4.74 (25)	1.95 (25) [lq]	31.36	0.089 4

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
1-Bromooctane		6.35 (−50)	1.99 (20) [lq] 1.88 (25) [lq]	31.00	0.092 8
1-Bromopenta- decane		3.9 (20)			
1-Bromopentane		9.9 (−90) 6.32 (25)	2.21 [g] 2.09 (20) [lq]	29.51	0.104 9
<i>p</i> -Bromophenol				48.88	0.107 0
1-Bromopropane	0.539 (15) 0.459 (30)	8.09 (25)	2.17 [g] 3.16 (20) [lq]	28.30	0.121 8
2-Bromopropane	0.536 (15) 0.437 (30)	9.46 (25)	2.21 [g] 2.10 (25) [lq]	26.21	0.118 3
1-Bromotetra- decane		3.84 (25)	1.92 (20) [lq] 1.83 (25) [lq]	32.93	0.087 8
<i>o</i> -Bromotoluene	1.3 (25)	4.28 (58)	1.45 (20) [B]	36.62	0.099 8
<i>m</i> -Bromotoluene		5.36 (58)	1.77 (20) [B]		
<i>p</i> -Bromotoluene		5.49 (58)	1.95 (20) [B]	36.40	0.099 7
Bromotrifluoro- methane	0.15 (25)		0.65 [g]	4 (25)	
1-Bromoundecane		4.73 (−9)		31.94	0.086 1
Butane	0.007 39 (20) [g] 0.008 39 (60) [g]		0	14.87	0.120 6
1,3-Butanediol	130.3 (20) 89 (25)	28.8 (25)		37.8 (25)	
1,4-Butanediol	65–70 (25)	33 (15) 30 (30)	3.93 (20) [lq] 2.4 (15) [D]		
2,3-Butanediol	121 (25)			36 (25)	
Butanesulfonyl chloride			3.94 (25) [D]	37.33	0.097 7
1-Butanethiol	0.501 (20) 0.450 (30)	5.07 (25) 4.59 (50)	1.54 (25) [lq] or [B]	28.07	0.114 2
1,2,4-Butanetriol	1227 (25)				
1-Butanol	2.948 (20) 1.782 (40)	17.8 (20) 8.2 (118)	1.66 [g] 20 [B]	27.18	0.089 8
DL-2-Butanol	3.907 (20) 0.527 (100)	16.6 (25)	1.66 (30) [B]	23.47 (20)	22.62 (30)
2-Butanone	0.428 (20) 0.349 (40)	18.5 (20) 15.3 (60)	3.2 (30) [lq] 2.76 (25) [B]	26.77	0.112 2
2-Butanone oxime		3.4 (20)		31.89	0.102 2
1-Butene [g]	0.007 6 (20) 0.010 0 (120)	1.003 2 (20)	0.30	15.19	0.132 3[lq]
2-Butene			0.33 [g, <i>cis</i>] 0 [g, <i>trans</i>]	16.11	0.128 9
3-Butenenitrile		28.1 (20)	4.53 [g]	31.40	0.108 5
2-Butoxyethanol	3.15 (25) 1.51 (60)	9.30 (25)	2.08 (25) [B]	28.18	0.081 6
Butoxyethyne		6.62 (25)	2.05 (25) [lq]		

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
2-(2-Butoxyethoxy)ethanol	4.76 (25)			30.0 (25)	
1-Butoxy-2-propanol	2.55 (25)			26.5 (25)	
Butyl acetate	0.734 (20) 0.688 (25)	6.85 (−73) 5.01 (20)	1.86 (22) [B]	27.55	0.106 8
DL- <i>sec</i> -Butyl acetate				23.33 (22)	21.24 (42)
<i>tert</i> -Butyl acetate			1.91 (25) [B]	24.69	0.110 2
Butylamine	0.681 (20)	4.88 (20)	1.00 [g] 1.22 (20) [lq]	26.24	0.112 2
<i>sec</i> -Butylamine		4.4 (21)	1.28 (25) [B]	23.75	0.105 7
<i>tert</i> -Butylamine			1.29 (25) [B]	19.44	0.102 8
Butylbenzene	1.035 (20) 0.960 (25)	2.36 (20)	0.36 (20) [lq]	31.28	0.102 5
<i>sec</i> -Butylbenzene		2.36 (20)	0.37 (20) [lq]	30.48	0.097 9
<i>tert</i> -Butylbenzene		2.37 (20)	0.36 (20) [lq]	30.10	0.098 5
Butyl butyrate	0.84 (25)			27.65	0.096 5
Butyl decyl <i>o</i> -phthalate	55 (20)				
<i>N</i> -Butyldiethanolamine	55 (25)				
4- <i>tert</i> -Butyl-2,5-dimethylphenol	8.30 (80)				
4- <i>tert</i> -Butyl-2,6-dimethylphenol	2.72 (80)				
6- <i>tert</i> -Butyl-2,4-dimethylphenol	2.10 (80)				
6- <i>tert</i> -butyl-3,4-dimethylphenol	3.50 (80)				
<i>N</i> -Butylethanolamine	17.4 (25)				
Butyl ethyl ether	0.421 (20) 0.397 (25)		1.24	22.75	0.104 9
Butyl formate	0.691 (20) 0.940 (0)	2.43 (80)	2.08 (26) [lq] 2.03 (25) [B]	27.08	0.102 6
Butyl methyl ether			1.25 (25) [B]	22.17	0.105 7
2- <i>tert</i> -Butyl-4-methylphenol	2.55 (80)		1.31 (20) [B]		
Butyl nitrate		13 (20)	2.99 (20) [B]	30.35	0.112 6
2-(2- <i>sec</i> -Butylphenoxy)ethanol	65.1 (25)				
2-(4- <i>tert</i> -Butylphenoxy)ethanol	122.5 (25)				
Butyl propionate			1.79 (22) [B]	27.37	0.099 3

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
4- <i>tert</i> -Butyl- pyridine	1.495 (20)		2.87 (25) [C]	35.48	0.095 1
Butyl stearate	8.26 (25) 4.9 (50)	3.11 (30)	1.88 (24) [B]	33.0 (25)	32.7 (30)
Butyl vinyl ether	0.5 (20)		1.25 (25) [H]	21.99 (20)	
Butyraldehyde	0.455 (20) 0.367 (39)	13.4 (26)	2.45 (40) [Iq]	26.67	0.092 5
Butyric acid	1.540 (20) 0.980 (40)	2.97 (20)	1.65 (30) [B]	28.35	0.092 0
Butyric anhydride	1.615 (20) 1.486 (25)	13 (20)		28.93 (20)	28.44 (25)
4-Butyrolactone	1.75 (25)	39.1 (20)	4.12 (25) [B]		
Butyronitrile	0.624 (15) 0.515 (30)	20.3 (21)	4.07 [g] 3.6 (20) [B]	29.51	0.103 7
Camphor		11.35 (20)	2.91 (20) [B] 3.10 (25) [B]		
Carbon disulfide	0.363 (20)	3.0 (−112) 2.64 (20)	0 [g] 0.12 (20) [Iq]	35.29	0.148 4
Carbon tetra- chloride	0.965 (20) 0.793 (25)	2.24 (20) 2.23 (25)	0	29.49	0.122 4
Carbon tetra- fluoride	0.020 (25)	1.000 6 (25) [g]	0	14 (−73)	
Carvone		11 (22)	2.8 (15) [B]	36.54	0.092 0
Chloroacetic acid	3.15 (50) 1.92 (75)	20 (20) 12.3 (60)	2.31 (30) [B]	43.27	0.111 7
<i>o</i> -Chloroaniline	0.925 (25)	13.4 (25)	1.78 (20) [B]	43.41	0.090 4
<i>m</i> -Chloroaniline		13.4 (19)	2.68 (20) [B]		
<i>p</i> -Chloroaniline			2.99 (25) [B]	48.69	0.109 9
Chlorobenzene	0.799 (20) 0.631 (40)	5.71 (20) 4.2 (120)	1.72 [g] 1.56 (20) [Iq]	35.97	0.119 1
1-Chlorobutane	0.469 (15)	9.07 (−30) 7.39 (20)	2.13 [g] 2.0 (20) [B]	25.97	0.111 7
2-Chlorobutane	0.439 (15)	7.09 (30)	2.14 [g] 2.1 (20) [B]	24.40	0.111 8
Chlorocyclohexane		10.9 (−47) 7.6 (25)	2.2 (25) [B]	33.90	0.110 1
Chlorodifluoromethane	0.23 (25) 0.013 (25) [g]	6.11 (24)	1.4 [g]	8 (25)	
1-Chlorododecane		4.2 (20)	2.11 (25) [Iq] 1.94 (20) [B]	31.56	0.090 4
1-Chloro-2,2,3- epoxypropane	1.03 (25)	25.6 (1) 22.6 (22)	1.8 (25) [C]	39.76	0.136 0
Chloroethane	0.279 (10)	1.013 (19) [g]	2.0 [g] 1.96 (20) [Iq]	21.18 (5)	20.58 (10)
2-Chloroethanol	3.913 (15)	25.8 (25) 13 (132)	1.77 [g] 1.90 (25) [B]	38.9 (20)	

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Chloroform	0.596 (15) 0.514 (30)	4.81 (20) 4.31 (50)	1.1 [g] 1.1 (25) [lq]	29.91	0.129 5
1-Chloroheptane		4.48 (20)	1.86 (22) [B]	28.94	0.096 1
2-Chloroheptane		6.52 (22)	2.05 (22) [B]		
3-Chloroheptane		6.70 (22)	2.06 (22) [B]		
4-Chloroheptane		6.54 (22)	2.06 (22) [B]		
1-Chlorohexane			1.94 (20) [B]	28.32	0.103 8
Chloromethane [g]	0.0106 (20) 0.012 9 (80)	1.006 9 (100)	1.87		
[lq]		12.6 (−20)	1.86 (20)	19.5	0.165 0
1-Chloro-3- methylbutane		7.63 (−70) 6.05 (20)	1.94 (20) [B]	25.51	0.107 6
Chloromethyl methyl ether			1.88 [C]		
1-Chloro-2- methylpropane	0.462 (20) 0.373 (40)	7.87 (−38) 6.49 (14)	2.06 [g] 2.0 (25) [B]	24.40	0.109 9
2-Chloro-2- methylpropane	0.543 (15)	10.95 (0) 9.96 (20)	2.11 [g] 2.13 (25) [B]	20.06 (15)	18.35 (30)
1-Chloronaph- thalene	2.940 (25)	5.04 (25)	1.33 (25) [lq] 1.52 (25) [B]	44.12	0.103 5
<i>o</i> -Chloronitro- benzene		38 (50) 32 (80)	4.62 [g] 6.22 (50) [lq]	48.10	0.117 1
<i>m</i> -Chloronitro- benzene		21 (50) 18 (80)	3.72 [g] 3.30 (50) [lq]	49.71	0.141 7
<i>p</i> -Chloronitro- benzene		8 (120)	2.81 [g] 2.83 (90) [lq]	45.84	0.104 6
1-Chlorooctane		5.05 (25)	2.14 (25) [lq]	29 64	0.096 1
Chloropenta- fluoroethane	0.26 (25) 0.013 (25) [g]		0.5 [g]	5 (25)	
1-Chloropentane	0.580 (20)	6.6 (11)	2.14 [g] 1.94 (20) [B]	27.09	0.107 6
<i>o</i> -Chlorophenol	2.250 (45) 4.11 (25)	6.31 (25)	2.19 [g] 1.46 (20) [lq]	42.5	0.112 2
<i>m</i> -Chlorophenol	4.722 (45) 11.55 (25)		2.19 (25) [B]	43.7	0.100 9
<i>p</i> -Chlorophenol	4.99 (50)		2.09 (20) [B]	19.51	0.087 5
1-Chloropropane	0.372 (15) 0.318 (30)	7.7 (20)	2.05 [g] 1.96 (20) [B]	24.41	0.124 6
2-Chloropropane	0.335 (15) 0.299 (30)	9.82 (20)	2.17 [g] 2.1 (20) [B]	21.37	0.088 3
1-Chloro-2- propanone		30 (19)	2.22 [g] 2.37 (20), [H]		
3-Chloro-1- propene	0.347 (15)	8.2 (20)	2.0 [g] 1.8 (20) [B]	25.50	0.094 6

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
<i>o</i> -Chlorotoluene		4.45 (20) 4.2 (55)	1.57 [g] 1.41 (20) [lq]		
<i>m</i> -Chlorotoluene		5.5 (20) 5.0 (60)	1.77 (20) [lq] 1.8 (22) [B]		
<i>p</i> -Chlorotoluene		6.08 (20) 5.6 (55)	2.21 [g] 1.90 (20) [lq]	34.93	0.108 2
Chlorotrifluoro- methane	0.016 (25)	1.001 3 (29) [g]	0.50 [g]	14 (−73)	
Chlorotrimethy- lsilane			2.09 (20) [B]	19.51	0.087 5
Cinnamaldehyde		17 (20) 16.9 (24)	3.74 [g] 3.30 (30) [lq]		
<i>o</i> -Cresol	3.506 (46)	11.5 (25)	2.32 (25) [lq] 1.45 (25) [B]	39.43	0.101 1
<i>m</i> -Cresol	18.42 (20) 5.057 (45)	11.8 (25)	2.39 (20) [lq] 1.61 (25) [B]	38.00	0.092 4
<i>p</i> -Cresol	5.607 (45)	9.91 (58)	2.35 (20) [lq] 1.54 (20) [B] 2.13 (30) [B]	38.58	0.096 2
Crotonic acid					
Cyanoacetic acid		33.4 (19)			
Cycloheptanol		2.6 (−89)	0.38 (20) [B]	35.02	0.092 3
1,3-Cyclohex- adiene					
Cyclohexane	0.980 (20) 0.534 (60)	2.05 (15) 2.02 (25) 2.6 (31)	0	27.62	0.118 8
Cyclohexane- carboxylic acid					
1,4-Cyclohex- anedione		15.0 (25)	1.41 [g] 1.3 (30) [B]		
Cyclohexanol	41.07 (30) 17.19 (45)	15.0 (25) 7.24 (100)	1.86 (25) [C]	35.33	0.096 6
Cyclohexanone	2.453 (15) 1.803 (30)	20 (−40) 18.2 (20) 3.0 (89)	3.11 (20) [B] 3.01 (25) [B] 0.83 (25) [B]	37.67	0.124 2
Cyclohexanone oxime					
Cyclohexene	0.650 (20)	2.6 (−105) 2.22 (25)	0.61 [g] 0.28 (20) [lq]	29.23	0.122 3
Cyclohexylamine	1.662 (20) 1.16 (49) 3.681 (0)	4.73 (20)	1.22 (20) [lq] 1.26 (20) [B] 0.62 (20) [B]	34.19	0.118 8
Cyclohexyl- benzene					
Cyclohexyl- methanol		9.7 (60) 8.1 (80)	1.68 (20) [B]		
<i>o</i> -Cyclohexyl- phenol		3.97 (55)			

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
<i>p</i> -Cyclohexyl-phenol	0.439 (20)	4.42 (131)			
Cyclooctane			0	32.02	0.109 0
Cyclopentane		1.965 (20)	0	25.53	0.146 2
Cyclopentanol		25 (−20) 18 (20)	1 72 (25) [C]	35.04	0.101 1
Cyclopentanone	3.402 (20)	16 (−51)	3.30 [g] 2.93 (25) [B]	35.55	0.110 0
Cyclopentene			0.98 (25) [H]	25.94	0.149 5
<i>p</i> -Cymene		2.243 (20)	0 [lq]	28.83	0.087 7
<i>cis</i> -Decahydro-naphthalene		2.18 (20)	0	32.18 (20)	31.01 (30)
<i>trans</i> -Decahydro-naphthalene	2.128 (20)	2.17 (20)	0	29.89 (20)	28.87 (30)
Decamethylcy-clopentasiloxane		2.5 (20)		19.56	0.056 5
Decamethylte-trasiloxane	1.28 (20)	2.4 (20)	0.79 (25) [lq]	86.20 (25)	
Decane	0.928 (20) 0.775 (22)	1.991 (20) 1.844 (130)	0	25.67	0.092 0
1-Decanol	0.805 (20)	8.1 (20)	1.71 (20) [B] 1.62 (25) [B]	30.34	0.073 2
1-Decene			0.42 (20) [B]	25.84	0.091 9
Diallyl sulfide		4.9 (20)	1.33 (25) [B]		
Dibenzofuran		3.0 (100)	0.88 (25) [B]		
Dibenzylamine	3.711 (25)	3.6 (20)	0.97 (20) [lq] 1.02 (20) [B]	43.27	0.108 6
Dibenzyl decanedioate		4.6 (25)			
Dibenzyl ether			1.39 (21) [B]	38.2 (35)	
<i>o</i> -Dibromobenzene		7.35 (20)	2.13 (20) [B]		
<i>m</i> -Dibromobenzene		3.80 (20)	1.5 (20) [B]		
<i>p</i> -Dibromobenzene		2.57 (95)	0	41.84	0.100 7
1,4-Dibromobutane			2.16 (20) [lq] 2.06 (20) [B]	48.24	0.119 0
2,3-Dibromobutane		5.75 (25)	2.20 [g] 1.7 (25) [lq]		
1,2-Dibromoethane	1.721 (20) 1.286 (40)	4.78 (25) 4.09 (131)	1.11 [g] 1.14 (20) [lq]	35.43	0.142 8
<i>cis</i> -1,2-Dibro-moethylene		7.7 (0) 7.08 (25)	1.35 (B)		
<i>trans</i> -1,2-Dibro-moethylene		2.9 (0) 2.88 (25)	0		
1,2-Dibro-moheptane		3.8 (25)	1.78 (25) [D]		

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
2,3-Dibromoheptane		5.1 (25)	2.15 (25) [B]		
3,4-Dibromoheptane		4.7 (25)	2.15 (25) [B]		
Dibromomethane		7.77 (10) 6.7 (40)	1.43 [g] 1.85 (20) [lq]	42.77	0.148 8
1,2-Dibromopropane	1.5 (25)	4.3 (20)	1.43 (25) [B]	36.81	0.115 5
Dibromotetrafluoroethane	0.72 (25)	2.34 (25)		18.9 (20)	18.1 (25)
Dibutylamine	0.95 (20)	2.978 (20)	1.06 (20) [lq] 1.05 (20) [B]	26.50	0.095 2
Dibutyl decanedioate	9.03 (25)	4.54 (30)	2.64 (25) [B]		
Dibutyl ether	0.602 (30)	3.06 (25)	1.18 [g] 1.19 (20) [lq]	24.78	0.093 4
Dibutyl maleate	5.62 (20) 4.76 (25)		2.70 (25) [B]	32.46	0.086 5
2,6-Di- <i>tert</i> -butyl-4-methylphenol	3.47 (80)		1.68 (20) [B]		
Dibutyl <i>o</i> -phthalate	19.91 (20) 7.85 (45)	6.436 (30) 5.99 (45)	2.97 (20) [lq] 2.85 (30) [B]	33.40 (20)	
Dichloroacetic acid	3.23 (50) 1.92 (75)	8.2 (22) 7.8 (61)		37.8	0.092 7
<i>o</i> -Dichlorobenzene	1.324 (25)	9.93 (25) 7.10 (90)	2.51 [g] 2.26 (24) [B]	26.84 (20)	35.55 (30)
<i>m</i> -Dichlorobenzene	1.045 (23) 0.955 (33)	5.04 (25) 4.22 (90)	1.68 [g] 1.38 (24) [B]	38.30	0.114 7
<i>p</i> -Dichlorobenzene	0.839 (55) 0.668 (79)	2.41 (50)	0	34.66	0.087 9
1,4-Dichlorobutane		8.9 (25)	2.22 [g] 2.13 (25) [lq]	37.79	0.117 4
Dichlorodifluoromethane	0.26 (25) 0.013 (25) [g]	2.13 (29)	0.51 [g]	9 (25)	
1,1-Dichloroethane	0.505 (25) 0.430 (30)	10.1 (18) 10.86 (16)	2.06 [g] 2.00 (25) [B]	27.03	0.118 6
1,2-Dichloroethane	0.887 (15) 0.730 (30)	12.7 (–10) 10.65 (20)	1.48 [g] 1.7 (20) [B]	35.43	0.142 8
1,1-Dichloroethylene	0.442 (0) 0.358 (20)	4.67 (16)	1.30 (25) [B]		
<i>cis</i> -1,2-Dichloroethylene	0.467 (20) 0.444 (25)	9.20 (25)	2.95 [g] 1.90 (25) [B]	28 (20)	
<i>trans</i> -1,2-Dichloroethylene	0.423 (15) 0.404 (20)	2.14 (25)	0.70 (25) [B]	25 (20)	

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , mN · s · m ⁻²	Dielectric constant, ϵ	Dipole moment, D	Surface tension, dyn · cm ⁻¹	
				<i>a</i>	<i>b</i>
2,2'-Dichloro-ethyl ether	2.41 (20) 2.065 (25)	21.2 (20)	2.61 (20) [B]	40.57	0.130 6
Dichlorofluoromethane	0.34 (25) 0.011 (25) [g]	5.34 (28)	1.3 [g]	18 (25)	
Dichloromethane	0.449 (15) 0.393 (30)	9.14 (20) 1.006 5 (100) [g]	1.60 [g] 1.90 (20) [B] 1.60 (25) [B]	30.41	0.128 4
2,4-Dichlorophenol				46.59	0.122 1
1,2-Dichloropropane	0.865 (20) 0.700 (25)	8.925 (26) 7.90 (35)	1.87 (25) [B]	31.42	0.124 0
1,3-Dichloropropane			2.08 [g] 2.2 (25) [B]	36.40	0.123 3
2,2-Dichloropropane	0.769 (15) 0.619 (30)	11.37 (20)	2.62 [g] 2.20 (25) [B]	23.60 (20)	22.53 (30)
1,1-Dichloro-2-propanone		14 (20)			
1,2-Dichlorotetrafluoroethane	0.38 (25) 0.011 (25) [g]	2.26 (25)	0.53 [g]	12 (25)	
α,α -Dichlorotoluene		6.9 (20)	2.07 (20) [B] 2.05 (25) [B]	41.26	0.103 5
Diethanolamine	368 (30) 196 (40)	2.81 (25)	2.84 (25) [B]		
1,1-Diethoxyethane		3.80 (25)	1.08 [g]	23.46	0.103 0
1,2-Diethoxyethane	0.65 (20)		1.99 (20) [B] 1.65 (25) [B]		
Diethoxymethane				23.87	0.129 1
Diethylamine	0.388 (10) 0.273 (38)	3.6 (22)	0.92 [g] 1.11 (25) [lq]	22.71	0.114 3
<i>N,N</i> -Diethylaniline	1.15 (30) 0.750 (75)	5.5 (19)	1.40 (20) [lq] 1.80 (20) [B]	36.59	0.104 0
Diethyl carbonate	0.868 (15) 0.748 (25)	2.82 (20)	1.07 [g] 0.91 (25) [B]	28.62	0.110 0
Diethyl decanedioate		5.0 (30)	2.38 (20) [lq] 2.52 (20) [B]	34.68	0.095 9
Diethyl ether	0.247 (15) 0.245 (20)	4.335 (20) 3.97 (40)	1.15 [g] 1.22 (16) [lq]	18.92	0.090 8
Diethyl ethyl phosphonate	1.627 (15) 0.969 (45)	11.00 (15) 9.86 (45)	2.95 (32) [lq] 2.91 (20) [C]	30.63	0.097 5
Diethyl fumarate		6.5 (23)	2.40 (20) [B]		
Diethyl glutarate		6.7 (30)	2.46 (30) [lq]	34.34	0.101 0
Di(2-ethylhexyl)-2-ethylhexylphosphonate	6.00 (45) 3.61 (65)	4.09 (45) 3.94 (65)			
Di(2-ethylhexyl)- <i>o</i> -phthalate	33.67 (35) 21.40 (45)	4.91 (35) 4.77 (45)			

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Diethyl maleate	3.57 (20) 3.14 (25)	8.58 (23)	2.56 (25) [B]	34.67	0.103 9
Diethyl malonate	2.15 (20) 1.94 (25)	8.03 (25)	2.49 (20) [lq] 2.54 (25) [B]	33.91	0.104 2
Diethyl nonanedioate		5.13 (30)			
Diethyl oxalate	2.311 (15) 1.618 (30)	8.1 (21)	2.49 (20) [D]	34.32	0.111 9
Diethyl <i>o</i> -phthalate	9.18 (35) 6.41 (45)	7.34 (35) 7.13 (45)	2.8 (25) [B]	38.47	0.096 3
Diethyl succinate		6.64 (30)	2.3 [g] 2.37 (30) [lq]	33.97	0.104 1
Diethyl sulfate		29 (20)	4.46 (25) [D]	35.47	0.097 6
Diethyl sulfide	0.446 (20) 0.422 (25)	5.72 (25) 5.24 (50)	1.52 [g] 1.58 (20) [B]	27.33	0.110 6
Diethyl sulfite		16 (20) 14 (50)			
Diethylzinc		2.5 (20)	0.62 (25) [B]		
1,1-Difluoroethane	0.243 (21)	2.30 [g]			
1,2-Dihydroxy- benzene		2.6 (−89)	2.60 (25) [B]	47.6	0.084 9
1,3-Dihydroxy- benzene		3.2 (18)	2.09 (44) [B]	54.8	0.071 7
1,4-Dihydroxy- benzene			1.4 (44) [B]		
1,2-Diiodobenzene		5.7 (20)	1.70 (20) [B]		
1,3-Diiodobenzene		4.3 (25)	1.22 (20) [B]		
1,4-Diiodobenzene		2.9 (120)	0.19 (20) [B]		
<i>cis</i> -1,2-Diiodo- ethylene		4.46 (83)	0.71 [B]		
<i>trans</i> -1,2-Diiodo- ethylene		2.19 (83)	0		
Diiodomethane	3.043 (15) 2.392 (30)	5.316 (25)	1.08 (25) [B]	70.21	0.161 3
Diisobutylamine		2.7 (22)	1.10 (25) [B]	24.00	0.091 2
Diisobutyl <i>o</i> -phthalate	30 (20)				
Diisopentylamine		2.5 (18)	1.48 (30) [B]	26.04	0.085 8
Diisopentyl ether	1.40 (11) 1.012 (20)	2.82 (20)	0.98 (20) [lq] 1.23 (25) [B]	24.76	0.087 1
Diisopropylamine	0.40 (25)		1.26 (25) [B]	21.83	0.107 7
Diisopropyl ether	0.379 (25)	3.88 (25)	1.13 [g] 1.26 (25) [B]	19.89	0.104 8
1,2-Dimethoxy- benzene	3.281 (25) 2.184 (40)	4.09 (25)	1.32 (25) [B]	34.4	0.064 2

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
1,1-Dimethoxyethane				23.90	0.115 9
1,2-Dimethoxyethane	0.530 (10) 0.455 (25)	7.60 (10) 7.20 (25)	1.71 (25) [B]	48.0 (25)	
Dimethoxymethane	0.340 (15) 0.325 (20)	2.65 (20)	0.74 [g]	23.59	0.119 9
<i>N,N</i> -Dimethylacetamide	2.141 (20) 0.838 (30)	37.78 (25)	3.80 [g] 4.60 (20) [lq]	32.43 (30)	29.50 (50)
Dimethylamine	0.207 (15) 0.186 (25)	6.32 (0) 5.26 (25)	1.03 [g] 1.14 (25) [lq]	29.50	0.126 5
<i>N,N</i> -Dimethylaniline	1.285 (25) 0.91 (50)	4.9 (20) 4.4 (70)	1.61 [g] 1.55 (25) [B] 1.40 (25) [B]	38.14	0.104 9
2,4-Dimethylaniline				39.34	0.099 6
2,2-Dimethylbutane	0.351 (25) 0.330 (30)	1.873 (25)	0	18.29	0.099 0
2,3-Dimethylbutane	0.361 (25) 0.342 (30)	1.890 (25)	0	19.38	0.100 0
2,3-Dimethyl-1-butanol				26.22	0.099 2
<i>N,N</i> -Dimethylbutyramide	1.271	2.00			
Dimethyl carbonate			0.90 [g] 0.96 (25) [B]	31.94	0.134 3
1,1-Dimethylcyclopentane			0	23.78	0.101 6
2,2-Dimethyl-1,3-dioxolane-4-methanol	11 (20)				
Dimethyl ether	0.010 4 (60)	5.02 (25) 2.97 (110)	1.30 [g] 1.25 (25) [B]	14.97	0.147 8
<i>N,N</i> -Dimethylformamide	0.845 (20) 0.598 (50)	38.3 (20) 36.71 (25)	3.86 (25) [B]	36.76 (20)	34.40 (40)
2,4-Dimethylheptane		1.9 (20)	0	23.21	0.092 9
2,5-Dimethylheptane		1.9 (20)	0	23.21	0.092 9
2,6-Dimethylheptane		2 (20)	0	22.77	0.088 7
2,6-Dimethyl-4-heptanone	1.03 (20)		2.66 (25) [C]		
Dimethyl hexanedioate	14 (20)		2.28 (20) [B]	38.26	0.113 8
Dimethyl hydrogen phosphonate	1.08 (25)				

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Dimethyl maleate	3.54 (20) 3.21 (25)		2.48 (25) [C]	40.73	0.122 0
Dimethyl malonate		10 (20)	2.41 (20) [B]	39.72	0.120 8
2,2-Dimethyl- pentane		1.91 (20)	0	19.94	0.095 7
2,3-Dimethyl- pentane	0.406 (20)	1.939 (20)	0	21.96	0.099 5
2,4-Dimethyl- pentane	0.361 (20)	1.914 (20)	0	20.09	0.097 2
3,3-Dimethyl- pentane		1.94 (20)	0	21.59	0.099 6
2,4-Dimethyl- phenol			1.48 (20) [B] 1.98 (60) [B]	34.57	0.086 9
2,5-Dimethyl- phenol	1.55 (80)		1.43 (20) [B] 1.52 (60) [B]	36.72	0.085 0
3,4-Dimethyl- phenol	3.00 (80)	4.8 (17)	1.77 (20) [B]	35.75	0.091 0
3,5-Dimethyl- phenol	2.42 (80)		1.76 (20) [B]	34.09	0.080 7
Dimethyl <i>o</i> -phthalate	17.2 (25) 6.41 (45)	8.25 (25) 8.11 (45)	2.8 (25) [B]		
2,2-Dimethyl- propane	0.328 (0) 0.303 (5)	1.80 (20) 1.678 (98)	0	12.05 (20)	10.98 (30)
<i>N,N</i> -Dimethyl- propionamide	0.935	33.1			
2,5-Dimethyl- pyrazine		2.43 (20)	0		
2,3-Dimethyl- quinoxaline		2.3 (25)	0		
Dimethyl succinate		5.1 (20)	2.09 (20) [B]	39.00	0.119 1
Dimethyl sulfate		48.3 (20) 46.4 (20)	4.31 (25) [D]	41.26	0.116 3
Dimethyl sulfide	0.289 (20) 0.265 (36)	6.2 (20)	1.45 (25) [B]	26.07	0.080 5
Dimethyl sulfite	0.715 (30) 0.436 (80)	22.5 (23)	2.93 (20) [B]	36.48	0.125 3
Dimethyl sulfoxide	2.47 (20) 1.192 (55)	48.9 (20) 41.9 (55)	3.9 (25) [B]	43.54 (20)	42.41 (30)
2,4-Dimethyl- tetrahydrothi- ophene-1, 1- dioxide	9.04	29.5			

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN}\cdot\text{s}\cdot\text{m}^{-2}$	Dielectric constant, ε	Dipole moment, D	Surface tension, $\text{dyn}\cdot\text{cm}^{-1}$	
				a	b
<i>N,N</i> -Dimethyl- <i>o</i> -toluidine	37 (20)	3.4 (20)	0.88 (25) [B]		
<i>N,N</i> -Dimethyl- <i>p</i> -toluidine		3.9 (20)	1.29 (25) [B]		
Dinonyl hexanedioate			2.53 (25) [B]		
Dinonyl <i>o</i> -phthalate		4.65 (35) 4.52 (45)			
Diocetyl decanedioate		4.0 (27)			
Diocetyl <i>o</i> -phthalate		5.1 (25)	3.06 (25) [C]		
1,4-Dioxane	1.439 (15) 1.087 (30)	2.24 (20) 2.21 (25)	0	36.23	0.139 1
Dipentyl ether	1.188 (15) 0.922 (30)	2.77 (25)	0.98 (20) [lq] 1.24 (25) [B]	26.66	0.092 5
Dipentyl <i>o</i> -phthalate	17.03 (35) 11.51 (45)	5.79 (35) 5.62 (45)	2.71 (20) [lq]	32.56	0.073 9
Dipentyl sulfide		3.83 (25)	1.59 (25) [B]	29.55	0.087 6
Diphenylamine	4.66 (55) 1.04 (130)	3.3 (52)	1.31 (20) [C] 1.01 (25) [B]	45.36	0.101 7
1,2-Dipheny- lethane		2.4 (110)	0 (110) [lq] 0.45 (25) [B]		
Diphenyl ether	2.61 (40) 2.09 (50)	3.65 (30)	1.16	28.70	0.078 0
Diphenylmethane		2.7 (18) 2.57 (26)	0.26 (30) [lq] 0.3 (25) [B]		
1,1-Dipropo- xyethane				25.03	0.097 2
Dipropo- xymethane				25.17	0.095 3
Dipropylamine	0.534 (20) 0.427 (37)	3.07 (20)	1.01 (20) [lq] 1.03 (20) [B]	24.86	0.102 2
Dipropyl carbonate				28.94	0.101 5
Dipropylene glycol butyl ether	4.23 (25)			28.2 (25)	
Dipropylene glycol ethyl ether	3.11 (25)			27.7 (25)	
Dipropylene glycol isopropyl ether	386 (25)			25.9 (25)	

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Dipropylene glycol methyl ether	3.1 (25)			28.8 (25)	
Dipropyl ether	0.448 (15) 0.376 (30)	3.39 (26)	1.21 [g] 1.17 (30) [H] 1.07 (20) [lq]	22.60	0.104 7
Divinyl ether		3.9 (20)			
Dodecamethyl- cyclohexasil- oxane		2.6 (20)			
Dodecamethyl- pentasiloxane		2.5 (20)		17.08 (25)	
Dodecane	1.508 (20) 1.378 (25)	2.05 (−10) 2.01 (20)	0	27.12	0.088 4
1-Dodecanol		5.15 (20) 6.5 (25)	1.52 (20) [B]	31.25	0.0748
6-Dodecyne		2.17 (25)			
1,2-Epoxybutane	0.41 (20) 0.40 (25)		2.01 (20) [B]	23.9 (20)	
Erythritol		28 (128)			
Ethane [g]	0.009 0 (20) 0.011 4 (100)	1.001 5 (0)	0	1.24	0.166 0 [lq]
1,2-Ethanedia- mine	1.54 (20) 1.226 (30)	16.8 (18) 14.2 (20)	1.96 [g] 1.92 (25) [B]	44.77	0.139 8
1,2-Ethanediol	26.09 (15) 13.55 (30)	38.66 (20) 37.7 (25)	2.28 [g] 2.3 (25) [D]	50.21	0.089 0
1,2-Ethanediol diacetate	3.13 (20)	13 (30)	2.34 (30) [B]		
Ethanesulfonic acid				45.74	0.082 4
Ethanesulfonyl chloride			3.89 (25) [B]	43.43	0.117 7
Ethanethiol	0.003 16 [g]	6.9 (15)	1.57 [g] 1.40 (20) [B]	25.06	0.079 3
Ethanol	1.209 (19) 0.991 (30)	25.00 (20) 20.21 (55)	1.69 [g] 1.71 (25) [B]	24.05	0.083 2
Ethoxybenzene	1.364 (15) 1.040 (30)	4.22 (20)	1.41 [g] 1.36 (25) [CS ₂]	35.17	0.110 4
2-Ethoxyethanol	2.04 (20) 1.85 (25)	29.6 (24)	2.24 (30) [B]	30.59	0.089 7
2-(2-Ethoxyeth- oxy)ethanol	3.71 (25)			31.8 (25)	27.2 (75)
2-Ethoxyethyl acetate	1.025 (25)	7.567 (30)	2.25 (30) [B]	31.8 (25)	

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
1-Ethoxy-2-methylbutane		3.96 (20)			
1-Ethoxynaphthalene		3.3 (19)			
1-Ethoxypentane		3.6 (23)			
1-Ethoxy-2-propanol	1.68 (25)			25.9 (25)	
α -Ethoxytoluene		3.9 (20)			
Ethyl acetate	0.473 (15) 0.426 (25)	6.11 (20) 5.30 (77)	1.78 [g] 1.84 (25) [lq]	26.29	0.116 1
Ethyl acetoacetate	1.419 (20) 1.508 (25)	15.7 (22)	3.22 (18) [B keto form] 2.04 (−80) [CS ₂ , enol form]	34.42	0.101 5
Ethylamine		6.94 (10)	1.40 (25) [B]	22.63	0.137 2
2-(Ethylamino)ethanol	12.40 (25)				
<i>N</i> -Ethylaniline	2.04 (25) 1.08 (55)	5.76 (20)		39.00	0.107 0
Ethylbenzene	0.669 (20) 0.531 (40)	2.41 (20)	0.37 (25) [lq]	31.48	0.109 4
Ethyl benzoate	2.407 (15) 1.751 (30)	6.02 (20)	1.95 [g] 1.93 (25) [B] 2.40 (25) [B]	37.16	0.105 9
Ethyl α -bromobutyrate		8 (20)			
2-Ethyl-1-butanol	8.021 (15) 5.892 (25)	6.19 (90)		25.06 (15)	24.32 (25)
Ethyl butyrate	0.771 (15) 0.613 (25)	5.10 (18)	1.74 (22) [B]	26.55	0.104 5
2-Ethylbutyric acid	3.3 (20)			26.3 (20)	
Ethyl carbamate	0.916 (105) 0.715 (120)	14.2 (50)	2.59 (30) [D]		
Ethyl chloroacetate		11.4 (21)	2.65 (25) [B]	34.18	0.117 7
Ethyl chloroformate		11 (20)	2.56 (35) [B]	28.90	0.108 4
Ethyl cinnamate	8.7 (20)	6.1 (18)	1.86 (20) [B]	39.99	0.104 5
Ethyl crotonate		5.4 (20)	1.95 (24) [B]	29.31	0.106 6
Ethyl cyanoacetate	3.256 (15) 2.148 (30)	26.9 (20)	4.04 (30) [B]	38.80	0.109 2
Ethylcyclohexane	0.843 (20) 0.787 (25)	2.054 (20)	0 [g]	27.78	0.105 4
Ethyl dichloroacetate		12 (2) 10 (22)	2.63 (25) [B]	34.89	0.115 8

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
<i>N</i> -Ethyl-diethanolamine	53 (25)				
Ethyl dodecanoate		3.4 (20) 2.7 (143)	1.3 (20) [lq]	30.05	0.086 3
Ethylene		1.001 44 (0)	0 [g]	−2.7	0.185 4
Ethylene carbonate	1.85 (40)	89.6 (40) 69.4 (91)	4.87 (25) [B]		
Ethylenediamine	1.540 (18)	16.0 (18) 14.2 (20)	1.98 [g] 1.92 (25) [B]	44.77	0.139 8
Ethylene dinitrate		28.3 (20)	3.58 (25) [B]	49.1 (0)	46.7 (45)
2,2'-(Ethylenedioxy)diethanol	38 (20)	23.69 (20)	5.58 [lq]	47.33	0.088 0
Ethylene glycol	26.09 (15) 13.35 (30)	41.2 (20) 37.7 (25)	2.27 [g] 2.20 (15) [lq]	50.21	0.089 0
Ethylene oxide	0.3 (0)	14 (−1)	1.88 [g] 1.92 (20) [lq]	27.66	0.166 4
Ethyleneimine	0.418 (25)	18.3 (25)	1.89 [g] 1.77 (25) [B]	7.9 (20)	
Ethyl formate	0.419 (15) 0.358 (30)	7.16 (25)	1.94 [g] 1.96 (25) [lq]	26.47	0.131 5
Ethyl fumarate		6.5 (23)		33.90	0.105 6
Ethyl hexadecanoate		3.2 (20) 2.71 (104)	1.2 [lq]	32.86	0.085 9
2-Ethyl-1, 3-hexanediol	323 (20)				
Ethyl hexanoate			1.80 (20) [B]	27.73	0.096 0
2-Ethylhexanoic acid	7.7 (20)				
2-Ethyl-1-hexanol	9.8 (20)	4.41 (90)	1.74 (25) [B]	30.0 (22)	
2-Ethylhexyl acetate	1.5 (20)				
Ethyl isobutyrate				25.33	0.104 6
Ethyl isopentyl ether		3.96 (20)			
Ethyl isothiocyanate		19.5 (21)	3.67 (20) [B]	38.69	0.132 6
Ethyl lactate	2.44 (25)	13.1 (25)	2.4 (20) [B]	30.72	0.098 3
Ethyl maleate		8.6 (23)			
Ethyl 3-methylbutyrate		4.71 (18)		25.79	0.100 6
Ethyl methyl ether			1.22 [g]	18.56	0.131 7
Ethyl methyl sulfide	0.373 (20) 0.354 (25)			27.63	0.128 6
Ethyl nitrate		19.4 (20)	2.93 (20) [B]	30.81	0.134 5

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Ethyl 9-octadecenoate		3.2 (25)	1.83 (20) [lq]		
Ethyl 4-oxopentanoate		12 (21)			
3-Ethylpentane		1.94 (20)	0	22.52	0.103 2
Ethyl pentanoate	0.847 (20)	4.7 (18)	1.76 (28) [B]	27.15	0.099 9
Ethyl pentyl ether		3.6 (23)	1.2 (20) [B]	24.19	0.099 2
Ethyl phenylacetate	5.3 (21)	1.82 (30)			
Ethyl phenyl sulfide			4.08 (25) [B]	39.30	0.113 1
Ethyl propionate	0.564 (15)	5.65 (19)	1.75 (22) [B]	26.72	0.116 8
	0.473 (30)				
Ethyl propyl ether	0.323 (20)			21.92	
	0.225 (60)		1.16 (25) [B]		0.105 4
Ethyl salicylate	1.772 (45)	7.99 (30)	2.85 (25) [B]	31.00	0.109 1
Ethyl stearate		2.98 (40)	1.65 (40) [lq]		
		2.69 (100)			
Ethyl thiocyanate		29.3 (21)	3.33 (20) [B]	37.28	0.122 6
<i>o</i> -Ethyltoluene				32.33	0.106 0
<i>p</i> -Ethyltoluene		2.24 (25)	0	30.98	0.107 5
Ethyl trichloroacetate		7.8 (20)	2.56 (25) [B]	32.97	0.107 3
Ethyl vinyl ether	0.2		1.26 (20) [B]	19.00 (20)	
Ethynyl acetate				32.81 (20)	30.20 (40)
Fluorobenzene	0.620 (15)	5.42 (25)	1.61 [g]	29.67	0.120 4
	0517 (30)	4.7 (60)			
1-Fluorohexane				23.41	0.100 1
2-Fluoro-2-methylbutane		5.89 (20)	1.92 (25) [B]		
1-Fluoropentane		4.24 (20)	1.85 (25) [B]	22.81	0.131 5
<i>o</i> -Fluorotoluene	0.680 (20)	4.22 (30)	1.35 [g]		
	0.601 (30)	3.9 (60)	1.26 (30) [lq]		
<i>m</i> -Fluorotoluene	0.608 (20)	5.42 (30)	1.86 [g]	32.31	0.125 7
	0.534 (30)	4.9 (60)	1.66 (30) [lq]		
<i>p</i> -Fluorotoluene	0.622 (20)	5.86 (30)	2.00 [g]	30.44	0.110 9
	0.522 (30)	5.3 (60)	1.76 (30) [lq]		
Formamide	4.320 (15)	111.0 (20)	3.73 [g]	59.13	0.084 2
	2.296 (30)	103.5 (40)			
Formanilide	1.65 (120)		3.37 (25) [C]	44.30	0.087 5
Formic acid	1.966 (15)	58.5 (15)	1.35 [g]	39.87	0.109 8
	1.219 (40)	57.0 (21)	1.20 (25) [B]		
2-Furaldehyde	2.475 (0)	41.9 (20)	2.13 (25) [lq]	46.41	0.132 7
	1.494 (25)	34.9 (50)	3.63 (25) [B]		
Furan	0.380 (20)	2.95 (25)	0.66 [g]	24.10 (20)	23.38 (25)
	0.361 (25)		0.67 (20) [B]		

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Furfuryl alcohol	4.62 (25)		1.92 (25) [Iq]	ca 38 (20)	
Glycerol	945 (25) 134 (50)	42.5 (25)	2.68 (25) [D]	63.14 (17)	62.5 (25)
Glycerol triacetate		7.2 (20)	2.73 (25) [B]	37.88	0.081
Glycerol trinitrate	36.0 (20) 13.6 (40)	19 (20)	3.38 (25) [B]	55.74	0.250 4
Glycerol trioleate		3.2 (26)	3.11 (23) [B]	36.03	0.069 9
Glycerol tripalmitate		2.9 (65)	2.80 (23) [B]	32.26	0.067 2
Glycerol tristearate		2.8 (70)	2.86 (23) [B]	32.73	0.068 5
Heptanaldehyde	0.977 (15)	9.1 (20)	2.26 (40) [Iq] 2.58 (22) [B]	28.64	0.092 0
Heptane	0.416 (20) 0.341 (40)	1.924 (20) 1.85 (70)	0	22.10	0.098 0
Heptanoic acid	3.40 (30)	2.6 (71)		29.88	0.084 8
1-Heptanol	7.014 (20) 8.53 (15)	12.1 (22)	1.73 (20) [B]		
DL-2-Heptanol	5.06 (25)	9.21 (22)	1.73 (20) [B]		
DL-3-Heptanol		6.9 (22)	1.73 (20) [B]		
4-Heptanol		6.2 (22)	1.72 (20) [B]		
2-Heptanone	0.854 (15) 0.686 (30)	11.95 (20) 8.27 (100)	2.61 (22) [B]	28.76	0.105 6
3-Heptanone		12.9 (22)	2.81 (22) [B]	28.24	0.101 5
4-Heptanone	0.736 (20)	12.60 (20) 9.46 (80)	2.74 (20) [B]	28.11	0.106 0
1-Heptene	0.35 (20) 0.34 (25)	2.07 (20)	0.34 (20) [Iq]	22.28	0.099 1
Hexadeca- methylcyclo- octasiloxane		2.7 (20)			
Hexadecane	3.591 (22)		0	29.18	0.085 4
1-Hexadecanol		3.8 (50)	1.67 (25) [B]		
1,5-Hexadiene	0.275 (20) 0.244 (36)				
2,4-Hexadiene		2.2 (25)	0.31 (25) [B]		
Hexafluoro- benzene			0	22.6 (20)	
Hexamethyl- disiloxane		2.2 (20)	0.37 (25) [Iq]	17.01	0.076 3
Hexamethyl- phosphoramide	3.47 (20)	30 (20)	4.31 (25) [Iq]	33.8 (20)	
Hexane	0.313 (20) 0.271 (40)	1.904 (15) 1.890 (20)	0	20.44	0.102 2
Hexanedinitrile	5.99	32.45	3.8 (25) [B]	47.88	0.097 3

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
2,4-Hexanedione				32.22	0.100 2
Hexanenitrile	1.041 (15) 0.830 (30)	17.26 (25)		29.64	0.090 7
Hexanoic acid	3.525 (15) 2.511 (3)	2.63 (71)	1.13 (25) [lq]	28.05 (20)	27.55 (25)
1-Hexanol	6.203 (15) 3.872 (30)	13.3 (25) 8.5 (75)	1.55 (20) [B]	27.81	0.080 1
2-Hexanone	0.584 (25)	14.6 (15)	2.68 (22) [B]	28.18	0.109 2
1-Hexene	0.26 (20) 0.25 (25)	2.051 (20)	0.34 (20) [lq]	20.47	0.102 7
Hexyl acetate				28.44	0.097 0
4-Hydroxy-4-methyl-2-pentanone	2.9 (25)	18.2 (25)	3.24 (20) [B]	31.0 (20)	
Iodobenzene	1.774 (17) 0.488 (149)	4.62 (20)	1.71 [g] 1.3 (20) [B]	41.52	0.112 3
1-Iodobutane		6.22 (20) 4.52 (130)	2.10 [g] 1.90 (20) [B]	30.82	0.013 1
2-Iodobutane			2.06 (20) [B]	30.32	0.105 6
1-Iodododecane		3.9 (20)	1.87 (20) [C]		
Iodoethane	0.617 (15) 0.540 (30)	10.2 (–50) 7.82 (20)	1.91 [g] 1.69 (20) [lq]	31.67	0.128 6
1-Iodoheptane		4.9 (22)	1.86 (22) [B]	32.18	0.088 7
3-Iodoheptane		6.4 (22)	1.95 (22) [B]		
1-Iodoheptadecane		3.5 (20)		34.49	0.088 0
1-Iodohexane		5.37 (20)	1.94 (20) [C]	31.63	0.084 5
Iodomethane	0.500 (20) 0.424 (40)	7.00 (20)	1.64 [g] 1.42 (20) [B]	33.42	0.123 4
1-Iodo-3-methylbutane		5.6 (19)	1.85 (20) [B]	30.37	0.091 5
2-Iodo-2-methylbutane		8.19 (20)	2.20 (20) [B]		
1-Iodo-2-methylpropane	0.875 (20) 0.697 (40)	6.5 (20)	1.89 (20) [B]	30.26	0.017 2
1-Iodoctane		4.6 (25)	1.80 (25) [lq] 1.90 (20) [C]	32.51	0.091 5
2-Iodoctane		5.8 (20)	2.07 (20) [C]		
1-Iodopentane		5.81 (20)	1.90 (20) [B]	31.41	0.101 4
1-Iodopropane	0.837 (15) 0.670 (30)	7.00 (20)	2.03 [g] 1.86 (20) [B]	31.64	0.113 6
2-Iodopropane	0.732 (15) 0.620 (30)	7.87 (20)	2.01 (20) [B]	29.35	0.1107
<i>p</i> -Iodotoluene		4.4 (35)	1.72 (22) [B]	39.23	0.096 5
α -Ionone		11 (18)		34.10	0.094 9
β -Ionone		12 (20)		35.36	0.095 0

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Iron pentacarbonyl		2.6 (20)			
Isobutyl acetate		5.29 (20)	1.87 (22) [B]	25.59	0.101 3
Isobutylamine	0.553 (25)	4.43 (21)	1.27 (25) [B]	24.48	0.109 2
Isobutylbenzene		2.319 (20)	0.31 (20) [lq]	29.39	0.096 1
		2.298 (30)			
Isobutyl butyrate		4.1 (20)		24.47	0.084 3
Isobutyl formate	0.680 (20)	6.41 (19)	1.89 (20) [B]	26.14	0.112 2
Isobutyl isobutyrate				30.92	0.127 0
Isobutyl nitrate		2.7 (20)			
Isobutyl pentanoate		3.8 (19)			
Isobutyl propionate				28.97	0.116 6
Isobutyric acid	1.44 (15)	2.7 (20)	1.09 (25) [lq]	26.88	0.092 0
Isobutyric anhydride	14 (20)				
Isobutyronitrile	0.551 (15)	20.4 (24)	3.61 (25) [B]	24.93 (20)	23.84 (30)
	0.456 (30)				
Isopentyl acetate	0.872 (20)	4.81 (20)	1.84 (22) [B]	26.75	0.098 9
	0.790 (25)	4.63 (30)	1.76 (30) [lq]		
Isopentyl butyrate		4.0 (20)		27.32	0.091 8
Isopentyl pentanoate		3.6 (19)	1.8 (28) [B]		
Isopentyl propionate	4.2 (20)				
Isopropyl acetate	0.559 (20)		1.86 (22) [B]	24.44	0.107 2
Isopropylamine	0.36 (25)	5.45 (20)	1.45 (25) [B]	19.91	0.097 2
Isopropylbenzene	0.791 (20)	2.39 (20)	0.65 [g]	30.32	0.105 4
	0.739 (25)		0.39 (20) [lq]		
Isopropyl formate	0.512 (20)			24.56	0.114 7
1-Isopropyl-4- methylbenzene	3.402 (20)	2.24 (20)	0	29.44 (20)	
	1.600 (30)				
Isoquinoline	3.253 (30)	10.7 (20)	2.75 [g] 2.55 (25) [B]		
Lactamide					
Lactic acid	40.33 (25)	22 (17)			
Lactonitrile	2.01 (30)	38 (20)		38.31	0.096 0
D-Limonene		2.4 (20)	1.57 (25) [B]	29.50	0.092 9
DL-Limonene		2.3 (20)	0.63 (25) [B]	29.11	0.091 3
DL-Mandelonitrile		17.8 (23)		45.90	0.098 8
Menthol	6.89 (35)		1.55 (20) [B]		
2-Mercaptoethanol	3.4 (20)				
Methacrylic acid	1.32 (20)		1.65	26.5 (25)	
Methacrylonitrile	0.392 (20)		3.69 [g]	24.4 (20)	
Methane [g]	0.010 9 (20)	1.000 94 (0)	0	*	
	0.013 3 (100)				
Methanesulfonic acid				52.28	0.089 3

* 38.618–0.1873T–0.000356T²

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Methanethiol			1.26 [g]	28.09	0.169 6
Methanol	0.676 (10) 0.544 (25)	41.8 (−20) 33.62 (20)	1.69 [g] 1.68 (22) [B] 4.34 (20) [B]	24.00 45.34	0.077 3 0.110 5
<i>o</i> -Methoxy- benzaldehyde					
<i>p</i> -Methoxy- benzaldehyde		22.3 (22) 10.4 (248)	3.26 (35) [B]	44.69	0.104 7
Methoxybenzene	1.152 (15) 0.789 (30)	4.33 (25) 3.9 (70)	1.36 [g] 1.24 (20) [B]	38.11	0.120 4
2-Methoxyethanol	1.72 (20) 1.60 (25)	16.93 (25) 16.0 (30)	2.04 (25) [B]	33.30	0.098 4
2-(2-Methoxy- ethoxy)ethanol	3.48 (25) 1.61 (60)			34.8 (25)	29.9 (75)
2-Methoxyethyl acetate		8.25 (20)	2.13 (30) [B]		
1-Methoxy-2- nitrobenzene			4.83 [g]	48.62	0.118 5
<i>o</i> -Methoxyphenol		12 (25)		41.2	0.094 3
2-Methoxy-4- (2-propenyl) phenol	6.931 (25)		2.46 (25) [B]		
<i>o</i> -Methoxytoluene		3.5 (20)			
<i>m</i> -Methoxytoluene		3.5 (20)			
<i>p</i> -Methoxytoluene		4.0 (20)		36.20	0.107 1
<i>N</i> -Methyl- acetamide	3.88 (30) 2.54 (45)	178.9 (30) 138.6 (60)	4.39 (20) [D]	33.67 (30)	30.62 (50)
Methyl acetate	0.388 (20) 0.320 (40)	7.03 (20) 6.68 (25)	1.70 [g] 1.75 (25) [B]	27.95	0.128 9
Methyl acetoacetate	1.704 (20)			34.98	0.094 4
Methyl acrylate	1.398 (20)		1.77 (25) [B]		
Methylamine	0.285 (15) 0.236 (0)	11.4 (−10) 10.0 (18)	1.29 [g]	22.87	0.148 8
<i>N</i> -Methylaniline	2.02 (25) 1.084 (55)		1.67 (25) [B]	39.32	0.097 0
Methyl benzoate	2.298 (15) 1.673 (30)	6.59 (20)	1.86 (25) [B]	40.10	0.117 1
2-Methyl-1, 2-butadiene	0.266 (0.3) 0.223 (20)	2.1 (25)	0.15 [g]		
2-Methylbutane	0.237 (15) 0.215 (25)	1.871 (0) 1.845 (20)	0.13 [g]	17.20	0.110 3
2-Methyl-1- butanol	5.50 (20) 1.44 (60)	14.7 (25)		21.5 (25)	
2-Methyl-2- butanol	5.48 (15) 2.81 (30)	5.82 (25)	1.72 (20) [B]	24.18	0.074 8

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
3-Methyl-1-butanol	4.81 (15)	14.7 (25)	1.82 (25) [B]	25.76	0.082 0
3-Methyl-2-butanol	2.96 (30)	5.82 (130)			
2-Methyl-1-butene	3.51 (25)			23.0 (25)	
2-Methyl-2-butene		2.20 (20)	0.52 (20) [Iq]	18.81	0.1148
			0.11 (25) [Iq]	19.70	0.127 1
			0.34 (25) [B]		
3-Methyl-1-butene		1.002 8 (100) [g]	0.25 [g]	16.42	0.103 1
2-Methylbutyl acetate	0.872 (20)	4.63 (30)	1.82 (22)	26.75	0.098 9
Methyl butyrate	0.580 (20)	5.6 (20)	1.72 (22) [B]	27.48	0.114 5
	0.459 (40)				
3-Methylbutyric acid	2.731 (15)	2.64 (20)	0.63 (25)	27.28	0.088 6
	2.411 (20)				
3-Methylbutyronitrile		18 (220)	3.62 (25) [C]	27.58	0.082 7
Methyl chloroacetate		12.9 (21)		37.90	0.130 4
Methyl cyanoacetate	3.82 (50)	19.23 (50)		41.32	0.107 4
	2.69 (65)	17.57 (65)			
Methylcyclohexane	0.734 (20)	2.02 (20)	0	26.11	0.113 0
	0.685 (25)	2.07 (25)			
<i>cis</i> -2-Methylcyclohexanol	18.08 (25)	13.3*	2.58 (30) [Iq]*	32.45	0.077 0*
	13.60 (30)		1.95 (25) [B]*		
<i>trans</i> -2-Methylcyclohexanol	37.13 (25)				
	25.14 (30)				
<i>cis</i> -3-Methylcyclohexanol	19.7 (25)	16.47 (20)	1.91	29.08	0.062 9*
	17.23 (30)				
<i>trans</i> -3-Methylcyclohexanol	25.52 (16)	8.05	1.75	28.80 (30)	
	15.60 (30)				
<i>cis</i> -4-Methylcyclohexanol	0.247 (25)	13.3*	2.70 (30) [Iq]*	29.07	0.069 0*
			1.9 (25) [B]*		
<i>trans</i> -4-Methylcyclohexanol	0.385 (25)				
2-Methylcyclohexanone		16 (−15)	2.98 (25) [B]	34.06	0.102 7
		14 (20)			
3-Methylcyclohexanone		18 (−80)	3.06 (25) [B]	33.06	0.092 5
		12 (20)			
4-Methylcyclohexanone		15 (−41)	3.07 (25) [B]	32.83	0.093 5
		12 (20)			
Methylcyclopentane	0.507 (20)	1.985 (20)	0	24.63	0.116 3
	0.478 (25)				
Methyl decanoate			1.65 (20) [H]	30.33	0.091 2
Methyl dichloroacetate				37.00	0.121 9

* Mixed isomers.

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Methyl dodecanoate			1.70 (20) [H]	31.37	0.089 3
<i>N</i> -Methyl- formamide	1.99 (15) 1.65 (25)	200.1 (15) 182.4 (25)	3.86 (25) [B]	37.96 (30)	35.02 (50)
Methyl formate	0.360 (15) 0.319 (29)	8.5 (20)	1.77 [g]	28.29	0.157 2
Methyl heptanoate				28.29	0.157 2
2-Methyl-2- heptanol		3.38 (−7) 2.46 (25)			
2-Methyl-3- heptanol		3.37 (20) 3.75 (60)	1.63 (20) [B]		
2-Methyl-4- heptanol		3.30 (20) 3.65 (60)			
3-Methyl-3- heptanol		3.74 (20) 2.89 (60)			
3-Methyl-4- heptanol		9.1 (−20) 7.4 (20)			
4-Methyl-3- heptanol		5.25 (20) 4.62 (55)			
4-Methyl-4- heptanol		2.87 (20) 3.27 (60)			
Methyl hexadecanoate				31.50	0.077 5
2-Methylhexane	0.378 (20)	1.92 (20)	0	21.22	0.096 64
3-Methylhexane	0.372 (20)	1.93 (20)	0	21.73	0.097 0
Methyl hexanoate			1.70 (20) [H]	28.47	0.104 5
Methyl isobutyrate	0.523 (20) 0.419 (40)		1.98 (20) [B]	25.99	0.113 1
Methyl methacrylate	0.632 (20)	2.9 (20)	1.68 (25) [B]	28–29 (30)	
Methyl <i>o</i> -metho- xybenzoate		7.7 (21)			
Methyl <i>p</i> -metho- xybenzoate		4.3 (33)			
1-Methylnaph- thalene		2.7 (20)	0.23 (20) [B]	39.96	0.0934
Methyl <i>o</i> -nitro- benzoate		28 (25)	3.67 (30) [B]		
Methyl octadecanoate				32.20	0.77 5
2-Methyloctane		1.97 (20)	0	23.76	0.094 0
4-Methyloctane		1.97 (20)	0	24.22	0.094 0
Methyl octanoate				29.93	0.100 2
Methyl oleate	4.88 (20)	3.211 (20)		31.3 (25)	25.4 (100)
2-Methylpentane	0.310 (20) 0.295 (25)	1.88 (20)	0	19.37	0.099 7

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
3-Methylpentane	0.307 (25) 0.292 (30)	1.895 (20)	0	20.26	0.106 0
2-Methyl-2, 4-pentanediol	34.4 (20)		2.9 (0)	33.1 (20)	
4-Methylpen- tanenitrile	0.980 (20) 9.843 (30)	15.5 (22)	3.53 (25) [B]	28.89	0.091 7
Methyl pentanoate	0.713 (20)	4.3 (19)	1.62 (22) [B]	27.85	0.104 4
2-Methyl-1- pentanol				26.98	0.081 9
3-Methyl-1- pentanol				26.92	0.078 9
4-Methyl-1- pentanol				25.93	0.074 3
2-Methyl-2- pentanol				25.07	0.086 1
3-Methyl-2- pentanol				27.14	0.091 9
4-Methyl-2- pentanol	4.074 (25)			24.67	0.082 1
2-Methyl-3- pentanol				26.43	0.091 4
3-Methyl-3- pentanol				25.48	0.088 8
4-Methyl-2- pentanone	0.585 (20) 0.522 (30)	13.11 (20) 11.78 (40)		23.64 (20)	19.62 (60)
4-Methyl-3- penten-2-one	0.879 (25)	15.6 (0) 15.1 (20)	3.20 (25) [B]		
1-Methyl-1- phenylhy- drazine		7.3 (19)	1.84 (15) [B]		
Methyl phenyl sulfide			1.38 (20) [B]	42.81	0.123 8
2-Methylpropane	0.007 44 (20) [g]		0	12.83	0.123 6
2-Methylpro- panenitrile	0.551 (15) 0.456 (30)	20.2	4.07 [g] 3.60 (20) [B]		
2-Methyl-1- propanol	4.70 (15) 2.876 (30)	26 (−34) 17.93 (25)	2.96 (30) [lq] 1.78 (20) [B]	24.53	0.079 5
2-Methyl-2- propanol	3.316 (20) 2.039 (40)	10.9 (30) 8.49 (50)	1.67 (22) [B]	20.02 (15)	19.10 (30)
2-Methylpropene			0.50 [g]	14.84	0.131 9
<i>N</i> -Methylpro- pionamide	6.06 (20) 3.56 (40)	185 (20) 151 (40)	3.59 [g]	31.20 (20)	29.12 (50)
Methyl propionate	0.477 (15)	6.21	1.70 (22) [B]	27.58	0.125 8
2-Methylpro- pionic acid	1.213 (25) 1.126 (30)	2.73 (40)	1.08 (25) [lq]	25.55 (20)	25.13 (25)

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
1-Methylpropyl acetate				25.72	0.105 4
2-Methylpropyl acetate	0.702 (20) 0.366 (78)	5.29 (20)	1.87 (22) [B]	25.59	0.101 3
2-Methylpropylamine	21.7 (25)	4.43 (21)	1.27 (27)	24.48	0.109 2
2-Methylpropyl formate	0.680 (20)	6.41 (19)	1.88 (22)	26.14	0.112 2
Methyl propyl ketoxime		3.3 (20)			
2-Methylpyridine	0.805 (20) 0.710 (30)	9.8 (20)	1.96 (25) [B]	36.11	0.124 3
3-Methylpyridine			2.41 (25) [B]	37.35	0.115 3
4-Methylpyridine			2.60 (25) [B]	37.71	0.114 1
<i>N</i> -Methyl-2-pyrrolidinone	1.666 (25)	32.0 (25)	4.09 (30) [B]		
Methyl salicylate		9.41 (30)	2.47 (25) [B]	42.15	0.117 4
Methyl tetradecanoate			1.62 (25) [B]	31.00	0.080 0
2-Methyltetrahydrofuran	0.601 (0) 0.536 (10)	6.92 (0) 6.63 (10)			
Methyl thiocyanate	64.3 (0)	4.3 (19)	3.34 (20) [B]	40.66	0.130 5
Morpholine	2.53 (15) 1.79 (30)	7.33 (25)	1.75 (25) [lq] 1.52 (25) [B]	37.63 (20)	36.24 (30)
Naphthalene	0.780 (100) 0.967 (80)	2.54 (85)	0	42.84	0.110 7
1-Naphthonitrile		16 (70)			
2-Naphthonitrile		17 (70)			
<i>o</i> -Nitroaniline		34.5 (90)	4.28 (20) [B]		
<i>p</i> -Nitroaniline		56.3 (160)	6.3 (25) [B]	60.62	0.092 3
<i>o</i> -Nitroanisole			4.83 [g]	48.62	0.118 5
Nitrobenzene	2.165 (15) 1.55 (35)	34.82 (25) 24.9 (90)	4.22 [g] 3.96 (25) [B]	46.34	0.115 7
<i>m</i> -Nitrobenzyl alcohol		22 (20)			
2-Nitrobiphenyl	12 (45)		3.82 (20) [B]		
Nitroethane	0.677 (20) 0.63 (35)	28.06 (30) 27.4 (35)	3.61 [g]	35.27	0.125 5
Nitromethane	0.692 (15) 0.596 (30)	35.87 (30) 35.1 (35)	3.46 [g]	40.72	0.167 8
1-Nitro-2-methoxybenzene			4.83 [g]	48.62	0.118 5
<i>o</i> -Nitrophenol	2.343 (45)	17 (50)	3.14 (25) [B]	47.35	0.117 4
1-Nitropropane	0.798 (25) 0.70 (35)	23.24 (30) 22.7 (35)	3.60 [g]	32.62	0.100 9

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
2-Nitropropane	0.750 (25)	25.52 (30)	3.76 [g]	32.18	0.115 8
<i>N</i> -Nitrosodime- thylamine		53 (20)	4.01 (20) [B]		
<i>o</i> -Nitrotoluene	2.37 (20)	27.4 (20)	3.72 (20) [B]	44.10	0.117 4
	1.63 (40)	22.0 (58)			
<i>m</i> -Nitrotoluene	2.33 (20)	24 (20)	4.20 (20) [B]	43.54	0.111 8
	1.60 (40)	22 (58)			
<i>p</i> -Nitrotoluene	1.20 (60)	22 (52)	4.47 (25) [B]	42.26	0.097 4
Nonane	0.713 (20)	1.972 (20)	0	24.72	0.093 5
	0.666 (25)	1.85 (110)			
1-Nonanol	14.3 (20)		1.72 (20) [B]	29.79	0.078 9
1-Nonene	0.620 (20)		0.59 (20) [B]	24.90	0.093 8
	0.586 (25)				
(<i>Z,Z</i>)-9,12- Octadeca- dienoic acid		2.70 (70) 2.60 (120)	1.40 (18) [Hx]		
Octamethylcy- clotetrasiloxane	2.20 (20)	2.4 (20)	0.42 (25) [lq] 0.67 (25) [B]	20.19	0.081 1
Octamethyltri- siloxane	0.82 (20)	2.3 (20)	0.64 (25) [lq]	67.56 (25)	
Octane	0.546 (20)	1.95 (20)	0	23.52	0.095 1
	0.433 (40)	1.83 (110)			
Octanenitrile	1.811 (15)	13.90 (25)		29.61	0.080 2
	1.356 (30)				
Octanoic acid	5.828 (20)	2.45 (20)	1.15 (25) [lq]	29.2 (20)	28.7 (25)
	4.690 (25)				
1-Octanol	10.64 (15)	11.3 (10)	1.72 (20) [B]	29.09	0.079 5
	6.125 (30)	10.34 (20)			
2-Octanol		8.20 (20)	1.65 (20) [B]	27.96	0.082 0
		6.52 (40)			
2-Octanone		10.39 (20)	2.72 (15) [B]		
		7.42 (100)			
1-Octene	0.470 (20)	2.084 (20)	0.34 (20) [lq]	23.68	0.095 8
	0.447 (25)				
Oleic acid	38.80 (20)	2.46 (20)	1.44 (25) [lq]	32.80 (20)	27.94 (90)
	27.64 (25)	2.45 (60)			
Oxalyl chloride		3.5 (21)	0.93 (20) [B]		
2-Oxohexame- thyleneimine	9 (78)		3.88 (25) [B]		
4-Oxopentanoic acid				41.69	0.076 3
Palmitic acid		2.3 (70)			
Paraldehyde		13.9 (25)	1.91 (25) [lq]	28.28	0.106 2
Parathion	15.30 (25)		4.98 (25) [B]	39.2 (25)	

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN}\cdot\text{s}\cdot\text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn}\cdot\text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Pentachloroethane	2.741 (15) 2.070 (30)	3.73 (20)	0.92 [g] 0.98 (25) [lq]	37.09	0.117 8
Pentadecane	2.814 (22)		0	28.78	0.085 7
<i>cis</i> -1,3-Pentadiene		2.32 (25)	0.50 (25) [B]		
Pentanaldehyde		10.1 (17)	2.59 (20) [B]	27.96	0.101 0
Pentane	0.237 (15) 0.215 (25)	2.011 (−90) 1.84 (20)	0	18.25	0.112 1
1,5-Pentanediol	128 (20)		2.45 (20) [D]	43.2 (20)	
2,4-Pentanedione	0.6 (20)	25.7 (20) 17.39 (25)	3.03 [g] 2.5 (20) [B]	33.28	0.1144
Pentanenitrile	0.779 (15) 0.637 (30)	17.4 (21)	3.57 (25) [B]	27.44 (20)	26.33 (30)
1-Pentanethiol		4.55 (25) 4.23 (50)	1.54 (25) [lq]		
Pentanoic acid	2.359 (15) 1.774 (30)	2.66 (20)	1.61 (20) [D]	28.90	0.088 7
1-Pentanol	4.650 (15) 2.987 (20)	16.9 (20) 13.9 (25)	1.71 (20) [B]	27.54	0.087 4
2-Pentanol	5.130 (15) 2.780 (30)	13.82 (22)	1.66 (22) [B]	25.96	0.100 4
3-Pentanol	7.337 (15) 3.306 (30)	13.02 (22)	1.64 (22) [B]	24.60 (20)	23.76 (30)
2-Pentanone	0.473 (25)	15.45 (20) 11.73 (80)	2.72 (22) [B]	24.89	0.065 5
3-Pentanone	0.493 (15) 0.423 (30)	19.4 (−20) 17.00 (20)	2.72 (20) [B]	27.36	0.104 7
1-Pentene	0.24 (0)	2.10 (20)	0.34 (20) [lq]	18.20	0.109 9
<i>cis</i> -2-Pentene				19.73	0.117 2
<i>trans</i> -2-Pentene				18.90	0.099 7
Pentyl acetate	0.924 (20) 0.862 (25)	4.75 (20)	1.72 [g] 1.91 (25) [B]	27.66	0.099 4
Pentylamine	1.018 (20)	4.5 (22)	1.55 (30) [B]	24.4 (13)	
Pentyl formate		6.5 (20)		28.09	0.102 3
Pentyl nitrate		9 (18)			
Phenanthrene		2.8 (20)	0		
Phenol	6.024 (35) 3.421 (50)	9.78 (60)	1.53 (20) [B]	43.54	0.106 8
Phenoxyacetal- dehyde		4.8 (20)			
Phenoxyacetylene		4.8 (20)	1.42 (25) [lq]		
2-Phenyl- acetamide				46.26	0.078 8
Phenyl acetate	1.799 (45)	5.23 (20)	1.54 (22) [B]		
Phenylacetoneitrile	1.93 (25)	19.0 (25) 8.5 (234)	3.47 (27) [B]	44.57	0.115 5

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Phenylacetylene		3.0 (20)	0.72 (20) [B]		
1-Phenylethanol		13 (20) 7.6 (90)	1.51 (20) [B]	42.88	0.103 8
Phenylhydrazine		7.2 (21)	1.67 (25) [B]	48.14	0.129 2
Phenyl isocyanate		8.8 (20)			
Phenyl isothio- cyanate		10 (20)		42.73	0.108 6
1-Phenylpropene		2.7 (20)			
2-Phenylpropene		2.3 (20)			
3-Phenylpropene		2.6 (20)			
Phenyl propyl ether				34.27	0.105 6
Phenyl salicylate		6.3 (50)		45.20	0.097 6
Phosgene		4.7 (0) 4.3 (22) 36 (75)			
Phthalide					
DL- α -Pinene	1.61 (25)	2.64 (25)	0.60 (25) [B]	28.35	0.094 4
L- β -Pinene	1.70 (20) 1.41 (25)	2.76 (20)		28.26	0.093 4
Piperidine	1.679 (15) 1.224 (30)	5.8 (20)	1.19 (25) [B]	31.79	0.115 3
Propane [g]	0.008 1 (20) 0.010 7 (125)	1.6 (0)	0	9.22	0.087 4 [lq]
1,2-Propane- diamine	1.46	10.2			
1,3-Propane- diamine	17.85	9.55	1.96 (25) [B]		
1,2-Propanediol	56.0 (20) 18.0 (40)	32.0 (20)	2.27 (25) [D]	72.0 (25)	
1,3-Propanediol	56.0 (20) 18.0 (40)	35.0 (20)	2.52 (25) [D]	47.43	0.090 3
1-Propanethiol			1.55 (25) [lq]	27.38	0.127 2
2-Propanethiol			1.64 (25) [lq]	24.26	0.117 4
1-Propanol	2.522 (15) 1.722 (30)	22.2 (20) 20.33 (25)	1.67 [g] 1.75 (25) [B]	25.26	0.077 7
2-Propanol	2.859 (15) 1.765 (30)	18.3 (25) 16.24 (40)	1.69 [g] 1.66 (30) [B]	22.90	0.078 9
2-Propenaldehyde			3.04 [g] 2.90 (25) [B]		
Propene [g]	0.008 43 (20) 0.009 33 (50)	1.88 (20) 1.44 (90)	0.35 [g]	9.99	0.142 7 [lq]
2-Propen-1-ol	1.363 (20) 0.914 (40)	21.6 (15)	1.63 [g]	27.53	0.090 2
Propionaldehyde	0.357 (15) 0.317 (27)	18.5 (17)	2.75 [g] 2.57 (20) [B]		

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Propionamide			3.4 (30) [B]	39.05	0.090 9
Propionic acid	1.175 (15) 0.956 (30)	3.30 (10) 3.44 (40)	1.76 [g] 1.77 (25) [D]	28.68	0.099 3
Propionic anhydride	1.144 (20) 1.061 (25)	18.3 (16)		30.30 (20)	29.70 (25)
Propionitrile	0.454 (15) 0.389 (30)	22.2 (20) 24.2 (50)	4.06 [g] 3.60 (20) [B]	29.63	0.115 3
Propyl acetate	0.585 (20) 0.460 (40)	5.69 (19)	1.86 (25) [B]	26.60	0.112 0
Propylamine	0.343 (25)	5.31 (20)	1.17 [g] 1.36 (20) [B]	24.86	0.124 3
Propylbenzene		2.37 (20) 2.351 (30)	0.35 (25) [lq]	31.13	0.107 5
Propyl benzoate				36.55	0.106 9
Propyl butyrate	0.831 (20)	4.3 (20)		27.06	0.100 0
Propyl chloroacetate				32.91	0.108 3
Propylene carbonate	2.53	64.4			
Propylene oxide	0.327 (20) 0.28 (25)		2.00 [g]		
Propyleneimine	0.491 (25)		1.77 [g, <i>cis</i>] 1.60 [g, <i>trans</i>]		
Propyl formate	0.574 (20) 0.417 (40)	7.72 (19)	1.91 (22) [B]	26.77	0.111 9
Propyl isobutyrate	0.831 (20)			25.83	0.101 5
Propyl nitrate		14 (18)	3.01 (20) [B]	29.67	0.123 7
Propyl pantoate	1.053 (20)	4 (19)		27.72	0.098 4
Propyl propionate	0.673 (20)	4.7 (20)	1.79 (22) [B]	26.85	0.105 9
Propyne			0.75 [g]	14.51	0.148 2
2-Propyn-1-ol	1.68 (20)	24.5 (20)	1.78 (25) [B]	38.59	0.127 0
Pulegone		9.5 (20)	2.00 (25) [B]		
Pyrazadine			3.97 (35) [D]	50.55	0.103 6
Pyrazine		2.8 (54)	0		
Pyridine	1.130 (10) 0.829 (30)	12.3 (25) 9.4 (116)	2.20 (20) [B] 2.25 [g]	39.82	0.130 6
Pyrimidine			2.44 (35) [D]	32.85	0.101 0
Pyrrole	1.352 (20) 1.233 (25)	7.48 (18) 8.13 (25)	1.80 (25) [B]	39.81	0.110 0
Pyrrolidine			1.58 (20) [B]	31.48	0.090 0
2-Pyrrolidone	13.3 (25)		3.55 (25) [B]		
Quinoline	4.354 (15) 3.37 (25)	9.00 (25)	2.18 (25) [B]	45.25	0.106 3
Safrole	2.294 (25)	3.1 (21)			
Salicylaldehyde	2.90 (20) 1.67 (45)	13.9 (20)	3.1 (30) [lq] 2.86 (20) [B]	45.38	0.124 2

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Squalane	6.08 (20)		0		
Squalene	12 (25)		0.68 (25) [B]		
D-Sorbitol		33 (80)			
Stearic acid	11.6 (70)	2.29 (70)	1.76 (25) [D]		
		2.26 (100)			
Styrene	0.751 (20)	2.43 (25)	0.13 (25) [Iq]	32.0 (20)	30.98 (30)
	0.696 (25)	2.32 (75)			
Succinonitrile	2.591 (60)	56.5 (57)	3.68 (30)	53.26	0.107 9
	2.008 (75)	54 (68)	[toluene]		
1, 1,2,2-	13.950 (11)	8.6 (3)	1.29 (20) [H]	52.37	0.146 3
Tetrabromo-	9.797 (20)	7.0 (22)			
ethane					
1, 1,2,2-	1.21 (25)	2.52 (25)		26.13	0.113 3
Tetrachloro-	1.208 (30)				
difluoroethane					
1, 1,2,2-Tetrachloroethane	1.844 (15)	8.20 (20)	1.29 [g]	38.75	0.126 8
	1.456 (30)		1.45 (25) [H]		
Tetrachloroethylene	1.932 (15)	2.30 (25)	0	32.86 (15)	31.27 (30)
	0.798 (30)				
Tetradecamethyl-cycloheptasiloxane		2.7 (20)			
Tetradecamethyl-hexasiloxane		2.5 (20)	1.58 (20) [Iq]	17.42 (25)	
Tetradecane	2.131 (22)		0	28.30	0.086 9
Tetradecanoic acid		0.76 (25) [B]	33.90	0.093 2	
1-Tetradecanol		4.72 (38)	1.69 (25) [C]	32.72	0.070 3
		4.40 (48)			
Tetraethylene glycol	44.9 (25)		5.84 (20) [Iq]	45 (25)	
Tetraethyllead			0.3 (20) [B]	30.50	0.096 9
Tetraethylsilane			0	25.22	0.107 9
Tetraethyl silicate		4.1 (20)	1.72 (32) [B]	23.63	0.097 9
Tetrahydrofuran	0.55 (20)	11.6 (−70)	1.75 (25) [B]	26.5 (25)	
	0.460 (25)	7.58 (25)			
2,5-Tetrahydrofuran-dimethanol	225 (25)				
Tetrahydro-2-furanmethanol	6.24 (20)	13.61 (23)	2.12 (35) [Iq]	39.96	0.100 8
1,2,3,4-Tetrahydronaphthalene	2.202 (20)	2.76 (20)	0.60 (25) [Iq]	35.55	0.095 4
	2.003 (25)				
1,2,3,4-Tetrahydro-2-naphthol		11.7 (20)			
		6.7 (90)			

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Tetrahydropyran	0.826 (20) 0.764 (25)	5.61 (25)	1.55 (25) [B]		
Tetrahydropyran- 2-methanol	11.0 (20)			34.1 (25)	
Tetrahydrothi- ophene-1, 1-dioxide	9.87 (30)	43.3 (30)	4.81 (25) [B]	35.5 (30)	
Tetrahydrothio- phene oxide	52 (30) 19 (80)	42.5 (30)			
1,1,2,2-Tetra- methylurea		23.06	3.47 (25) [B]		
Tetranitromethane	1.76 (20)	2.32 (20)	0		
Tetrathiomethyl- methane		2.82 (70)			
Thiacyclohexane				36.06 (20)	33.74 (40)
Thiacyclopentane	1.042 (20) 0.971 (25)		1.90 (25) [B]	38.44	0.134 2
Thioacetic acid		12.8 (20)			
2,2'-Thiodiethanol	65.2 (20)			53.8 (20)	
Thiophene	0.662 (20) 0.353 (82)	2.76 (16) 2.57 (25)	0.55 [g] 0.52 (25) [B] 1.55 (25) [B]	34.00	0.132 8
Thymol			0.45 (20) [lq]	33.95	0.082 1
Toluene	0.623 (15) 0.523 (30)	2.385 (20) 2.364 (30)		30.90	0.118 9
<i>p</i> -Toluenesulfonyl chloride				42.41	0.090 3
<i>o</i> -Toluidine	5.195 (15) 4.39 (20)	6.34 (18) 5.71 (58)	1.60 (25) [B]	42.87	0.109 4
<i>m</i> -Toluidine	4.418 (15) 2.741 (30)	5.95 (18) 5.45 (58)	1.45 (25) [B]	40.33	0.097 9
<i>p</i> -Toluidine	1.945 (45) 1.557 (60)	4.98 (54)	1.52 (25) [B]	39.58	0.095 7
<i>m</i> -Tolunitrile			4.21 (22) [B]	38.85	0.101 3
<i>p</i> -Tolunitrile			4.47 (20) [B]	39.79	0.110 0
Tribenzylamine			0.65 (20) [B]	42.41	0.095 3
Tributyl phosphite	1.9 (25)		1.92 (20) [C]	27.57	0.086 5
2,2,2-Tribromo- acetaldehyde		7.6 (20)	1.70 (20) [B]		
Tribromoethane	2.152 (15) 1.741 (30)	4.39 (20)	0.99 [g]	48.14	0.130 8
1,2,3-Tribro- mopropane		6.45 (20)	1.59 (25) [B]	47.99	0.126 7
Tributylamine	1.35 (25)		0.78 (25) [B]	26.47	0.083 1
Tributyl borate	1.776 (20) 1.601 (25)		0.78 (25) [C]	26.2 (20)	25.8 (25)

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Tributyl phosphate	111.1 (15)	3.39 (25)	7.96 (30) [B]	3.07 (25) 28.71	0.066 6
Trichloroace- taldehyde		7.6 (−40) 4.9 (20)	1.96 (25) [B]	27.66	9.119 7
Trichloroacetic acid		4.6 (60)	1.1 (25) [B, dimer]	35.4	0.089 5
Trichloro- acetonitrile		7.85 (19)	1.93 (19) [Iq]		
1,1,1-Trichlo- roethane	0.903 (15) 0.725 (30)	7.1 (7) 7.52 (20)	1.79 [g] 1.6 (25) [B]	28.28	0.124 2
1,1,2-Trichlo- roethane	0.119 (20) 0.110 (25)	8.78 (23)	1.45 [g]	37.40	0.135 1
Trichloroethylene	0.566 (20) 0.532 (25)	3.42 (16)	0.77 (30) [Iq] 0.95 (30) [B]	29.5 (20)	28.8 (25)
Trichlorofluoro- methane	0.42 (25) 0.011 (25) [g]	2.28 (29)	0.45 [g] 0.49 [Iq]	18 (25)	
Trichloro- methylsilane	0.47 (20)		1.87 (25) [B]	20.3 (20)	
2,4,6-Trichloro- phenol			1.88 (25) [D]	43.13	0.095 5
1,2,3-Trichloro- propane		7.5 (20)	1.61 [g]	37.8 (20)	37.05 (25)
Trichlorosilane	0.332 (20) 0.316 (25)		0.86 [g] 0.98 (25) [B]	20.43	0.107 6
α,α,α -Trichloro- toluene	3.07 (10) 2.55 (17)	6.9 (21)	2.17 (20) [B]		
1,1,2-Trichloro- 1,2,2,-trifluoro- ethane	0.711 (20) 0.627 (30)	2.41 (25)		17.75 (20)	16.56 (30)
Tridecane	1.883 (20) 1.55 (23)		0	27.73	0.087 2
1-Tridecene				28.01	0.088 4
Triethanolamine	613.6 (25) 208.1 (40)	29.36 (25)	3.57 (25) [B]		
Triethylaluminum		2.9 (20)			
Triethylamine	0.394 (15) 0.363 (30)	2.42 (25)	0.66 [g] 0.9 (25) [B]	22.70	0.099 2
Triethylene glycol	49.0 (20) 8.5 (60)	23.7 (20)	5.58 (20) [Iq]	47.33	0.088 0
Triethyl phosphate	1.684 (40) 1.376 (55)	13.43 (15) 10.93 (65)	3.08 (25) [B]	31.81	0.092 8
Triethyl phosphite	0.72 (25)	5.0	1.82 (25) [D]	25.73	0.087 8

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Trifluoroacetic acid	0.926 (20) 0.653 (40)	8.55 (20) 5.76 (50)	2.28 [g]	15.64	0.184 4
2,2,2-Trifluoroethanol	1.996 (20)		2.03 (25) [cH]	20.6 (33)	
α,α,α -Trifluorotoluene		9.2 (30) 8.1 (60)			
Trimethylamine	0.321 (–33)	2.4 (25)		16.24	0.113 3
1,2,3-Trimethylbenzene		2.636 (20) 2.609 (30)	0.56 (20) [lq]	30.91	0.104 0
1,2,4-Trimethylbenzene	0.894 (15) 0.730 (30)	2.38 (20) 2.36 (30)	0.30 (20) [lq]	31.76	0.102 5
1,3,5-Trimethylbenzene	1.154 (20)	2.28	0	29.79	0.089 7
Trimethyl borate		8 (20)	0.82 (25) [C]		
2,2,3-Trimethylbutane	0.579 (20)	1.93 (20)	0	20.70	0.097 3
<i>cis</i> , <i>cis</i> -1,3,5-Trimethylcyclohexane	0.632 (20) 0.558 (30)				
<i>trans</i> -1,3,5-Trimethylcyclohexane	0.714 (20) 0.624 (30)				
Trimethylene sulfide	0.638 (20) 0.607 (25)		1.78 (25) [B]	36.3 (20)	35.0 (30)
3,5,5-Trimethyl-1-hexanol	11.06 (25)				
2,6,8-Trimethyl-4-nonanone	1.9 (20)				
1,3,5-Trimethyl-2-oxabicyclo-[2.2.2]octane		4.57 (24)	1.54 (25) [C]	32.1 (20)	31.1 (25)
2,2,3-Trimethylpentane	0.598 (20)	1.962 (20)	0	22.46	0.089 5
2,2,4-Trimethylpentane	0.502 (20)	1.940 (20)	0	20.55	0.088 8
Trimethyl phosphite	0.61 (20)		1.83 (20) [C]	27.18 (20)	24.88 (40)
2,4,6-Trimethylpyridine	1.498 (20) 1.496 (25)	6.6	1.95 (25) [B]		
Triphenylamine				46.2	0.095 5
Triphenyl phosphite	25.18 (15) 6.95 (45)	3.67 (45) 3.57 (65)	2.04 (25) [B]		
Tripropylamine			0.58 (20) [lq] 0.76 (20) [B]	24.58	0.087 8

TABLE 4.10 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Organic Substances (*continued*)

Substance	Viscosity η , $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
Tripropylene glycol	56.1 (25)			34 (25)	
Tripropylene glycol butyl ether	6.58 (25)			28.8 (25)	
Tripropylene glycol ethyl ether	5.17 (25)			28.2 (25)	
Tripropylene glycol isopropyl ether	7.7 (25)			27.4 (25)	
Tripropylene glycol methyl ether	5.96 (25)			30.0 (25)	
Tris(dimethylamino) phosphine oxide	3.34 (30)	30 (20)			
Tris(4-ethylphenyl) phosphite	30.22 (15) 9.047 (45)	3.74 (15) 3.61 (45)	2.08 (25) [B]		
Tris(<i>m</i> -tolyl) phosphite	37.55 (15) 9.132 (45)	3.67 (15) 3.53 (45)	1.62 (25) [B]		
Tris(<i>p</i> -tolyl) phosphite	35.52 (15) 8.794 (45)	3.88 (15) 3.74 (45)	1.77 (25) [B]		
Tritolyl phosphate	38.8 (35) 16.8 (55)	6.92 (40)	2.84 (40) [C]	40.9 (20)	
Undecane	1.186 (20) 0.761 (50)	2.00 (20) 1.84 (150)	0	26.26	0.090 1
2-Undecanone	1.61 (30)		2.71 (15) [B] 4.59 (25) [D]		
Urea					
Vinyl acetate	0.421 (20)		1.79 (25) [B]	23.95 (20)	22.54 (30)
<i>o</i> -Xylene	0.809 (20) 0.627 (40)	2.57 (20) 2.54 (30)	0.62 [g] 0.52 (25) [lq]	32.51	0.110 1
<i>m</i> -Xylene	0.617 (20) 0.497 (40)	2.37 (20) 2.35 (30)	0.33 (20) [lq] 0.37 (20) [B]	31.23	0.110 4
<i>p</i> -Xylene	0.644 (20) 0.513 (40)	2.26 (20) 2.22 (50)	0	30.69	0.107 4
Xylitol		40 (20)			

TABLE 4.11 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substance

Temperature in degree celsius are indicated in parentheses. The physical state of the substance is indicated in square brackets

Substance	Viscosity, mN · s · m ⁻²	Dielectric constant, ε	Dipole moment, D	Surface tension, dyn · cm ⁻¹	
				<i>a</i>	<i>b</i>
Air (20 °C)	0.018 2	1.000 536 4	5.2		
AlBr ₃		3.38 ¹⁰⁰			
Ar	0.022 3	1.000 517 2			
[g] (20 °C)		1.538 ⁻¹⁹¹	0	34.28	0.249 3
AsBr ₃		8.83 ³⁵	1.61	54.51	0.1043
AsCl ₃		12.6 ²⁰	1.59	41.67	0.097 81
AsH ₃ (arsine)		2.05 ²⁰	0.20		
BBr ₃		2.58 ⁰	0	31.90	0.128 0
BCl ₃			0		
BF ₃			0	-2.92	0.230 0
B ₂ H ₆ (diborane)		1.872 ^{-92.5}	0	-3.13	0.178 5
B ₅ H ₉			2.13		
B ₃ H ₆ N ₃ (triborotriazine)			0		
Br ₂					
[g] (20 °C)		1.012 8			
[lq]	1.03 ¹⁶	3.09 ²⁰	0	45.5	0.182 0
BrF ₃	2.22 ²⁰		1.1	38.30	0.099 9
BrF ₅	0.62 ²⁴	7.91 ^{24.5}	1.51	25.24	0.109 8
Cl ₂					
[g] (20 °C)	0.013 2		0		
[lq]		1.91 ¹⁴			
ClF ₃	0.48 ¹²	4.29 ²⁵	0.554	26.9	0.166 0
ClO ₃ F (perchloryl fluoride)			0.023	12.24	0.157 6
Co					
[g]	0.017 5 ²⁰	1.000 70 ⁰	0.112		
[lq]				-30.20	0.207 3
CO ₂					
[g] (20 °C)	0.014 7	1.000 922	0		
[lq]	0.071 ²⁰	1.60 ^{0 °C, 50 atm}			
COCl ₂		4.34 ²²	1.17	22.59	0.145 6
COF ₂			0.95		
COS			0.712	12.12	0.177 9
COSe		3.47 ¹⁰	0.73		
CS			1.98		
CS ₂					
[g]		1.002 9 ⁰	0		
[lq]	0.375 ²⁰	2.6 ²⁰			
CrO ₂ Cl ₂ [chromyl(VI) chloride]		2.6 ²⁰	0.47		
D ₂ (deuterium)		1.277 ⁻²⁵³			
DH				6.537	0.188 3
D ₂ O	1.098 ²⁵	78.25 ²⁵	1.87	(71.72 ²⁰)*	(68.38 ⁴⁰)*

*Actual values of surface tension.

TABLE 4.11 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*continued*)

Substance	Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
F ₂		1.54 ⁻²⁰²		-16.10	0.164 6
GaCl ₃			0.85	35.0	0.100 0
GeCl ₄		2.430 ²⁵	0	(22.44 ³⁰)*	
H ₂					
[g] (20°C)	0.008 8	1.000 253 8	0		
[lq]		1.228 ^{20.4 K}			
HBr					
[g]		1.003 13 ⁰	0.82		
[lq]	0.83 ⁻⁶⁷	3.82 ²⁵		13.10	0.207 9
HCl					
[g]		1.004 6 ⁰	1.08		
[lq]	0.51 ⁻⁹⁵	4.60 ²⁸			
HCN	0.206 ¹⁸	116 ²⁰	2.98	(19.45 ¹⁰)*	(18.33 ²⁰)*
HCNO (isocyanate)			1.6		
HCNS (isothiocyanate)			1.7		
HF	0.256 ⁰	83.6 ⁰	1.82	10.41	0.078 67
HI					
[g]		1.002 34 ⁰	0.44		
[lq]		2.90 ²²			
NH ₃ (azide)			0.8		
H ₂ O (see Table 4.12)					
H ₂ O ₂	1.25 ²⁰	84.2 ⁰	2.2	78.97	0.154 9
HNO ₃			2.17		
H ₂ S					
[g]		1.00 4 0 ⁰	0.97		
[lq]	0.412 ⁰	5.93 ¹⁰		48.95	0.175 8
H ₂ Se			0.24	22.32	0.148 2
H ₂ SO ₄	24.54 ²⁵	100 ²⁵			
HSO ₃ Cl (chlorosulfonic acid)	2.43 ²⁰	60 ²⁰			
HSO ₂ F (fluorosulfonic acid)	1.56 ²⁵	~120 ²⁵			
H ₂ Te			<0.2	29.03	0.261 9
He					
[g] (20°C)	0.019 6	1.000 065 0	0		
Hg	1.552 ²⁰		0	490.6	0.204 9
I ₂	1.98 ¹¹⁶	11.1 ¹¹⁸	0		
IF ₅			2.18	33.16	0.131 8
Kr					
[g] (20°C)	0.025 0		<0.05		
[lq]				40.576	0.289 0
Ne[g] (20°C)	0.031 3	1.000 063 9	0		
N ₂					
[g] (20°C)	0.017 6	1.000 548 0	0		
[lq]		1.454 ⁻²⁰³		26.42	0.226 5

*Actual values of surface tension.

TABLE 4.11 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*continued*)

Substance	Viscosity, mN · s · m ⁻²	Dielectric constant, ε	Dipole moment, D	Surface tension, dyn · cm ⁻¹	
				<i>a</i>	<i>b</i>
NH ₃					
[g]		1.007 2 ⁰	1.47		
[lq]	0.254 ^{-33.5}	22.4 ^{-33.4}		(37.91 ⁻⁵⁰)*	(35.38 ⁻⁴⁰)*
N ₂ H ₄ (hydrazine)	0.97 ²⁰	52.9 ²⁰	1.75		
NO			0.153	-67.48	0.585 3
N ₂ O					
[g]	0.014 6 ²⁰	1.001 13 ⁰	0.167		
[lq]		1.52 ¹⁵		5.09	0.203 2
NO ₂			0.316		
N ₂ O ₄		2.56 ¹⁵	0.5		
NOBr (nitrosyl bromide)		13.4 ¹⁵	1.8		
NOCl		18.2 ¹²	1.9	29.49	0.149 3
NOF			1.81	14.00	0.116 5
NO ₂ F (nitryl fluoride)			0.47	8.26	0.185 4
O ₂					
[g] (20 °C)	0.020 4	1.000 494 7	0		
[lq]		1.507 ⁻¹⁹³		-33.72	0.256 1
O ₃			0.53	(38.1 ⁻¹⁸³)*	
OF ₂ (oxygen difluoride)			0.297		
OsO ₄			0		
PBr ₃		3.9 ²⁰	0.5	45.34	0.128 3
PCl ₃		3.43 ²⁵	0.78	31.14	0.126 6
PCl ₅		2.7 ¹⁶⁵	0.9		
PF ₅			0		
PH ₃		2.9 ¹⁵	0.58		
PI ₃		4.12 ⁶⁵	0	61.66	0.067 71
POCl ₃	1.065 ²⁵	13.7 ²⁵	2.41	35.22	0.127 5
POF ₃			1.76		
PSCl ₃		5.8 ²²	1.42	37.00	0.127 2
PbCl ₄		2.78 ²⁰			
S ₂ Cl ₂ dimer		4.79 ¹⁵	1.0	46.23	0.146 4
S ₂ F ₂					
FSSF isomer			1.45		
S=SF ₂ isomer			1.03		
SF ₄			0.632	12.87	0.173 4
SF ₆			0	5.66	0.119 0
S ₂ F ₁₀		2.020 ²⁰	0		
SO ₂					
[g]	0.012 6 ²⁹	1.009 3 ⁰	1.63		
[lq]		15.0 ⁰		26.58	0.194 8
SO ₃		3.11 ¹⁸	0		
SOBr ₂ (thionyl bromide)		9.06 ²⁰	9.11		
SOCI ₂		9.25 ²⁰	1.45	36.10	0.141 6

*Actual values of surface tension.

TABLE 4.11 Viscosity, Dielectric Constant, Dipole Moment, and Surface Tension of Selected Inorganic Substances (*continued*)

Substance	Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Dipole moment, D	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$	
				<i>a</i>	<i>b</i>
SO_2Cl_2 (sulfuryl chloride)		9.15^{20}	1.81	32.10	0.132 8
SbCl_3		33.2^{75}	3.93	47.87	0.123 8
SbCl_5		3.22^{20}	0		
SbF_5				49.07	0.193 7
SbH_3			0.12		
SeF_4				38.61	0.127 4
SeF_6			0		
SeOCl_2		55^{25}	2.64		
SiCl_4		2.40^{16}	0	20.78	0.099 62
SiF_4			0		
SiH_4			0		
SiHCl_3			0.86	20.43	0.107 6
SnBr_4			0		
SnCl_4		2.89^{20}	0	29.92	0.113 4
TeF_6			0		
TiCl_4		2.80^{20}	0	$(33.54^{20})^*$	$(31.06^{40})^*$
UF_6					
[g]		$1.002\,92^{67}$	0		
[lq]		2.18^{65}		25.5	0.124 0
VCl_4		3.05^{25}	0		
VOBr_3		3.6^{25}			
VOCl_3		3.4^{25}	0.3	$(36.36^{20})^*$	$(33.60^{40})^*$
Xe [g] (20 °C)	0.022 8	1.001 23	0		

*Actual values of surface tension.

TABLE 4.12 Refractive Index, Viscosity, Dielectric Constant, and Surface Tension of Water at Various Temperatures

Temperature, °C	Refractive index, n_D	Viscosity, $\text{mn} \cdot \text{s} \cdot \text{m}^{-2}$	Dielectric constant, ϵ	Surface tension, $\text{dyn} \cdot \text{cm}^{-1}$
0	1.333 95	1.770 2	87.74	75.83
5	1.333 88	1.510 8	85.76	75.09
10	1.333 69	1.303 9	83.83	74.36
15	1.333 39	1.137 4	81.95	73.62
20	1.333 00	1.001 9	80.10	72.88
21	1.332 90	0.976 4	79.73	72.73
22	1.332 80	0.953 2	79.38	72.58
23	1.332 71	0.931 0	79.02	72.43
24	1.332 61	0.910 0	78.65	72.29
25	1.332 50	0.890 3	78.30	72.14
26	1.332 40	0.870 3	77.94	71.99
27	1.332 29	0.851 2	77.60	71.84
28	1.332 17	0.832 8	77.24	71.69
29	1.332 06	0.814 5	76.90	71.55
30	1.331 94	0.797 3	76.55	71.40
35	1.331 31	0.719 0	74.83	70.66
40	1.330 61	0.652 6	73.15	69.92
45	1.329 85	0.597 2	71.51	69.18
50	1.329 04	0.546 8	69.91	68.45
55	1.328 17	0.504 2	68.35	67.71
60	1.327 25	0.466 9	66.82	66.97
65	1.326 16	0.434 1	65.32	66.23
70	1.325 11	0.405 0	63.86	65.49
75	1.323 99	0.379 2	62.43	64.75
80		0.356 0	61.03	64.01
85		0.335 2	59.66	63.28
90		0.316 5	58.32	62.54
95		0.299 5	57.01	61.80
100		0.284 0	55.72	61.80

COMBUSTIBLE MIXTURES**TABLE 4.13** Properties of Combustible Mixtures in Air

Additional compounds can be found in National Fire Protection Association, *Fire Protection Handbook*, 14th ed., 1976.

Substance	Autoignition temperature, °C	Flammable limits, percent by volume of fuel (25°C, 760 mm)	
		Lower	Upper
Acetaldehyde	175	4.0	6.0
Acetic acid, glacial	465	5.4	16.0
Acetic anhydride	390	2.9	10.3
Acetone	465	2.6	12.8
Acetonitrile	524	4.4	16.0
Acetylene	305	2.5	100
Acrolein	235*	2.8	31.0
Acrylonitrile	481	3.0	17
Allyl alcohol	378	2.5	18.0
Allylamine	374	2.2	22
Ammonia, anhydrous	651	16	25
Aniline	615	1.3	
Benzene	560	1.3	7.1
Biscyclohexyl	245	0.7 (100°C)	5.1 (150°C)
1-Bromobutane	265	2.6 (100°C)	6.6 (100°C)
3-Bromopropene	295	4.4	7.3
Butane	405	1.9	8.5
Butanol	365	1.4	11.2
2-Butanone	516	1.8	10
1-Butene	385	1.6	10.0
3-Buten-1-ol		4.7	34
Butyl acetate	425	1.7	7.6
Butylamine	312	1.7	9.8
Butylbenzene	410	0.8	5.8
Butylene oxide		1.5	18.3
Butyl formate	322	1.7	8.2
Butyraldehyde	230	2.5	12.5
Butyric acid	450	2.0	10.0
Carbon disulfide	90	1.3	50.0
Carbon monoxide	609	12.5	74
Carbonyl sulfide		12	29
Chlorobenzene	640	1.3	7.1
2-Chloro-1,3-butadiene		4.0	20.0
1-Chlorobutane		1.8	10.1
2-Chloro-2-butene		2.3	9.3
1-Chloro-1,1-difluoroethane		6.2	17.9
2-Chloroethanol	425	4.9	15.9
Chloromethane	632	10.7	17.4

*Unstable.

TABLE 4.13 Properties of Combustible Mixtures in Air (*continued*)

Substance	Autoignition temperature, °C	Flammable limits, percent by volume of fuel (25 °C, 760 mm)	
		Lower	Upper
1-Chloropentane	260	1.6	8.6
2-Chloropropane	593	2.8	10.7
1-Chloro-1-propene		4.5	16
3-Chloro-1-propene	485	2.9	11.1
Chlorotrifluoroethylene		8.4	38.7
Crotonaldehyde	232	2.1	15.5
Cumene	425	0.9	6.5
Cyanogen		6.6	42.6
Cyclohexane	245	1.3	8
Cyclopropane	500	2.4	10.4
Decahydronaphthalene	250	0.7	4.9
Decane	210	0.8	5.4
Diborane	38–52 [†]	0.8	88
Dibutyl ether	194	1.5	7.6
<i>o</i> -Dichlorobenzene	648	2.2	9.2
1,2-Dichloroethylene		9.7	12.8
Dichloropropane	557	3.4	14.5
Diisopropyl ether	443	1.4	7.9
Diethylamine	312	1.8	10.1
Diethyl ether	160	1.9	36.0
2,2-Dimethylbutane	425	1.2	7.0
Dimethyl ether		3.4	27.0
<i>N,N</i> -Dimethylformamide	445	1.2	7.0
1,1-Dimethylhydrazine	249	2	95
2,3-Dimethylpentane	335	1.1	6.7
2,2-Dimethylpropane	450	1.4	7.5
Dimethyl sulfide	206	2.2	19.7
Dimethyl sulfoxide	215	2.6	28.5
1,4-Dioxane	180	2.0	22.0
Divinyl ether	360	1.7	27
Ethane	515	3.0	12.5
Ethanol	365	3.3	19
2-Ethoxyethanol	235	1.8	14.0
1-Ethoxypropane		1.7	9.0
Ethyl acetate	427	2.2	11.0
Ethylamine	385	3.5	14.0
Ethylbenzene	432	1.0	6.7
Ethylcyclobutane	210	1.2	7.7
Ethylene	490	2.7	36.0
Ethyleneimine	320	3.6	46
Ethylene oxide	429	3.6	100
Ethyl formate	455	2.8	16.0
1,3-Ethylidene dichloride	440	6.2	16
Ethyl nitrite	90	3.0	50

[†]Ignites in moist air.

TABLE 4.13 Properties of Combustible Mixtures in Air (*continued*)

Substance	Autoignition temperature, °C	Flammable limits, percent by volume of fuel (25°C, 760 mm)	
		Lower	Upper
Ethyl propionate	440	1.9	11
Ethyl vinyl ether	202	1.7	28
Formaldehyde	429	7.0	73
2-Furaldehyde	316	2.1	19.3
Furan		2.3	14.3
Furfuryl alcohol	491	1.8	16.3
Gasoline, 92 octane	~280	1.4	7.6
Heptane	215	1.0	6.7
Hexane	225	1.1	7.5
2-Hexanone	533	1.2	8
Hydrocyanic acid, 96%	538	5.6	40.0
Hydrogen	400	4.0	75
4-Hydroxy-4-methyl-2-pentanone	603	1.8	6.9
Isobutyl acetate	421	2.4	10.5
Isobutylbenzene	430	0.8	6.0
Isopentane	420	1.4	7.6
Isopentyl acetate	360	1.0	7.5
Isoprene	220	2	9
Isopropyl acetate	460	1.8	8
Isopropyl alcohol	399	2.0	12
Methane	540	5.4	15.0
Methanethiol		3.9	21.8
Methanol	385	6.7	36.0
2-Methoxyethyl acetate		1.7	8.2
Methyl acetate	502	3.1	16
Methyl acrylate		2.8	25
Methylamine	430	4.9	20.6
2-Methyl-2-butanol	437	1.2	9.0
3-Methyl-1-butene	365	1.5	9.1
Methylcyclohexane	250	1.2	6.7
Methyl formate	465	5.0	23
2-Methylpropene	465	1.8	9.6
4-Methyl-2-pentanone	460	1.4	7.5
2-Methylpropene	465	1.8	9.6
α -Methylstyrene	574	1.9	6.1
Methyl propionate	469	2.5	13
Nicotine	244	0.7	4.0
Nitrobenzene	482	1.8 (93°C)	
Nonane	205	0.8	2.9
Octane	220	1.0	6.5

TABLE 4.13 Properties of Combustible Mixtures in Air (*continued*)

Substance	Autoignition temperature, °C	Flammable limits, percent by volume of fuel (25°C, 760mm)	
		Lower	Upper
Pentanamine		2.2	22
Pentane	260	1.5	7.8
2-Pentanone	505	1.5	8.2
Pentyl acetate	360	1.1	7.5
Petroleum ether	550	1.1	5.9
Propane	450	2.2	9.5
1,3-Propanediol	371	2.6	12.5
Propanol	440	2.1	13.5
Propene	460	2.0	11.1
Propanamine	318	2.0	10.4
Propionaldehyde	207	2.9	17.0
Propyl acetate	450	2.0	8
Propylene oxide		2.8	37.0
Propyl nitrate	175	2	100
Pyridine	482	1.8	12.4
Styrene	490	1.1	6.1
Tetrahydrofuran	321	2	11.8
Tetrahydrofurfuryl alcohol	282	1.5	9.7
Tetrahydronaphthalene	385	0.8	5.0
Toluene	480	1.2	7.1
Trichloroethylene	420	12.5	90
Triethylamine		1.2	8.0
Triethylene glycol	371	0.9	9.2
Trimethylamine	190	2.0	11.6
Trioxane	414	3.6	29
Vinyl acetate	427	2.6	13.4
Vinyl butyrate		1.4	8.8
Vinyl chloride	461	3.6	33.0
Vinyl fluoride		2.6	21.7
Xylene, <i>m</i> - and <i>p</i> -	530	1.1	7.0
Xylene, <i>o</i> -	465	1.0	6.0

SECTION 5

THERMODYNAMIC PROPERTIES

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ENTHALPIES AND GIBBS (FREE) ENERGIES OF FORMATION, ENTROPIES, AND HEAT CAPACITIES

The tables in this section contain values of the enthalpy (ΔH_f) and Gibbs (ΔG_f , free) energy of formation, entropy (S), and heat capacity (C_p) at 298.15 K (25°C). The tables cover common organic compounds. No values are given in these tables for metal alloys or other solid solutions, for fused salts, or for substances of undefined chemical composition.

For a more complete listing of compounds see the tables in *Selected Values of Chemical Thermodynamical Properties*, by D. D. Wagman *et al.*, National Bureau of Standards Technical Notes 270-3, 270-4, 270-5, 270-6, 270-7, and 270-8, Washington; *JANAF Thermochemical Tables*, by D. R. Stull and H. Prophet, National Bureau of Standards Publication 37, Washington; supplements to JANAF appearing in *J. Phys. Chem. Ref. Data*; D. R. Stull, E. F. Westrum, Jr., and G. C. Sinke, *The Chemical Thermodynamics of Organic Compounds*, Wiley-Interscience, New York, 1969; and I. Barin and O. Knacke, *Thermochemical Properties of Inorganic Substances*, Springer-Verlag, Berlin, 1973.

The values of the thermodynamic properties of the pure substances given in these tables are, for the substances in their standard states, defined as follows:

Pure solid (c) or liquid (liq). The substance is in the condensed phase under a pressure of 1 atm.

Gas (g). The standard state is the hypothetical ideal gas at unit fugacity, in which state the enthalpy is that of the real gas at the same temperature and at zero pressure.

The values of ΔH_f° and ΔG_f° given in the tables represent the change in the appropriate thermodynamic quantity when one gram formula weight of the substance in its standard state is formed, isothermally at the indicated temperature, from the elements, each in its appropriate standard reference state. The standard reference state at 25°C for each element has been chosen to be the standard state that is thermodynamically stable at 25°C and 1 atm pressure. The standard reference states are indicated in the tables by the fact that the values of ΔH_f° and ΔG_f° are exactly zero.

The values of S° represent the virtual or "thermal" entropy of the substance in the standard state at 298.15 K, omitting contributions from nuclear spins. Isotope mixing effects are also excluded except in the case of the ^1H – ^2H system.

The physical state of each substance is indicated in the column headed "State" as crystalline solid (c), liquid (liq), gaseous (g), or amorphous (amorp). Solutions in water are listed as aqueous (aq). Solutions in water are designated as aqueous, and the concentration of the solution is expressed in terms of the number of moles of solvent associated with 1 mol of the solute. If no concentration is indicated, the solution is assumed to be dilute. The standard state for a solute in aqueous solution is taken as the hypothetical ideal solution of unit molality (indicated as std state, $m = 1$). In this state the partial molal enthalpy and the heat capacity of the solute are the same as in the infinitely dilute real solution (aq. m).

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Acenaphthene	c	16.8			
Acenaphthylene	c	44.7			
Acetaldehyde	liq	-45.96	-30.64	38.3	65.6
	g	-39.76	-31.86	63.15	13.06
Acetaldoxime	c	-18.6			
	liq	-19.5			
Acetamide	c	-76.0			
Acetamidoguanidine nitrate	c	-118.1			
1-Acetamido-2- nitroguanidine	c	-46.3			
5-Acetamidotetrazole	c	-1.2			
Acetanilide	c	-50.3			
Acetic acid	liq	-115.71	-93.2	38.2	29.7
	g	-103.93	-90.03	67.52	15.90
Ionized; std state, $m = 1$	aq	-116.16	-88.29	20.7	-1.5
Nonionized; std state, $m = 1$	aq	-116.70	-94.78	42.7	
Acetic anhydride	liq	-149.14	-116.82	64.2	
	g	-137.60	-113.93	93.20	23.78
Acetone	liq	-59.18	-37.22	47.9	30.22
	g	-51.78	-36.58	70.49	17.90
Acetone glyceraldehyde	liq	-180			
Acetonitrile	liq	12.8	23.7	35.76	21.86
	g	21.00	25.24	58.19	12.48
Acetophenone	liq	-34.07	-4.06	59.62	
	g	-20.76	0.44	89.12	
Acetyl radical	g	-4.0			
<i>N</i> -Acetylbenzidine	c	-38.0			
Acetyl bromide	liq	-53.5			
Acetyl chloride	liq	-65.44	-49.73	48.0	28
	g	-58.30	-46.29	70.47	16.21
Acetylene	g	54.19	50.00	48.00	10.50
Std state, $m = 1$	aq	50.54	51.88	29.5	
Acetylenedicarbonitrile	liq	119.6			
	g	127.50	122.10	69.31	20.53
Acetylene dicarboxylic acid	c	-138.1			
Acetyl fluoride	liq	-112.4			
<i>N</i> -Acetylhydrazobenzene	c	-2.0			
<i>o</i> -Acetylhydroxybenzoic acid	c	-194.93			
<i>N</i> -Acetylimidazole	c	-28.6			
Acetyl iodide	liq	-39.3			
4-Acetylresorcinol	c	-137.1			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
<i>N</i> -Acetyltetrazole	c	19.49			
Acridine	c	44.8			
Acrolein	liq	-29.97	-16.17		
	g	-20.50	-15.45		
Acrylic acid	liq	-91.8			
	g	-80.36	-68.37	75.29	18.59
Acrylonitrile	liq	36.1			
	g	44.20	46.68	65.47	15.24
Adenine	c	23.21	71.58	36.1	
Adipic acid	c	-237.60			
	liq	-235.51	-177.17		
Aetioporphyrin I	c	-6.0			
Aetioporphyrin II	c	0.4			
α -Alanine					
D	c	-134.03	-88.23	31.6	
L	c	-133.96	-88.49	30.88	
DL	c	-134.55	-88.92	31.6	
Alanine anhydride	c	-128.0			
α -Alanylglycine					
DL	c	-185.64	-117.00	51.0	
L	c	-197.52	-127.30	46.62	
DL-Alanylphenylalanine	c	-170.2			
Alanylphenylalanyl anhydride	c	-89.3			
Allantoin (5-ureidohydantoin)	c	-171.50	-106.65	46.6	
Allomucic acid	c	-142			
Alloxan monohydrate	c	-239.08	-182.08	44.6	
Alloxantin dihydrate	c	-510.3			
Allyl radical	g	38			
1-Allyl-5-allylamino- tetrazole	c	83.7			
1-Allyl-5-aminotetrazole	c	63.4			
2-Allyl-5-aminotetrazole	c	67.6			
Allyl chloride	g	-0.15	10.42	73.29	18.01
Allylcyclopentane	liq	-15.74			
Allyl ethyl sulfoxide	liq	-41.83			
Allyl trichloroacetate	liq	-94.5			
Amalic acid	c	-367.0			
Amarine	c	63			
<i>p</i> -Aminoacetophenone	c	70.2			
3-Aminoacridine	c	39.8			
5-Aminoacridine	c	38.1			
2-Aminobenzoic acid	c	-95.8			
3-Aminobenzoic acid	c	-98.2			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
4-Aminobenzoic acid	c	-98.8			
2-Aminobiphenyl	c	26.8			
4-Aminobiphenyl	c	19.4			
1-Aminobutane (butylamine)	liq	-30.52			
	g	-22.00	11.76	86.76	28.33
2-Aminobutane (<i>sec</i> -butylamine)	g	-24.90	9.71	83.90	27.99
4-Aminobutanoic acid	c	-138.1			
2-Aminoethanesulfonic acid	c	-187.7	-134.3	36.8	33.6
Ionized; std state, $m = 1$	aq	-171.92	-121.76	47.8	
Nonionized; std state, $m = 1$	aq	-181.92	-134.12	55.7	
2-Aminohexanoic acid (norleucine)	c	-152.7			
4-Aminohexanoic acid	c	-154.5			
5-Aminohexanoic acid	c	-153.7			
6-Aminohexanoic acid	c	-152.7			
3-Amino-2-methylpropane (2-butylamine)	liq	-31.68			
5-Aminopentanoic acid	c	-144.5			
5-Aminotetrazole	c	49.7			
5-Aminotetrazole nitrate	c	-6.6			
3-Amino-1,2,4-triazole	c	18.4			
Amygdalin	c	-455			
1,2-Anhydroglucose- 3,5,6-triacetate	c	-411.7			
Aniline	liq	7.55	35.63	45.72	45.90
	g	20.76	39.84	76.28	25.91
Anisine	c	-51			
Anisoyl glycine	c	-180.9			
Anthracene	c	29.0	68.30	49.58	49.7
9,10-Anthracenedione	c	-49.6			
β -D-Arabinose	c	-252.84			
β -L-Arabinose	c	-252.84			
D-Arabonic acid- γ -lactone	c	-238.2			
L-Arginine	c	-148.66			
D-Arginine	c	-149.05	-57.43	59.9	
L-Ascorbic acid (vitamin C)	c	-278.34			
L-Asparagine	c	-188.50	-126.73	41.7	
L-Aspartic acid	c	-232.47	-174.53	40.66	
Azobenzene					
<i>cis</i>	c	86.7			
<i>trans</i>	c	76.6			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Azodicarbamide	c	-69.90			
Azulene	g	66.90	84.10	80.75	30.69
Barbituric acid	c	-152.2			
Benzaldehyde	liq	-21.23	2.24		
	g	-9.57	5.85		
Benzamide	c	-48.42			
Benzanilide	c	-22.3			
1,2-Benzanthracene	c	41			
2,3-Benzanthracene	c	38.3	85.79	51.48	
1,2-Benzanthra-9,10-quinone	c	-55.4			
Benzene	liq	11.71	29.72	41.41	19.52
	g	19.82	30.99	64.34	
Benzenethiol (thiophenol)	liq	15.32	32.02	53.25	41.40
	g	26.66	35.28	80.51	25.07
Benzidine	c	16.9			
Benzil	c	-36.8			
Benzoic acid	c	-92.03	-58.62	40.05	34.97
Benzoic anhydride	c	-103.0			
Benzonitrile	g	52.30	62.33	76.73	26.07
Benzophenone	c	-8.0	33.5	58.6	
<i>p</i> -Benzoquinone	c	-44.33			
Benzotriazole	c	59.74			
DL-Benzoylalanine	c	-147.9			
Benzoyl bromide	liq	-25.58			
Benzoyl chloride	liq	-39.17			
Benzoyl iodide	liq	-12.31			
Benzoylphenylalanine	c	-129.6			
Benzoyl sarcosine	c	-135.7			
3,4-Benzphenanthrene	c	44.2			
Benzyl radical	g	45			
Benzyl alcohol	liq	-38.49	-6.57	51.8	
Benzyl bromide	liq	5.6			
(2-bromotoluene)					
Benzyl chloride	liq	-7.8			
<i>N</i> -Benzyl diphenylamine	c	44.2			
Benzyl ethyl sulfide	liq	-1.17			
Benzyl iodide	liq	13.8			
Benzyl mercaptan	liq	10.4			
Benzyl methyl ketone	liq	-36.30			
Benzyl methyl sulfide	liq	6.27			
Bicyclo[4.1.0]heptane	g	0.33			
Bicyclo[3.1.0]hexane	g	9.09			
Bicyclo[4.2.0]octane	g	-6.39			
Bicyclo[5.1.0]octane	g	-3.85			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Bicyclopropyl	g	30.9			
Biphenyl	c	24.02	60.75	49.2	38.80
	liq	28.5	62.07	59.8	
Biphenylene	liq	84.4			
<i>N,N'</i> -Bisuccinimide	c	-169.5			
Brassicid acid	c	-214			
Bromal	liq	-31.13			
Bromal hydrate	c	-112			
Bromobenzene	liq	14.5	30.12	52.0	37.17
4-Bromobenzoic acid	c	-90.4			
1-Bromobutane	g	-25.65	-3.08	88.39	26.13
2-Bromobutane	liq	-37.2	-4.60		
	g	-28.70	-6.16	88.50	26.48
Bromochlorodi- fluoromethane	g	-112.7	-107.18	76.14	
Bromochloro- fluoromethane	g	-70.5	-66.58	72.88	
Bromochloromethane	g	-12.0	-9.39	68.67	
Bromodichloro- fluoromethane	g	-64.4	-58.98	78.87	
Bromodichloromethane	g	-14.0	-10.16	75.56	
Bromodifluoromethane	g	-110.8	-106.90	70.51	
Bromoethane	liq	-21.99	-6.64	47.5	24.1
	g	-15.30	-6.29	68.71	15.45
Bromoethene (vinyl bromide)	g	18.73	19.30	65.83	13.26
Bromofluoromethane	g	-60.4	-57.71	65.97	
1-Bromoheptane	liq	-52.21			
1-Bromohexane	liq	-46.42			
Bromiodomethane	g	12.0	9.36	73.49	
Bromomethane	g	-9.02	-6.75	58.76	10.15
2-Bromo-2-methylpropane	liq	-39.3			
	g	-32.00	-6.73	79.34	27.85
1-Bromooctane	liq	-58.57			
1-Bromopentane	liq	-40.68			
	g	-30.87	-1.37	97.70	31.60
1-Bromopropane	g	-21.00	-5.37	79.08	20.66
2-Bromopropane	g	-23.20	-6.51	75.53	21.37
<i>N</i> -Bromosuccinimide	c	-80.35			
Bromotrichloromethane	g	-8.9	-2.96	79.55	
Bromotrifluoromethane	g	-155.1	-148.8	71.16	16.57
Brucine	c	-188.6			
1,2-Butadiene	g	38.77	47.43	70.03	19.15
1,3-Butadiene	g	26.33	36.01	66.62	19.01
Butadiyne (biacetylene)	g	113.00	106.11	59.76	17.60

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Butane	liq	-35.29	-3.60	55.2	
	g	-30.15	-4.10	74.12	23.29
1,2-Butanediamine	liq	-28.74			
2,3-Butanedione (diacetyl)	liq	-87.44			
1,4-Butanedithiol	liq	-25.11			
1-Butanethiol (butyl mercaptan)	liq	-29.79	0.97	65.96	
	g	-21.05	2.64	89.68	28.24
2-Butanethiol	liq	-31.13	-0.04	64.87	
	g	-23.00	1.29	87.65	28.51
1-Butanol	liq	-78.18	-38.84	54.1	42.31
	g	-65.65	-36.04	86.7	26.29
2-Butanol	liq	-81.88	-42.31	53.8	47.5
	g	-69.94	-40.06	85.6	27.08
2-Butanone (methyl ethyl ketone)	liq	-65.29	-36.18	57.08	37.98
	g	-56.26	-34.91	80.81	24.59
1-Butene	g	-0.03	17.04	73.04	20.47
2-Butene					
<i>cis</i>	g	-1.67	15.74	71.90	18.86
<i>trans</i>	g	-2.67	15.05	70.86	20.99
1-Buten-3-yne	g	72.80	73.13	66.77	17.49
<i>tert</i> -Butoxy radical	g	-24.7			
<i>tert</i> -Butyl radical	g	6.7			
<i>N</i> -Butylacetamide	liq	-91.02			
Butyl acetate	liq	-126.52			
<i>tert</i> -Butylamine	liq	-35.97			
	g	-28.65	6.90	80.76	28.67
Butylbenzene	liq	-18.67 ^{18°C}	27.50		
	g	-3.30	34.58	105.04	41.85
<i>sec</i> -Butylbenzene	liq	-15.87			
<i>tert</i> -Butylbenzene	liq	-16.90			
<i>sec</i> -Butyl butyrate	liq	-141.6			
Butyl chloroacetate	liq	-128.7			
Butyl 2-chlorobutyrate	liq	-156.6			
Butyl 3-chlorobutyrate	liq	-146.0			
Butyl 4-chlorobutyrate	liq	-147.7			
Butyl 2-chloropropionate	liq	-136.7			
Butyl 3-chloropropionate	liq	-133.4			
Butyl crotonate	liq	-111.8			
Butylcyclohexane	g	-50.95	13.49	109.58	49.50
Butylcyclopentane	g	-40.22	14.67	109.04	42.42
Butyl dichloroacetate	liq	-131.5			
Butyl ether	liq	-156.1			
	g	-87.2	114.96	48.82	
<i>tert</i> - Butyl hydroperoxide	liq	-70.2			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Butyllithium	liq	-31.6			
Butyl trichloroacetate	liq	-130.6			
1-Butyne (ethyl acetylene)	g	39.48	48.30	69.51	19.46
2-Butyne (dimethylacetylene)	g	34.97	44.32	67.71	18.63
Butyraldehyde	g	-49.00	-27.43	82.44	24.52
Butyramide	c	-87.5			
Butyric acid	liq	-127.59	-90.27	54.1	42.1
Butyronitrile	g	8.14	25.97	77.98	23.19
Caffeine (methyl theobromine)	c	-76.2			
Capric acid (decanoic acid)	c	-170.59			
Caproic acid (hexanoic acid)	liq	-139.71			
ϵ -Caprolactam	c	-78.54	-22.72	40.3	
Caprylic acid (octanoic acid)	liq	-151.93			
Carbazole	c	30.3			
Carboxyl radical	g	-54			
CCH radical	g	114	105	49.6	8.87
Cellobiose	c	-532.5			
Chloroacetamide	c	-80.9			
Chloroacetic acid	c, l	-122.3			
Ionized	aq	-119.81			
Nonionized; std state, $m = 1$	aq	-118.92			
Chloroacetyl chloride	liq	-68.0			
2-Chlorobenzaldehyde	liq	-28.4			
3-Chlorobenzaldehyde	liq	-30.2			
4-Chlorobenzaldehyde	c	-35.1			
Chlorobenzene	liq	2.58	21.32	50.0	35.9
2-Chlorobenzoic acid	c	-95.3			
3-Chlorobenzoic acid	c	-101.2			
4-Chlorobenzoic acid	c	-102.19			
Chlorobenzoquinone	c	-52.7			
1-Chlorobutane	g	-35.20	-9.27	85.58	25.71
2-Chlorobutane	g	-38.60	-12.78	85.94	25.93
2-Chlorobutyric acid	liq	-137.6			
3-Chlorobutyric acid	liq	-133.0			
4-Chlorobutyric acid	liq	-135.4			
Chlorocyclohexane	liq	-49.54			
2-Chloro-1,1- difluoroethylene	g	-79.2	-72.90	72.28	
Chlorodifluoromethane	g	-115.6	-108.1	67.12	13.35

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Chloroethane (ethyl chloride)	g	-26.83	-14.46	65.91	14.97
Chloroethylene (vinyl chloride)	g	8.5	12.4	63.07	12.84
Chloroethyne	g	51	47	57.81	12.98
Chlorofluoromethane	g	-63.2	-57.11	63.16	11.24
Chloroform	liq	-31.6	-17.17	48.5	
	g	-24.60	-16.76	70.63	15.63
Chloriodomethane	g	3.0	3.69	70.78	
Chloromethane (methyl chloride)	g	-19.59	-13.97	55.97	9.74
Chloromethyloxirane	liq	-35.48			
1-Chloro-2-methylpropane	g	-38.10	-11.87	84.56	25.93
2-Chloro-2-methylpropane	g	-43.80	-15.32	77.00	27.30
1-Chloronaphthalene	liq	13.0			
2-Chloronaphthalene	c	13.2			
1-Chloropentane	g	-41.80	-8.94	94.89	31.18
3-Chlorophenol	c	-49.4			
4-Chlorophenol	c	-47.3			
1-Chloropropan-2,3-diol	liq	-125.58			
2-Chloropropan-1,3-diol	liq	-123.71			
1-Chloropropane	g	-31.10	-12.11	76.27	20.23
2-Chloropropane	g	-35.00	-14.94	72.70	20.87
3-Chloro-1-propene (allyl chloride)	g	-0.15	10.42	73.29	18.01
2-Chloropropionic acid	liq	-125.0			
3-Chloropropionic acid	c	-131.4			
N-Chlorosuccinimide	c	-85.58			
Chlorotrifluoromethane	g	-169.20	-159.38	68.16	15.98
Chlorotrinitromethane	liq	-6.54			
Chrysene	c	34.7			
Cinchonamine	c	-10.4			
Cinchonidine	c	7.1			
Cinchonine	c	7.4			
Cinnamic acid					
<i>cis</i>	c	-72.0			
<i>trans</i>	c	-80.53			
Cinnamic anhydride	c	-83.1			
Citraconic acid	c	-197.04			
Citric acid	c	-369.0	-295.5	39.73	
Citric acid monohydrate	c	-439.4	-352.0	67.74	1.276
Codeine monohydrate	c	-151.2			
Coniine	liq	-57.6			
Creatine	c	-128.16	-63.32	45.3	
Creatine hydrate	c	-199.1			
Creatinine	c	-56.77	-6.97	40.10	

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
<i>o</i> -Cresol (2-methylphenol)	g	-30.74	-8.86	85.47	31.15
<i>m</i> -Cresol (3-methylphenol)	g	-31.63	-9.69	85.27	29.27
<i>p</i> -Cresol (4-methylphenol)	g	-29.97	-7.38	83.09	29.75
<i>m</i> -Cresol acetate	liq	-89.41			
Crotonic acid <i>cis</i>	liq	-83			
<i>trans</i>	c	-102.9			
<i>trans</i> -Crotononitrile	g	35.77	46.22	71.31	19.62
Cyanamide	c	14.05			
1-Cyanoguanidine	c	5.4	42.9	30.90	28.40
3-Cyanopyridine	c	46.23			
5-Cyanotetrazole	c	96.1			
4-Cyanothiazole	c	52.63			
Cyclobutane	g	6.37	26.30	63.43	17.26
Cyclobutene	g	31.00	41.76	62.98	16.03
Cyclododecane	c	-73.29			
Cycloheptane	liq	-37.47	12.92	57.97	29.42
Cycloheptanone	liq	-71.5			
1,3,5-Cycloheptatriene	liq	34.22	58.09	51.30	38.90
1,3-Cyclohexadien-5-yl radical	g	49.4			
Cyclohexane	liq	-37.34	6.37	48.84	37.4
	g	-29.43	7.59	71.28	25.40
Cyclohexane- 1,2- dicarboxylic acid <i>cis</i>	c	-229.7			
<i>trans</i>	c	-232.0			
Cyclohexanethiol	g	-22.80			
Cyclohexanol	liq	-83.22	-31.87	47.7	
Cyclohexanone	g	-55.00	-21.69	77.00	26.21
Cyclohexene	liq	-9.28	24.28	51.67	34.9
	g	-1.28	25.54	74.27	25.10
Cyclohexen-3-yl radical	g	29			
1-Cyclohexenylmethanol	liq	-91.4			
Cyclohexyl radical	g	13			
Cyclooctane	liq	-40.58	18.60	62.62	
Cyclooctanone	liq	-77.9			
1,3,5,7-Cyclooctatetraene	liq	60.93	85.70	52.65	
Cyclopentadiene	g	32.00	42.86	64.00	
Cyclopentane	liq	-25.28	8.70	48.82	30.80
	g	-18.46	9.23	70.00	19.84
Cyclopentane-1,2-diol <i>cis</i>	c	-115.9			
<i>trans</i>	c	-117.1			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Cyclopentanethiol	g	-11.45	13.63	86.38	25.79
Cyclopentanol	liq	-71.74	-30.55	49.2	
Cyclopentanone	liq	-56.24			
	g	-46.03			
Cyclopentene	liq	1.02	25.93	48.10	29.24
	g	7.87	26.48	69.23	17.95
1-Cyclopentenylmethanol	liq	8.2			
Cyclopentyl-1-thiaethane	g	-15.41			
Cyclopropane	g	12.74	24.95	56.75	13.37
Cyclopropene	g	66.0	68.42	58.38	
Cyclopropyl radical	g	55			
L-Cysteine	c	-124.5			
L-Cystine	c	-245.7			
Decahydronaphthalene (decalin)					
<i>cis</i>	liq	-52.45	16.47	63.34	55.45
<i>trans</i>	liq	-55.14	13.79	63.32	54.61
Decanal	g	-79.09	-15.90	138.28	57.29
Decane	liq	-71.95	-4.19	101.70	75.16
1,10-Decanediol	c	-165.74			
1-Decanethiol	liq	-66.07			
	g	-50.54	14.68	145.82	61.08
1-Decanoic acid	c	-170.59			
1-Decanol	liq	-114.6	-31.6	102.9	
	g	-96.0	-24.9	142.8	59.1
1-Decene	liq	-41.73	25.10	101.58	
1-Decyne	g	9.85	60.28	125.36	52.51
Deoxybenzoin	c	-16.96			
Desoxyamalic acid	c	-285.7			
Diacetamide	c	-117			
Diacetyl peroxide	liq	-127.9			
<i>o</i> -Diallyl phthalate	liq	-131.6			
Dialuric acid	c	-314.4			
2,6-Diaminopyridine	c	-1.56			
Diamylose	c	-850			
Diazomethane	g	46.0	52.06	58.02	12.55
Dibenzoyl ethane	c	-61.1			
Dibenzoyl ethylene	c	-27.4			
Dibenzoyl methane	c	-53.6			
Dibenzoyl peroxide	c	-100			
Dibenzyl	c	10.53	62.15	64.4	61.0
Dibenzyl ketone	c	-20.1			
Dibenzyl sulfide	c	23.74			
Dibenzyl sulfone	c	-42.1			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1,2-Dibromobutane	g	-23.70	-3.14	97.70	30.38
Dibromochlorofluoro- methane	g	-55.4	-53.40	81.99	
Dibromochloromethane	g	-5.0	-4.50	78.31	
1,2-Dibromocycloheptane	liq	-37.67			
1,2-Dibromocyclohexane	liq	-38.8			
1,2-Dibromocyclooctane	liq	-41.41			
Dibromodichloromethane	g	-7.0	-4.67	83.23	
Dibromodifluoromethane	g	-102.7	-100.16	77.66	
1,2-Dibromoethane	liq	-19.4	-5.0	53.37	32.51
Dibromofluoromethane	g	-53.4	-52.84	75.70	
Dibromomethane	g	-3.53	-3.87	70.10	13.04
1,2-Dibromopropane	g	-17.40	-4.22	89.90	24.57
Dibutylborinic acid	liq	-146.3			
Dibutyl ether	g	-79.80	-21.16	119.60	48.76
Dibutylmercury	liq	-23.4			
Di- <i>tert</i> -butyl peroxide	liq	-91.0			
Dibutyl <i>o</i> -phthalate	c	-201			
Dibutyl sulfate	liq	-216.1			
Dibutyl sulfite	liq	-165.6			
Dibutyl sulfone	c	-145.76			
Dichloroacetic acid	liq	-119.0			
Ionized	aq	-122.4			
Nonionized	aq	-120.4			
Dichloroacetylene	g	50	47	65	15.67
1,2-Dichlorobenzene	g	7.16	19.76	81.61	27.12
1,3-Dichlorobenzene	g	6.32	18.78	82.09	27.20
1,4-Dichlorobenzene	g	5.50	18.44	80.47	27.22
Dichlorodifluoromethane	g	-117.90	-108.51	71.91	17.31
1,1-Dichloroethane	liq	-38.3	-18.1	50.61	30.18
	g	-31.10	-17.52	72.91	18.25
1,2-Dichloroethane	liq	-39.49	-19.03	49.84	30.9
	g	-31.00	-17.65	73.66	18.80
1,1-Dichloroethylene	liq	-5.8	5.85	48.17	26.60
	g	0.30	5.78	68.85	16.02
<i>cis</i> -1,2-Dichloroethylene	liq	-6.6	5.27	47.42	27
	g	0.45	5.82	69.20	15.55
<i>trans</i> -1,2-Dichloroethylene	g	1.00	6.35	69.29	15.93
Dichlorofluoromethane	g	-68.10	-60.77	70.04	14.58
Dichloromethane	liq	-29.7	-16.83	42.7	
	g	-22.80	-16.46	64.61	12.16
1,2-Dichloropropane	g	-39.60	-19.86	84.80	23.47
1,3-Dichloropropane	g	-38.60	-19.74	87.76	23.81
2,2-Dichloropropane	g	-42.00	-20.21	77.92	25.30
Dicyanoacetylene	liq	119.6			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1,4-Dicyano-2-butyne	c	87.6			
Dicyclohexadiene	liq	6.3			
Dicyclopentadiene	c	27.9			
Dicyclopentyl	liq	-41.8			
2,2-Diethoxypropane	liq	-128.83			
Diethylamine	g	-17.30	17.23	84.18	27.66
Diethylbarbituric acid (veronal)	c	-178.7			
1,2-Diethylbenzene	g	-4.53	33.72	103.81	43.63
1,3-Diethylbenzene	g	-5.22	32.67	104.99	42.27
1,4-Diethylbenzene	g	-5.32	32.95	103.73	42.10
Diethylenediamine	c	-3.2	57.4	20.5	
Diethylene glycol	liq	-150.2			
	g	-136.5		105.4	32.3
Diethyl ether (ethyl ether)	liq	-65.30	-27.88	60.5	40.8
	g	-60.26	-29.24	81.90	26.89
Diethylmercury	liq	7.1			
Diethylmethyl phos- phonate	liq	-245.3			
Diethylnitramine	liq	-25.4			
Diethyl oxalate	liq	-192.51			
Diethyl peroxide	liq	-53.4			
Diethyl <i>o</i> -phthalate	liq	-186			
Diethyl selenide	liq	-23.0			
Diethyl sulfate	liq	-194.28			
Diethyl sulfite	liq	-143.50			
Diethyl sulfone	c	-123.13			
Diethyl sulfoxide	liq	-63.97			
Diethylzinc	liq	4.0			
1,2-Difluorobenzene	liq	-79.04	-59.41	53.20	38.01
1,3-Difluorobenzene	g	-74.09	-61.43	76.57	25.40
1,4-Difluorobenzene	g	-73.43	-60.43	75.43	25.55
2,2'-Difluorobiphenyl	c	-70.73			
4,4-Difluorobiphenyl	c	-70.91			
2,2-Difluorochloroethylene	g	-75.4	-69.1	72.39	17.23
1,1-Difluoroethane	g	-119.70	-105.87	67.50	16.24
1,1-Difluoroethylene	g	-82.50	-76.84	63.38	14.14
Difluoromethane	g	-108.24	-101.66	58.94	10.25
9,10-Dihydroanthracene	c	15.87			
1,2-Dihydronaphthalene	liq	18.0			
1,4-Dihydronaphthalene	liq	21.0			
4 <i>H</i> -Dihydropyran	liq	-37.5			
5,12-Dihydrotetracene	c	25.44			
2,3-Dihydrothiophene	liq	12.73			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
2,5-Dihydrothiophene	liq	11.31			
1,2-Dihydroxybenzene	c	-86.3	-50.20	35.9	31.6
1,3-Dihydroxybenzene	c	-87.95	-50.00	35.3	31.3
1,2-Diiodobenzene	c	41.2			
1,3-Diiodobenzene	c	44.7			
1,4-Diiodobenzene	c	38.4			
1,2-Diiodoethane	g	15.90	18.76	83.30	19.67
Diiodomethane	g	28.30	24.24	73.95	13.80
Diisopropyl ether	liq	-83.94	-21.1	70.4	
	g	-76.20	-29.13	93.27	37.83
Diisopropyl ketone	g	-74.40			
Diisopropylmercury	liq	-3.1			
1,2-Dimethoxybenzene	liq	-69.4			
Dimethoxyborane	liq	-144.5			
1,2-Dimethoxyethane	liq	-90.02			
2,2-Dimethoxypropane	liq	-108.92			
<i>cis</i> - α,β -Dimethylacrylic acid	c	-117.3			
Dimethyl adipate	liq	-211.9			
Dimethylamine	g	-4.50	16.25	65.24	16.50
Std state, $m = 1$	aq	-16.88	13.85	31.8	
(CH ₃) ₂ NH ₂ ⁺ ; std state, $m = 1$	aq	-28.74	-0.80	41.2	
Dimethylaminotrimethyl- silane	liq	-66.8			
<i>N,N</i> -Dimethylaniline	liq	8.2			
2,2-Dimethylbutane	g	-44.35	-2.20	85.62	33.91
2,3-Dimethylbutane	g	-42.49	-0.98	87.42	33.59
2,3-Dimethyl-1-butene	g	-13.32	18.89	87.39	34.29
2,3-Dimethyl-2-butene	g	-14.15	18.18	87.15	29.54
3,3-Dimethyl-1-butene	g	-10.31	23.46	82.16	30.23
2,3-Dimethyl-2-butenic acid	c	-108.9			
Dimethylcadmium	g	9.528		72.40	31.5
Dimethylchlorosilane	liq	-79.8			
1,1-Dimethylcyclohexane	liq	-52.31	6.34	63.87	
	g	-43.26	8.42	87.24	36.90
1,2-Dimethylcyclohexane					
<i>cis</i>	g	-41.15	9.85	89.51	37.40
<i>trans</i>	g	-43.02	8.24	88.65	38.00
1,3-Dimethylcyclohexane					
<i>cis</i>	g	-44.16	7.13	88.54	37.60
<i>trans</i>	g	-42.20	8.68	89.92	37.60
1,4-Dimethylcyclohexane					
<i>cis</i>	g	-42.22	9.07	88.54	37.60
<i>trans</i>	g	-44.12	7.58	87.19	37.70

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1,1-Dimethylcyclopentane	g	-33.05	9.33	85.87	31.86
1,2-Dimethylcyclopentane					
<i>cis</i>	g	-30.96	10.93	87.51	32.06
<i>trans</i>	g	-32.67	9.17	87.67	32.14
1,3-Dimethylcyclopentane					
<i>cis</i>	g	-32.47	9.37	87.67	32.14
<i>trans</i>	g	-31.93	9.91	87.67	32.14
Dimethyldichlorosilane	g	-110.2		80.16	24.17
<i>cis</i> -2,4-Dimethyl-1,3-dioxane	liq	-111.79			
4,5-Dimethyl-1,3-dioxane	liq	-108.32			
5,5-Dimethyl-1,3-dioxane	liq	-110.53			
4,4'-Dimethyldiphenylamine	c	-2.8			
Dimethyl ether	g	-43.99	-26.99	63.83	15.73
<i>N,N</i> -Dimethylformamide	liq	-57.2		28.5	37.45
Dimethylfulvene	liq	21.5			
Dimethyl fumarate	liq	-174.3			
Dimethyl glutarate	liq	-205.9			
Dimethylglyoxime	c	-42.51			
2,2-Dimethylhexane					
liq	liq	-62.63	0.71	79.33	
g	g	-53.71	2.56	103.06	
2,3-Dimethylhexane	liq	-60.40	2.17	81.91	
2,3-Dimethylhexane	g	-51.13	4.23	106.11	
2,4-Dimethylhexane					
liq	liq	-61.47	0.89	82.62	
g	g	-52.44	2.80	106.51	
2,5-Dimethylhexane					
liq	liq	-62.26	0.60	80.96	
g	g	-53.21	2.50	104.93	
3,3-Dimethylhexane					
liq	liq	-61.58	1.23	81.12	
g	g	-52.61	3.17	104.70	
3,4-Dimethylhexane					
liq	liq	-60.23	2.03	82.97	
g	g	-50.91	4.14	107.15	
2,2-Dimethyl-3-hexene					
<i>cis</i>	liq	-30.22			
<i>trans</i>	liq	-34.64			
5,5-Dimethylhydantoin	c	-126.4			
1,1-Dimethylhydrazine	liq	11.8	49.4	47.32	39.21
1,2-Dimethylhydrazine	liq	13.3	50.8	47.60	40.88
Dimethyl maleate	liq	-168.2			
Dimethylmaleic anhydride	c	-139.0			
Dimethyl malonate	liq	-190.2			
Dimethylmercury	liq	14.0			
Dimethylnitramine	c	-16.9			
Dimethyl oxalate	liq	-181.0			
2,2-Dimethylpentane	g	-49.27	0.02	93.90	39.67

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
2,3-Dimethylpentane	g	-47.62	0.16	98.96	39.67
2,4-Dimethylpentane	g	-48.28	0.74	94.80	39.67
3,3-Dimethylpentane	g	-48.17	0.63	95.53	39.67
2,7-Dimethylphenanthrene	c	8.70			
4,5-Dimethylphenanthrene	c	21.26			
9,10-Dimethyl- phenanthrene	c	11.4			
Dimethyl <i>m</i> -phthalate	c	-171			
Dimethyl <i>o</i> -phthalate	liq	-162			
Dimethyl <i>p</i> -phthalate	c	-170			
2,2-Dimethylpropane	g	-39.67	-0.364	73.23	29.07
2,3-Dimethylpyridine	liq	4.62			
2,4-Dimethylpyridine	liq	3.85			
2,5-Dimethylpyridine	liq	4.45			
2,6-Dimethylpyridine	liq	3.02			
3,4-Dimethylpyridine	liq	4.36			
3,5-Dimethylpyridine	liq	5.36			
Dimethyl succinate	liq	-199.6			
1,1-Dimethylsuccinic acid	c	-236.08			
1,2-Dimethylsuccinic acid <i>cis</i>	c	-233.6			
<i>trans</i>	c	-235.1			
Dimethyl sulfate	liq	-175.23			
Dimethyl sulfite	liq	-125.07			
Dimethyl sulfone	c	-107.8	-72.3	34.77	
Dimethyl sulfoxide	liq	-48.6	-23.7	45.0	35.2
3,3-Dimethyl-2-thiabutane	liq	-37.49			
2,2-Dimethylthia- cyclopropane	liq	-5.78			
2,2-Dimethyl-3-thiapentane	liq	-44.7			
2,4-Dimethyl-3-thiapentane	g	-33.76	6.48	99.30	40.45
2,3-Dinitroaniline	c	-2.8			
2,4-Dinitroaniline	c	-16.3			
2,5-Dinitroaniline	c	-10.6			
2,6-Dinitroaniline	c	-12.1			
3,4-Dinitroaniline	c	-7.8			
3,5-Dinitroaniline	c	-9.3			
2,4-Dinitroanisole	c	-44.6			
2,6-Dinitroanisole	c	-45.2			
1,2-Dinitrobenzene	c	2.06	50.56	51.7	
1,3-Dinitrobenzene	c	-4.04	44.13	52.8	
2,4-Dinitrophenol	c	-55.6			
2,6-Dinitrophenol	c	-50.2			
2,4-Dinitroresorcinol	c	-99.3			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
4,6-Dinitroresorcinol	c	-105.1			
2,4-Dinitrotoluene	c	-17.1			
2,6-Dinitrotoluene	c	-12.2			
1,4-Dioxane	liq	-84.47	-44.96	46.67	
	g	-75.30	-43.21	71.65	22.48
1,3-Dioxane	liq	-89.99			
1,4-Dioxatetralin	liq	-60.9			
Dioxindole	c	-76.9			
1,3-Dioxolane	g	-71.1			
Dipentene	liq	-12.1			
<i>N,N</i> -Diphenylacetamide	c	-10.3			
Diphenylamine	c	31.07			
1,4-Diphenylbutadiene					
<i>cis,cis</i>	c	47.51			
<i>trans,trans</i>	c	42.73			
Diphenylbutadiyne	c	123.91			
1,4-Diphenylbutane	c	-2.36			
1,4-Diphenyl- 1,4-butanedione	c	-61.24	1.87	77.6	
1,4-Diphenyl-2-butene- 1,4-dione	c	-27.55	26.64	76.3	
Diphenylcarbinol	c	-25.04			
Diphenyl carbonate	c	-95.93	-42.05	66.54	
Diphenyldichlorosilane	liq	-66.5			
Diphenyl disulfide	c	35.8			
Diphenyl disulfone	c	-153.59			
1,1-Diphenylethane	liq	11.7	58.58	80.28	
1,2-Diphenylethane	liq	12.31	63.87	64.6	
1,1-Diphenylethene	liq	41.21			
Diphenyl ether	liq	-3.48	34.47	69.62	
Diphenylethyne	c	74.66			
Diphenylfulvene	c	7.1			
Diphenylmercury	c	66.8			
Diphenylmethane	liq	21.25	66.19	57.2	55.7
Diphenyl sulfide	liq	39.1			
Diphenyl sulfone	c	-53.71			
Diphenyl sulfoxide	c	2.40			
Dipropyl ether	g	-70.00	-25.23	100.98	37.83
Dipropylmercury	liq	-5.0			
Dipropyl sulfate	liq	-205.22			
Dipropyl sulfite	liq	-154.52			
Dipropyl sulfone	liq	-130.94			
Dipropyl sulfoxide	liq	-78.65			
2,3-Dithiabutane	liq	-14.82	1.67	56.26	34.92
5,6-Dithiadecane	g	-37.86	12.87	136.91	55.23

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
3,4-Dithiahexane	liq	-28.69	2.28	72.90	
1,3-Dithian-2-thione	c	-3.1			
4,5-Dithiaoctane	liq	-40.95	4.56	89.28	
<i>N,N</i> -Dithiodiethylamine	liq	-29.1			
1,3-Dithiolan-2-thione	c	3.1			
Di- <i>p</i> -tolyl sulfone	c	-74.32			
Divinyl ether	g	-9.53			
Divinyl sulfone	liq	-49.5			
Dodecane	liq	-84.16	6.71	117.26	89.86
Dodecanoic acid	c	-185.14			
1-Dodecene	g	-39.52	32.96	147.78	64.43
1-Dodecyne	g	-0.01	64.22	143.98	63.44
Dulcitol	c	-321.9			
Eicosane	g	-108.93	28.04	223.26	110.73
Eicosanoic acid (arachidic acid)	c	-241.9			
1-Eicosene	g	-78.93	49.03	222.26	108.15
Ergosterol	c	-188.8			
<i>meso</i> -Erythritol	c	-127.56	-152.12	39.9	
Ethane	g	-20.24	-7.84	54.76	12.54
1,2-Ethanedithiol	liq	-12.83			
Ethanethiol	g	-11.02	-1.12	70.77	17.37
Ethanol	liq	-66.20	-41.63	38.49	26.76
	g	-56.03	-40.13	67.54	15.64
Ethoxy radical	g	-6			
Ethyl radical	g	26.0	31	59.2	
Ethyl acetate	liq	-114.49	-79.52	62.0	
	g	-105.86	-78.25	86.70	27.16
Ethyl allyl sulfone	liq	-96.95			
Ethylamine	g	-11.00	8.91	68.08	17.36
<i>N</i> -Ethylaniline	liq	0.9	45.10	57.2	
Ethylbenzene	liq	-2.98	28.61	60.99	
	g	7.12	31.21	86.15	30.69
2-Ethyl-1-butene	g	-12.32	19.11	90.01	31.92
Ethyl carbamate (urethane)	c	-124.4			
Ethyl chloride	g	-26.83	-14.46	65.91	14.97
Ethyl crotonate	liq	-100.4			
Ethylcyclohexane	liq	-50.72	6.95	67.14	
1-Ethylcyclohexene	liq	-25.50			
Ethylcyclopentane	liq	-39.08	8.92	67.00	
	g	-30.37	10.65	90.42	31.49
Ethyl-diethylcarbamate	liq	-141.6			
Ethylene	g	12.50	16.31	52.39	10.24
Ethylene carbonate	c	-138.9			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Ethylene chlorohydrin	liq	-70.6			
1,2-Ethylenediamine	liq	-15.06		50	
	aq, 200	-13.32			
Ethylenediaminetetraacetic acid (EDTA)	c	-420.5			
Ethylenediammonium chloride	c	-122.7			
	aq, 5000	-115.92			
Ethylene glycol (2,1-ethanediol)	liq	-108.70	-77.25	39.9	35.8
	g	-93.05	-72.77	77.33	23.20
	aq, 1	-109.01			
Ethyleneimine (azirane)	g	29.50	42.54	59.90	12.55
Ethylene oxide	g	-12.58	-3.13	57.94	11.54
2-Ethyl-1-hexanal	liq	-83.30			
2-Ethyl-2-hexanal	liq	-62.44			
3-Ethylhexane	liq	-59.88	1.79	84.95	
Ethylidenecyclohexane	liq	-21.19			
Ethyl isovalerate	liq	-136.5			
Ethyllithium	c	-14.0			
Ethylmercury bromide	c	-25.7			
Ethylmercury chloride	c	-33.7			
Ethylmercury iodide	c	-15.7			
Ethyl methyl ether	g	-51.73	-28.12	74.24	21.45
Ethyl nitrate	g	-36.80	-8.81	83.25	23.27
Ethyl nitrite	g	-24.9		24.74	23.71
3-Ethylpentane	g	-45.33	2.63	98.35	39.67
Ethyl pentanoate	liq	-132.2			
Ethyl peroxy radical	g	(-2)			
2-Ethylphenol	c	-49.91			
3-Ethylphenol	c	-51.21			
4-Ethylphenol	c	-53.63			
Ethylphosphonic acid	c	-251.3			
Ethyl propanoate	liq	-122.16	-79.16		
2-Ethylpyridine	liq	-1.2			
Ethylsuccinic acid	c	-236.4			
Ethyl thioacetate	liq	-64.01			
Ethyl β -vinylacrylate	liq	-80.8			
Ethyl vinyl ether	g	-33.63			
Ethynylbenzene (phenyl-acetylene)	g	78.22	86.46	76.88	27.46
Fluoranthene	c	45.75	82.60	55.09	
Fluoroacetamide	c	-118.7			
Fluoroacetic acid	c	-164.5			
Fluorobenzene	g	-27.86	-16.50	72.33	22.57
2-Fluorobenzoic acid	c	-135.67			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
3-Fluorobenzoic acid	c	-139.13			
4-Fluorobenzoic acid	c	-140.00			
Fluoroethane	g	-62.90	-50.44	63.34	14.21
2-Fluoroethanol	liq	-111.3			
Fluoromethane	g	-56.80	-51.09	53.25	8.96
1-Fluoropropane	g	-67.20	-47.87	72.71	19.75
2-Fluoropropane	g	-69.00	-48.81	69.82	19.60
4-Fluorotoluene	liq	-44.80	-19.06	56.67	
Fluorotrinitromethane	liq	-52.8			
Formaldehyde	g	-27.70	-26.27	52.29	8.46
unhydrolyzed	aq	-35.9	-31.02		
Formamide	liq	-60.7			
	g	-44.5	-33.71	59.41	10.84
Formanilide	c	-36.2			
Formic acid	liq	-101.51	-86.38	30.82	23.67
	g	-90.49	-83.89	59.45	10.81
Ionized; std state, $m = 1$	aq	-101.71	-83.9	22	-21.0
Nonionized; std state, $m = 1$	aq	-101.68	-89.0	39	
Dimer	g	-195.08			
Formyl					
HCO	g	10.4	6.76	53.66	8.27
HCO ⁺	g	204	201	48.3	8.62
Formyl fluoride	g	-90	-88	59.0	9.66
<i>N</i> -Formyl-DL-leucine	c	-222.1			
Formyl urea	c	-118			
β -D-Fructose	c	-302.2			
D-Fucose	c	-262.7			
Fumaric acid	c	-193.84	-156.70	39.7	
Fumaronitrile	c	64.11			
Furan	g	-8.23	0.21	63.86	15.64
Furfural	liq	-47.8			
Furfuryl alcohol	liq	-66.05	-36.85	51.50	
2-Furoic acid	c	-119.12			
(pyromucic acid)					
Furylacrylic acid	c	-109.7			
Furylethylene	liq	-2.5			
D-Galactonic acid	c	-384.8			
D-Galactose	c	-304.1	-219.60	49.1	
D-Glucaric acid-	c	-343.2			
1,4-lactone					
D-Glucaric acid-	c	-343.6			
3,6-lactone					
D-Gluconic acid	c	-379.3			
D-Gluconic acid- δ -	c	-300.3			
lactone					

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
D-Glucose					
α	c	-304.26	-217.6	50.7	
β	c	-302.76			
D-Glutamic acid	c	-240.19	-173.87	45.7	
L-Glutamic acid	c	-241.32	-174.78	44.98	
L-Glutamine	c	-197.3			
Glutaric acid	c	-229.44			
Glyceraldehyde	liq	-143			
Glycerol	liq	-159.76	-114.01	48.87	35.9
Glyceryl-1-acetate	liq	-217.5			
Glyceryl-1-benzoate	c	-185.80			
Glyceryl-2-benzoate	c	-184.71			
Glyceryl-1-caprate	c	-265.05			
Glyceryl-2-caprate	c	-261.90			
Glyceryl-1,3-diacetate	liq	-268.2			
Glyceryl-1-laurate	c	-277.46			
Glyceryl-2-laurate	c	-275.48			
Glyceryl-2-myristate	c	-292.31			
Glyceryl-1-palmitate	c	-306.28			
Glyceryl-1-stearate	c	-319.64			
Glyceryl triacetate	liq	-318.3			
Glyceryl trilaurate	c	-489			
Glyceryl trimyristate	c	-520			
Glyceryl trinitrate	liq	-88.6			
Glycine	c	-126.22	-88.09	24.74	23.71
Ionized; std state, $m = 1$	aq	-112.28	-75.28	26.54	
Nonionized; std state, $m = 1$	aq	-122.85	-88.62	37.84	
NH ₃ ⁺ CH ₂ COOH; std state, $m = 1$	aq	-123.78	-91.82	45.46	
Glycol acetal	liq	-91.1			
Glycolic acid (hydroxyacetic acid)	c	-158.6			
Glycylglycine	c	-178.51	-117.25	45.4	
Glycylphenylalanine	c	-163.9			
Glycylvaline	c	-200.0			
Glyoxal	g	-50.66			
Glyoxime	c	-21.63			
Glyoxylic acid	c	-199.7			
Guanidine	c	-13.39			
Guanidine carbonate	c	-232.10	-133.23	70.6	61.87
Guanidine nitrate	c	-92.5			
Guanidine sulfate	c	-288.0			
Guanine	c	-43.72	11.33	38.3	

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Guanylurea nitrate	c	-102.1			
Heptadecane	g	-94.15	22.01	195.33	94.33
Heptadecanoic acid	c	-220.9			
1-Heptadecene	g	-64.15	43.00	194.33	91.76
1-Heptanal	g	-63.10	-20.71	110.34	40.89
Heptane	liq	-53.63	0.42	77.92	53.76
Heptanedioic acid	g	-44.88	1.91	102.27	39.67
1-Heptanethiol	g	-35.76	8.65	117.89	44.68
	liq	-145.75			
Heptanoic acid (enantic acid)	c	-241.75			
1-Heptanol	liq	-95.8	-34.0	76.5	66.5
	g	-79.3	-28.9	114.8	42.7
1-Heptene	liq	-23.41	21.22	78.31	50.62
	g	-14.89	22.90	101.24	37.10
1-Heptyne	g	24.62	54.18	97.44	36.11
Hexachlorobenzene	c	-31.30	0.25	62.20	48.11
	g	-8.10	10.56	105.45	41.40
Hexachloroethane	g	-33.20	-13.13	95.30	32.68
Hexadecafluoroethyl- cyclohexane	liq	-799.1			
Hexadecafluoroheptane	liq	-817.6	-739.24	134.28	
	g	-808.9	-737.87	158.88	
Hexadecane	g	-89.23	20.00	186.02	88.86
Hexadecanoic acid (palmitic acid)	c	-213.3	-75.54	108.12	
1-Hexadecanol (cetyl alcohol)	c, II	-163.4	-23.6	108.0	104.8
	liq	-151.86	-23.08	145.0	
1-Hexadecene	g	-59.23	40.99	185.02	86.29
Hexafluorobenzene	liq	-237.27	-211.43	66.90	52.96
	g	-228.64	-210.18	91.59	37.43
Hexafluoroethane	g	-320.90	-300.15	79.30	25.43
Hexahydroindane					
<i>cis</i>	g	-30.4			
<i>trans</i>	g	-31.4			
Hexamethylbenzene	c	-39.19	28.06	71.66	61.5
Hexamethyldisiloxane	liq	-194.7	-129.5	103.69	74.42
Hexamethylenetetramine (urotropine)	c	30.0	103.92	39.05	
	liq	-18.7	28.65	73.28	
Hexanal	g	-59.37	-23.93	101.07	35.43
Hexanamide	c	-101.48			
Hexane	liq	-47.52	-0.91	70.76	45.2
	g	-39.96	-0.06	92.83	34.20
1-Hexanethiol	g	-30.83	6.65	108.58	39.21
Hexanoic acid	liq	-139.71			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1-Hexanol	liq	-90.7	-36.4	69.2	56.6
	g	-75.9	-32.4	105.5	37.2
1-Hexene	liq	-17.30	19.93	70.55	43.81
	g	-9.96	20.90	91.93	31.63
2-Hexene					
<i>cis</i>	g	-12.51	18.22	92.37	30.04
<i>trans</i>	g	-12.27	18.27	90.97	31.64
3-Hexene					
<i>cis</i>	g	-11.38	19.84	90.73	29.55
<i>trans</i>	g	-13.01	18.55	89.59	31.75
1-Hexyne	g	29.55	52.24	88.13	30.65
Hippuric acid (benzoylglycine)	c	-145.63	-88.33	57.2	
Hydantoic acid	c	-179			
Hydantoin	c	-107.2			
Hydrazobenzene	c	52.9			
Hydroquinone	c	-87.08	-49.48	33.5	33.9
Hydrosorbic acid	liq	-110.2			
Hydroxyacetic acid	c	-158.6			
<i>o</i> -Hydroxybenzoic acid	c	-140.64	-100.7	42.6	38.03
<i>m</i> -Hydroxybenzoic acid	c	-139.8	-99.74	42.3	37.59
<i>p</i> -Hydroxybenzoic acid	c	-139.7	-99.55	42.0	37.08
β -Hydroxybutyric acid	liq	-162.3			
Hydroxyisobutyric acid	c	-177.9			
L-Hydroxyproline	c	-158.1			
8-Hydroxyquinoline	c	-19.9			
Hypoxanthene (6-oxypurine)	c	-26.47	18.39	34.8	
Imidazole	c	14.5			
Indane	liq	2.56	36.04	56.01	45.47
Indene	liq	26.39	52.00	51.19	44.68
Indole	c	29.8			
Iodobenzene	g	38.85	44.88	79.84	24.08
2-Iodobenzoic acid	c	-72.2			
3-Iodobenzoic acid	c	-75.7			
4-Iodobenzoic acid	c	-75.5			
Iodocyclohexane	liq	-23.5			
Iodoethane	liq	-9.6	3.5	50.6	27.5
	g	-2.00	5.10	70.82	15.76
Iodomethane	liq	-3.29	3.61	38.9	
	g	3.29	3.72	60.64	10.54
2-Iodo-2-methylpropane	g	-17.60	5.65	81.79	28.27
1-Iodonaphthalene	liq	38.6			
2-Iodonaphthalene	c	34.5			
2-Iodophenol	c	-22.9			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
3-Iodophenol	c	-22.6			
4-Iodophenol	c	-22.8			
1-Iodopropane	g	-7.30	6.68	80.32	21.48
2-Iodopropane	g	-10.00	4.80	77.55	21.53
3-Iodopropene (allyl iodide)	liq	13.7			
3-Iodopropionic acid	c	-109.9			
2-Iodotoluene	liq	18.7			
3-Iodotoluene	liq	18.9			
4-Iodotoluene	liq	16.1			
Isatin	c	-62.7			
Isobutylbenzene	liq	-16.68			
Isobutyl dichloroacetate	liq	-132.4			
Isobutyl phenyl ketone	liq	-52.63			
Isobutyl trichloroacetate	liq	-132.4			
Isobutyronitrile	g	6.07	24.76	74.88	23.04
L-Isoleucine	c	-151.8	-82.97	49.71	45.00
Isopropenyl acetate	liq	-92.31			
Isopropyl radical	g	17.6			
Isopropyl acetate	liq	-124.01			
Isopropylbenzene	liq	-9.85	29.70	66.87	
(cumene)	g	0.94	32.74	92.87	36.26
Isopropyl nitrate	g	-45.65	-9.72	89.20	28.84
Isopropyl thiolacetate	liq	-71.26			
Isopropyl trichloroacetate	liq	-128.2			
Isoquinoline	c	37.9			
L-Isoleucine	c	-177.8			
Isothiocyanic acid	g	30.50	26.98	59.28	11.09
Itaconic acid	c	-201.06			
Ketene	g	-14.60	-14.41	57.79	12.37
α -Ketoglutaric acid	c	-245.35			
D-Lactic acid	c	-165.88		34.3	
L-Lactic acid	c	-165.89	-124.98	34.00	
	liq	-161.2	-123.84	45.9	
β -Lactose	c	-534.1	-374.52	92.3	
Lauric acid (dodecanoic acid)	c	-185.14			
D-Leucine	c	-152.36	-82.97	49.71	
L-Leucine	c	-154.6	-82.76	50.62	48.03
DL-Leucine	c	-153.14	-83.54	49.5	
DL-Leucylglycine	c	-205.7	-112.14	67.2	
Leucylglycylglycine	c	-259.6			
Levulinic acid	c	-166.6			
Levulinic lactone	liq	-76.2			
(+)-Limonene	liq	-13.0			
DL-Lysine	c	-162.2			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Maleic acid	c	-188.94	-149.40	38.1	32.36
Maleic anhydride	c	-112.08			
L-Malic acid	c	-263.78	-211.45		
DL-Malic acid	c	-264.27			
Malonamide	c	-130.5			
Malonic acid	c	-212.96			
Malonic diamide	c	-130.52			
Malononitrile	c	44.6			
Maltose	c	-530.8	-412.60		
L-Mandelic acid	c	-138.8			
D-Mannitol	c	-139.61	-225.20	57.0	
D-Mannose	c	-301.9			
Melamine	c	-17.3	44.10	35.63	
(triaminotriazine)					
Melezitose	c	-815			
2-Mercaptopropionic acid	liq	-111.9	-82.19	54.70	
Mesaconic acid	c	-197			
Mesoxalic acid	c	-290.7			
2,2-Metacyclophane	g	40.8			
Methane	g	-17.89	-12.15	44.52	8.54
Methanethiol	g	-5.49	-2.37	60.96	12.01
(methyl mercaptan)					
Methanol	liq	-57.13	-39.87	30.41	19.40
	g	-48.06	-38.82	57.29	10.49
Std state, $m = 1$	aq	-58.78			
L-Methionine	c	-180.4	-120.88	55.32	
Methoxyl radical	g	(2)			
2-Methoxybenzaldehyde	c	-63.7			
3-Methoxybenzaldehyde	liq	-66.0			
4-Methoxybenzaldehyde	liq	-63.9			
Methoxybenzene (anisole)	g	-17.3			
Methoxymethyl radical	g	(-4)			
2-Methoxytetrahydropyran	liq	-105.7			
5-Methoxytetrazole	c	16.6			
Methyl (CH ₃) radical	g	34.82	35.35	46.38	9.25
Methyl acetate	liq	-106.4			
Methyl acrylate	g	-70.10	-56.78		
Methyl allantoin (pyvurile)	c	-177.0			
Methyl allyl sulfone	liq	-91.95			
Methylamido radical	g	35			
(CH ₃ NH)					
Methylamine	g	-5.50	7.71	57.98	11.97
Std state, $m = 1$	aq	-16.77	4.94	29.5	
Methylaminolithium	c	-22.92			
N-Methylaniline	liq	7.7			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Methyl benzoate	liq	-79.8			
Methyl benzyl sulfone	c	-88.65			
2-Methylbiphenyl	liq	25.8			
3-Methylbiphenyl	liq	20.4			
4-Methylbiphenyl	c	13.2			
2-Methyl-1,3-butadiene (isoprene)	g	18.10	34.86	75.44	25.00
3-Methyl-1,2-butadiene	g	31.00	47.47	76.40	25.20
2-Methylbutane	g	-36.92	-3.54	82.12	28.39
3-Methyl-1-butanethiol	g	-27.44			
2-Methyl-2-butanethiol	liq	-38.90	0.56	69.34	
	g	-30.36	2.20	92.48	34.30
2-Methyl-1-butanol	liq	-85.2			52.6
3-Methyl-1-butanol	liq	-85.2			50.3
2-Methyl-2-butanol	liq	-90.7	-41.9	54.8	59.2
	g	-78.8	-39.5	86.7	
3-Methyl-2-butanol	liq	-87.5			55.5
2-Methyl-1-butene	g	-8.68	15.68	81.15	26.28
3-Methyl-1-butene	g	-6.92	17.87	79.70	28.35
2-Methyl-2-butene	g	-10.17	14.26	80.92	25.10
Methyl butyl sulfone	liq	-128.00			
Methyl <i>tert</i> -butyl sulfone	c	-132.8			
3-Methyl-1-butyne	g	32.60	49.12	76.23	25.02
Methyl caprate	liq	-153.07			
Methyl caproate (methyl hexanoate)	liq	-129.10			
<i>N</i> -Methylcaprolactam	liq	-73.3			
5-Methylcaprolactam	c	-86.9			
7-Methylcaprolactam	c	-86.5			
Methyl caprylate (methyl octanoate)	liq	-141.07			
Methyl chloride	g	-19.59	-13.97	55.97	9.74
Methyl crotonate	liq	-91.5			
Methylcyclohexane	liq	-45.45	4.86	59.26	
	g	-36.99	6.52	82.06	32.27
2-Methylcyclohexanol					
<i>cis</i>	liq	-93.3			
<i>trans</i>	liq	-99.4			
3-Methylcyclohexanol					
<i>cis</i>	liq	-99.5			
<i>trans</i>	liq	-94.3			
4-Methylcyclohexanol					
<i>cis</i>	liq	-98.8			
<i>trans</i>	liq	-103.6			
2-Methylcyclohexanone	liq	-68.8			
Methylcyclopentane	g	-25.50	8.55	81.24	26.24

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1-Methylcyclopentanol	liq	-82.3			
2-Methylcyclopentanone	liq	-63.4			
1-Methylcyclopentene	g	-1.30	24.41	78.00	24.10
3-Methylcyclopentene	g	2.07	27.48	79.00	23.90
4-Methylcyclopentene	g	3.53	29.06	78.60	23.90
Methyldichlorosilane	liq	-105.9			
2-Methyl-1,3-dioxane	liq	-104.60			
4-Methyl-1,3-dioxane	liq	-99.80			
N-Methyldiphenylamine	liq	28.8			
4-Methyldiphenylamine	c	11.7			
Methylene	g	92.35	88.25	46.32	8.27
2-Methylenecyclohexanol	liq	-66.3			
2-Methylenecyclopentanol	liq	11.2			
β -Methylene- β -propio- lactone (diketene)	liq	-55.72			
Methylene sulfate	c	-164.6			
1-Methyl-2-ethylbenzene	g	0.29	31.33	95.42	37.74
1-Methyl-3-ethylbenzene	g	-0.46	30.22	96.60	36.38
1-Methyl-4-ethylbenzene	g	-0.78	30.28	95.34	36.22
2-Methyl-3-ethylpentane	liq	-59.69	3.03	81.41	
	g	-50.48	5.08	105.43	
3-Methyl-3-ethylpentane	liq	-60.46	2.69	79.97	
	g	-51.28	4.76	103.48	
2-Methyl-3-ethyl-1- pentene	g	-23.97			
Methyl ethyl sulfite	liq	-135.55			
Methyl ethyl sulfone	c	-116.17			
Methyl formate	liq	-90.60	-71.53	29	
	g	-83.70	-71.03	72.00	15.90
Methylglyoxal	g	-64.8			
Methylglyoxime	c	-30.3			
2-Methylheptane	liq	-60.98	0.92	84.16	
	g	-51.50	3.05	108.81	
3-Methylheptane	liq	-60.34	1.12	85.66	
	g	-50.82	3.28	110.32	
4-Methylheptane	liq	-60.17	1.87	83.72	
	g	-50.69	4.00	108.35	
Methyl heptanoate	liq	-135.54			
2-Methylhexane	liq	-54.93	-0.69	77.28	53.28
	g	-46.59	0.77	100.38	39.67
3-Methylhexane	liq	-54.35	-0.39	78.23	
	g	-45.96	1.10	101.37	39.67
Methyl hexanoate	liq	-129.11			
5-Methylhydantoin	c	-116.3			
Methylhydrazine	liq	12.9	43.0	39.66	32.25
	g	22.55	44.66	66.61	17.0

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Methyldiyne					
CH	g	142.00	134.02	43.72	6.97
CH ⁺	g	388.8	380.1	41.00	6.97
α -Methylindole	c	14.5			
Methyl isocyanide	g	35.6	39.6	58.99	12.65
1-Methyl-2-isopropyl- benzene (<i>o</i> -cymene)	liq	-18.19			
1-Methyl-3-isopropyl- benzene	liq	-18.69			
Methyl isopropyl ether	g	-60.24	-28.89	80.86	26.55
Methyl isopropyl ketone	g	-62.76			
Methyl isopropyl sulfone	liq	-120.44			
Methyl isothiocyanate (CH ₃ NCS)	g	31.3	34.5	69.29	15.65
3-Methylisoxazole	liq	-5.0			
5-Methylisoxazole	liq	-6.4			
Methyl laurate	liq	-165.66			
Methylmercury bromide	c	-20.6			
Methylmercury chloride	c	-27.8			
Methylmercury iodide	c	-10.4			
Methyl myristate	liq	-177.80			
1-Methylnaphthalene	liq	13.43	46.26	60.90	53.63
2-Methylnaphthalene	c	10.72	46.03	52.58	46.84
Methyl nitrate	liq	-38.0	-10.4	51.9	37.6
	g	-29.8	-9.4	76.1	
Methyl nitrite	g	-15.30	0.24	67.95	15.11
Methyl oleate	liq	-174.2			
Methyl pelargonate	liq	-147.29			
2-Methylpentane	g	-41.66	-1.20	90.95	34.46
3-Methylpentane	g	-41.02	-0.51	90.77	34.20
Methyl pentanoate	liq	-122.90			
2-Methyl-1-pentene	g	-12.49	18.55	91.34	32.41
3-Methyl-1-pentene	g	-10.76	20.66	90.06	34.04
4-Methyl-1-pentene	g	-10.54	21.52	87.89	30.23
2-Methyl-2-pentene	g	-14.28	17.02	90.45	30.26
3-Methyl-2-pentene					
<i>cis</i>	g	-13.80	17.50	90.45	30.26
<i>trans</i>	g	-14.02	17.04	91.26	30.26
4-Methyl-2-pentene					
<i>cis</i>	g	-12.03	19.63	89.23	31.92
<i>trans</i>	g	-12.99	19.03	88.02	33.80
Methyl pentanoate	liq	-122.89			
Methyl phenyl sulfone	c	-82.49			
(2-Methyl phenol)	g	-30.74	-8.86	85.47	31.15

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
(3-Methyl phenol)	g	-31.63	-9.69	85.27	29.27
(4-Methyl phenol)	g	-29.97	-7.38	83.09	29.75
Methylphosphonic acid	c	-252			
2-Methylpropanal	g	-52.25			
2-Methylpropane	g	-32.15	-4.99	70.42	23.14
2-Methyl- 1,2-propanediamine	liq	-32.00			
2-Methyl-1-propanethiol	g	-23.24	1.33	86.73	28.28
2-Methyl-2-propanethiol	g	-26.17	0.17	80.79	28.91
2-Methyl-1-propanol	g	-67.69	-39.99	85.81	26.6
2-Methyl-2-propanol	liq	-85.86	-44.14	46.10	52.61
	g	-74.67	-42.46	77.98	27.10
2-Methylpropene	g	-4.04	13.88	70.17	21.30
Methyl propyl ether	g	-56.82	-26.27	83.52	26.89
7-Methylpurine	c	51.3			
2-Methylpyridine (2-picoline)	liq	13.83	39.80	52.07	37.86
	g	24.05	42.32	77.68	23.90
3-Methylpyridine	liq	15.57	41.16	51.70	37.93
4-Methylpyridine	liq	13.58			
N-Methylpyrrolidone	liq	-62.64			
Methyl salicylate	liq	-127.1			
α -Methylstyrene	liq	16.8			
	g	27.00	49.84	91.70	34.70
β -Methylstyrene					
<i>cis</i>	g	29.00	51.84	91.70	34.70
<i>trans</i>	g	28.00	51.08	90.90	34.90
Methylsuccinic acid	c	-229.02			
3-Methyl-2-thiabutane	g	-21.61	3.21	85.87	28.00
2-Methylthiacyclopentane	g	-15.12			
2-Methyl-3-thiapentane	liq	-37.3			
4-Methylthiazole	liq	16.31			
2-Methylthiophene	liq	10.75	27.35	52.22	29.43
3-Methylthiophene	liq	10.38	27.00	52.19	29.38
4-Methyluracil	c	-109.2			
Methyl valerate (methyl pentanoate)	liq	-122.89			
Morphine monohydrate	c	-170.1			
Mucic acid	c	-423			
Murexide	c	-289.7			
Myrcene	liq	3.5			
Myristic acid (tetradecanoic acid)	c	-199.21			
Naphthalene	c	18.0	48.05	39.89	
	g	35.6	53.44	80.22	31.68
1-Naphthol	g	-5.1			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
2-Naphthol	g	-10.1			
1,4-Naphthoquinone	c	-43.83			
1-Naphthyl acetate	c	-68.89			
2-Naphthyl acetate	c	-72.72			
1-Naphthylamine	c	16.2			
2-Naphthylamine	c	14.4			
Narceine dihydrate	c	-421.2			
Narcotine	c	-210.9			
Nicotine	liq	9.4			
Nitrilotriacetic acid	c		-312.5		
2-Nitroaniline	c	-3.45	42.60	42.1	39.3
3-Nitroaniline	c	-4.46	41.60	42.1	40.2
4-Nitroaniline	c	-9.91	36.10	42.1	40.4
Nitrobenzene	liq	3.80	34.95	53.6	44.4
2-Nitrobenzoic acid	c	-94.25	-46.95	49.8	
3-Nitrobenzoic acid	c	-100.25	-52.71	49.0	
4-Nitrobenzoic acid	c	-101.25	-53.07	50.2	43.3
3-Nitrobiphenyl	c	15.6			
4-Nitrobiphenyl	c	9.7			
1-Nitrobutane	g	-34.40	2.42	94.28	29.85
2-Nitrobutane	g	-39.10	-1.49	91.62	29.51
3-Nitro-2-butanol	liq	-93.2			
2-Nitrodiphenylamine	c	15.4			
Nitroethane	g	-24.4	-1.17	75.39	18.69
aci form	aq	-30.7			
nitro form	aq	-32			
2-Nitroethanol	liq	-83.8			
Nitroguanidine	c	-22.1			
Nitromethane	liq	-27.03	-3.47	41.05	25.33
	g	-17.86	-1.66	65.73	13.70
1-Nitronaphthalene	c	10.2			
1-Nitropropane	g	-30.00	0.08	85.00	24.41
2-Nitropropane	g	-33.21	-3.06	83.10	24.26
4-Nitrosodiphenylamine	c	50.9			
Nonadecane	g	-104.00	26.03	213.95	105.26
1-Nonadecene	g	-74.00	47.02	212.95	102.69
1-Nonanal	g	-74.16	-17.91	128.97	51.82
Nonane	liq	-65.84	2.81	94.09	
	g	-54.74	5.93	120.86	50.60
1-Nonanethiol	g	-45.61	12.67	136.51	55.61
Nonanoic acid	liq	-157.68			
1-Nonanol	liq	-109.2	-32.4	91.3	67.50
1-Nonene	g	-24.74	26.93	119.86	48.03
Octadecane	g	-99.08	24.02	204.64	99.80
Octadecanoic acid	c	-226.5			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1-Octadecene	g	-69.08	45.01	203.64	97.22
Octafluorocyclobutane	g	-365.20	-334.33	95.69	37.32
1-Octanal	g	-69.23	-19.91	119.66	46.36
Octanamide	c	-113.1			
Octane	liq	-59.74	1.77	85.50	45.14
	g	-49.82	3.92	111.55	45.14
1-Octanethiol	g	-40.68	10.67	127.20	50.14
Octanoic acid (caprylic acid)	liq	-151.93			
1-Octanol	liq	-101.6	-34.2	90.2	77.7
2-Octanone	liq	-91.9	-33.54	89.35	65.31
1-Octene	liq	-29.52	22.49	86.15	57.65
	g	-19.82	24.91	110.55	42.56
1-Octyne	g	19.70	56.26	106.75	41.58
Oleic acid	c	-187.2			
DL-Ornithine	c	-156.0			
Oxacyclobutane (trimethylene oxide)	g	-19.25	-2.33	65.46	
Oxalic acid	c	-197.7	-166.8	28.7	
Std state, $m = 1$	aq	-197.2	-161.1	10.9	
Oxalic acid dihydrate	c	-341.0			
Oxalyl chloride	liq	-85.6			
Oxamic acid	c	-160.4			
Oxamide	c	-123.0	-81.9	28.2	
Oxindole	c	-41.2			
8-Oxypurine	c	-15.4			
Palmitic acid (hexadecanoic acid)	c	-213.10			
Papaverine	c	-120.2			
Parabanic acid	c	-138.0			
[1,8]-Paracyclophane	c	-19.6			
[2,2]-Paracyclophane	g	59.9			
[6,6]-Paracyclophane	c	-46.1			
Paraldehyde	liq	-164.2			
Pentachloroethane	g	-34.8	-16.79	91.17	28.22
Pentachlorofluoroethane	g	-75.8	-55.93	93.54	
Pentachlorophenol	c	-70.6	-34.44	60.21	48.27
Pentadecane	g	-84.31	17.98	176.71	83.40
1-Pentadecene	g	-54.31	38.97	175.71	80.82
1-Pentadecyne	g	-14.78	70.25	171.91	79.84
1,2-Pentadiene	g	34.80	50.29	79.70	25.20
1,3-Pentadiene					
<i>cis</i>	g	18.70	34.84	77.50	22.60
<i>trans</i>	g	18.60	35.07	76.40	24.70
1,4-Pentadiene	g	25.20	40.69	79.70	25.10

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
2,3-Pentadiene	g	33.10	49.21	77.60	24.20
Pentaerythritol	c	-220.0	-146.73	47.34	45.51
Pentaerythritol tetranitrate	c	-128.8			
Pentafluorobenzoic acid	c	-296.34			
Pentafluoroethane	g	-264.00	-246.00	79.76	22.88
Pentafluorophenol	c	-244.86			
Pentamethylbenzene	liq	-32.33	25.64	70.22	51.74
Pentamethylbenzoic acid	c	-128.13			
1-Pentanal	g	-54.45	-25.88	91.53	29.96
Pentanamide	c	-90.70			
Pentan-2,4-dione	liq	-101.33			
(acetylacetone)	g	-90.47		95.1	28.7
Pentan-1,5-dithiol	liq	-30.99			
Pentane	g	-35.00	-2.00	83.40	28.73
1-Pentanethiol	liq	-35.72	2.28	74.18	
Pentanoic acid	liq	-133.71	-89.10	62.10	50.48
(valeric acid)					
1-Pentanol	liq	-85.0	-38.3	62.0	49.8
2-Pentanol	liq	-87.7			
3-Pentanol	liq	-88.5	-40.4	57.4	60.0
2-Pentanone	g	-61.82	-32.76	89.91	28.91
3-Pentanone	liq	-70.87			
1-Pentene	g	-5.00	18.91	82.65	26.19
2-Pentene					
<i>cis</i>	g	-6.71	17.17	82.76	24.32
<i>trans</i>	g	-7.59	16.71	81.36	25.92
2-Pentenoic acid	liq	-106.7			
3-Pentenoic acid	liq	-103.9			
4-Pentenoic acid	liq	-102.9			
1-Pentyne	g	34.50	50.25	78.82	25.50
2-Pentyne	g	30.80	46.41	79.30	23.59
Perfluoropiperidine	liq	-482.9	-422.67	94.02	70.93
Perylene	c	43.69			
α -Phellandrene	liq	-14.3			
Phenacetin	c	-101.1			
9,10-Phenanthraquinone	c	-55.18			
Phenanthrene	c	27.3	64.12	50.6	
Phenazine	c	56.4			
Phenol	c	-39.44	-12.05	34.42	32.2
	liq	-37.80	-11.02		30.46
	g	-23.03	-7.86	75.43	24.75
Phenoxy radical	g	10			
Phenoxyacetic acid	c	-122.8			
Phenyl radical	g	71			
Phenyl acetate	liq	-80.02			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Phenylacetic acid	c	-95.3			
Phenylacetylene	g	78.22	86.46	76.88	27.46
β -Phenyl-L-alanine, DL- and L-	c	-111.9	-50.6	51.06	48.52
Phenyl benzoate	c	-57.7			
2-Phenylbenzoic acid	c	-83.4			
Phenylboronic acid	c	-172.0			
1-Phenylcyclohexene	liq	-4.0			
Phenylcyclopropane	liq	24.7			
N-Phenyldiacetamide	c	-86.63			
p-Phenylenediamine	c	0.73			
Phenyl ethyl sulfide	liq	5.29			
DL-Phenylglyceric acid	c	-178.5			
N-Phenylglycine	c	-96.2			
α -Phenylglycine	c	-103.2			
Phenylglyoxime					
α	c	-4.9			
β	c	10.1			
Phenylglyoxylic acid	c	-115.3			
Phenylhydrazine	liq	34.03			
Phenyl methyl sulfide	liq	11.5			
N-Phenyl-2-naphthylamine	c	38.2			
N-Phenylpyrrole	c	38.1			
2-Phenylpyrrole	c	34.5			
Phenyl salicylate	c	-104.3			
Phenyl thiolacetate	liq	-29.16			
Phosgene	g	-52.80	-49.42	67.82	13.79
Phthalamide	c	-104.4			
m-Phthalic acid	c	-191.91			
o-Phthalic acid	c	-186.91	-141.39	49.7	45.0
p-Phthalic acid	c	-195.05			
Phthalic anhydride	c	-110.1	-79.12	42.9	38.5
Phthalonitrile	c	65.82			
Pimelic acid (heptanedioic acid)	c	-241.25			
Pinene					
α	liq	-3.9			
β	liq	-1.8			
Piperazine	c	-10.90			
Piperidine	liq	-21.05			
α -Piperidone	c	-73.3	-26.79	39.4	
DL-Proline	c	-125.7			
Propadiene	g	45.92	48.37	58.30	14.10
Propane	g	-24.82	-5.63	64.58	17.59
1,2-Propanediamine	liq	-23.38			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1,2-Propanediol	liq	-119.6			
1,3-Propanediol	liq	-124.4			
1,3-Propanedithiol	liq	-18.83			
2,3-Propanedithiol	liq	-18.82			
1-Propanethiol	g	-16.22	0.52	80.40	22.65
2-Propanethiol	g	-18.22	-0.61	77.51	22.94
1-Propanol	liq	-72.66	-40.78	46.5	33.7
	g	-61.28	-38.67	77.61	20.82
2-Propanol	liq	-75.97	-43.09	43.16	36.06
	g	-65.11	-41.44	74.07	21.21
1,2,3-Propenetricarboxylic acid					
<i>cis</i>	c	-292.7			
<i>trans</i>	c	-294.7			
2-Propen-1-ol (allyl alcohol)	g	-31.55	-17.03	73.51	18.17
Propionaldehyde	g	-45.90	-31.18	72.83	18.80
Propionamide	c	-81.7			
Propionic acid	liq	-122.07	-91.65		
Propionic anhydride	liq	-161.53	-113.66		
Propionitrile	liq	3.5	21.31	45.25	
	g	12.10	22.98	68.50	17.46
1-Propylamine	g	-17.30	9.51	77.48	22.89
2-Propylamine	liq	-26.83			
Propylbenzene	g	1.87	32.80	95.76	36.41
Propylcarbamate	c	-132.07			
Propyl chloroacetate	liq	-123.3			
Propylcyclohexane	g	-46.20	11.31	100.27	44.03
Propylcyclopentane	g	-35.39	12.57	99.73	36.96
Propylene (propene)	g	4.88	15.02	63.72	15.37
Propylene oxide	g	-22.17	-6.16	68.53	17.29
Propyl nitrate	g	-41.60	-6.53	92.10	28.99
Propyl phenyl ketone	liq	-45.14			
Propyl thiolacetate	liq	-70.29			
Propyl trichloroacetate	liq	-122.7			
Propyne (methyl acetylene)	g	44.32	46.47	59.30	14.50
Pyrazine	c	33.41			
Pyrazole	c	28.3			
Pyrene	c	27.44	64.40	53.75	56.4
Pyridazine	liq	53.74			
Pyridine	liq	23.96	43.34	42.52	31.72
	g	33.61	45.46	67.59	18.67
Pyrimidine	liq	35.04			
Pyrrole	liq	15.08			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Pyrrole-2-aldehyde	c	-24.8			
Pyrrole-2-aldoxime	c	2.9			
Pyrrolidine	liq	-9.84	25.94	48.76	
	g	-0.86	27.41	73.97	19.39
2-Pyrrolidone	c	-68.3			
Pyruvic acid	liq	-139.7	-110.75	42.9	
Quinaldine	c	39.3			
Quinhydrone	c	-19.79	-77.19	77.9	66.2
Quinidine	c	-38.3			
Quinine	c	-37.1			
Quinoline	liq	37.33	65.90	51.9	
<i>p</i> -Quinone	c	-44.10	-20.0	38.9	
Raffinose	c	-761			
L-Rhamnose	c	-256.5			
Rhamnose triacetate	c	-455.4			
D-Ribose	c	-251.16			
Saccharinic acid lactone	c	-249.6			
Salicylaldehyde	liq	-66.9			
Salicylaldoxime	c	-43.91			
Salicyclic acid	c	-140.9	-99.93	42.6	
Sarcosine	c	-121.2			
Sebacic acid (decanedioic acid)	c	-258.8			
Semicarbazide, std state, <i>m</i> = 1	aq	-39.9	-9.7	71.2	
L-Serine	c	-173.6			
Serylserine	c	-281.8			
Sorbic acid	c	-93.4			
L-Sorbose	c	-303.68	-217.10	52.8	
5,5'-Spirobis(1,3-dioxane)	c	-167.8			
Spiropentane	g	44.27	63.41	67.45	21.06
Stearic acid (octadecanoic acid)	c	-226.5			
Stilbene					
<i>cis</i>	liq	43.81			
<i>trans</i>	c	32.27	75.90	60.0	
Strychnine	c	-41.0			
Styrene	liq	24.83	48.37	56.78	43.64
	g	35.22	51.10	82.48	29.18
Suberic acid (octanedioic acid)	c	-248.1			
Succinamide	c	-138.9			
Succinic acid	c	-224.79	-178.64	42.0	35.8
Sucrose	c	2531.9	2369.18	86.1	

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
L-Tartaric acid	c	-306.5			
DL-Tartaric acid	c	-308.5			
meso-Tartaric acid	c	-305.9			
Tetrabromomethane	g	19.00	15.61	85.53	21.78
Tetracene	c	37.95			
Tetrachlorobenzoquinone	c	-69.0			
1,1,1,2-Tetrachlorodi- fluoroethane	g	-117.1	-97.3	91.5	29.5
1,1,1,2-Tetrachloroethane	g	-35.7	-19.2	85.05	24.67
1,1,2,2-Tetrachloroethane	liq	-47.0	-22.7	59.0	39.6
	g	-36.50	-20.45	86.69	24.09
Tetrachloroethylene	g	-3.40	4.90	81.46	22.69
Tetrachloromethane	liq	-31.75	-14.97	51.67	
	g	-22.90	-12.80	74.07	19.94
1,1,2,2-Tetracyano- cyclopropane	c	141			
Tetracyanoethylene	c	149.1			
Tetradecane	g	-79.38	15.97	167.40	77.93
Tetradecanoic acid	c	-199.2			
1-Tetradecene	g	-49.36	36.99	166.40	75.36
Tetraethylene glycol	liq	-234.6			
Tetraethyllead	liq	12.7	80.4	112.92	
	g	26.3			
1,1,1,2-Tetrafluoroethane	g	-214.10	-197.46	75.58	20.62
Tetrafluoroethylene	g	-157.40	-149.07	71.69	19.24
Tetrafluoromethane	g	-223.0	-212.3	62.45	14.59
Tetrahydrofuran	liq	-51.67			
Tetrahydrofurfuryl alcohol	liq	-104.1			
1,2,3,4-Tetrahydro- naphthalene (Tetralin)	liq	-6.1			
Tetrahydropyran	liq	-61.1			
1,2,5,6-Tetrahydropyridine	liq	8.0			
Tetraiodomethane	g	62.84	51.89	93.60	22.91
1,2,3,4-Tetramethylbenzene	liq	-23.0	25.49	69.45	
1,2,3,5-Tetramethylbenzene	liq	-23.54	23.58	99.55	57.5
1,2,4,5-Tetramethylbenzene	liq	-29.48	24.20	71.83	51.6
2,2,3,3-Tetramethylbutane	g	-53.99	5.26	93.06	
Tetramethyllead	liq	23.5	62.8	76.5	
	g	32.6	64.7	100.5	34.42
Tetramethylsilane	g	-68.50	-23.92	86.30	31.12
Tetramethylsuccinic acid	c	-242.0			
Tetramethylthia- cyclopropane	c	-19.84			
Tetranitromethane	liq	8.9			
1,1,1,2-Tetraphenylethane	c	53.31			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1,1,2,2-Tetraphenylethane	c	51.63			
Tetraphenylethene	c	74.46			
Tetraphenylhydrazine	c	109.4			
Tetraphenylmethane	c	59.1	137.20		
Tetrazole	c	56.7			
Thebaine	c	-63.0			
Theobromine	c	-86.4			
Thiaadamantane	c	-34.22			
2-Thiabutane	liq	-21.89	1.79	57.14	
	g	-14.25	2.73	79.62	22.73
Thiacyclobutane	g	14.61	25.69	68.17	16.57
Thiacycloheptane	g	-14.66	20.09	86.50	29.78
Thiacyclohexane	liq	-25.32	9.96	52.16	
	g	-15.12	12.68	77.26	25.86
Thiacyclopentane	liq	-17.39	8.97	49.67	
	g	-8.08	11.00	73.94	21.72
Thiacyclopropane	liq	12.41	22.52	38.84	
	g	19.65	23.16	61.01	12.83
4-Thia-5,5-dimethylhex-1-ene	liq	-21.68			
2-Thiaheptane	g	-29.34	8.39	107.73	39.10
3-Thiaheptane	g	-29.92	7.65	108.27	38.71
4-Thiaheptane	liq	-40.62	5.12	80.85	
	g	-29.96	7.94	107.16	38.53
2-Thiahexane	liq	-34.15	4.08	73.49	
	g	-24.42	6.37	98.43	33.64
3-Thiahexane	liq	-34.58	3.50	73.98	
	g	-25.00	5.63	98.97	33.25
5-Thianonane	liq	-52.74	7.66	96.82	
	g	-39.99	11.76	125.76	49.46
2-Thiapentane	liq	-28.21	2.79	65.14	
	g	-19.54	4.40	88.84	28.05
3-Thiapentane	liq	-28.43	2.81	64.36	40.97
	g	-19.95	4.25	87.96	27.97
2-Thiapropane	g	-8.97	1.66	68.32	17.71
6-Thiaundecane	liq	-63.61			
Thioacetic acid	g	-43.49	-36.81	74.86	19.33
Thiohydantoic acid	c	-132.6			
Thiohydantoin	c	-59.5			
Thiolacetic acid	liq	-52.39			
β -Thiolactic acid	liq	-111.6			
Thiophene	liq	19.24	28.97	43.30	
	g	27.66	30.30	66.65	17.42
Thiosemicarbazide	c	6.0			
Thiourea	c	-21.13	5.2	27.7	
	aq, 100	-15.6			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	$C_{p,p}^\circ$, cal · deg ⁻¹ · mol ⁻¹
Threonine, L- and DL-	c	-181.4			
Thymine	c	-111.9			
Thymol	c	-74.0			
Tiglic acid	c	-117.3			
Toluene	liq	2.87	27.19	52.81	37.58
	g	11.95	29.16	76.64	24.77
2-Toluenethiol	liq	10.57			
<i>m</i> -Toluic acid	c	-101.85			
<i>o</i> -Toluic acid	c	-99.55			
<i>p</i> -Toluic acid	c	-102.59			
<i>o</i> -Toluic anhydride	c	-127.5			
<i>p</i> -Toluic anhydride	c	-124.5			
Trehalose	c	-531.3			
2,4,6-Triamino-	c	-17.3	44.10	35.63	
1,3,5-triazine	g	-17.13	42.33	74.10	20.93
(triaminotriazine)					
2-Triazoethanol	liq	22.6			
Tribenzylamine	c	33.6			
Tribromochloromethane	g	3.0	2.17	85.36	
Tribromofluoromethane	g	-45.4	-46.14	82.65	
Tribromomethane	g	4.00	1.78	79.01	16.96
Tributylamine	liq	-67.32			
Tributyl borate	liq	-286.7			
Tributylboron	liq	-83.4			
Tributyl phosphate	liq	-348			
Tributylphosphine oxide	c	-110			
Trichloroacetaldehyde	liq	-56.1			
Trichloroacetamide	c	-85.6			
Trichloroacetic acid	c	-120.7			
Ionized	aq	-123.4			
Trichloroacetyl chloride	liq	-66.4			
Trichlorobenzoquinone	c	-64.5			
1,1,1-Trichloroethane	g	-34.01	-18.21	76.49	22.07
1,1,2-Trichloroethane	g	-33.10	-18.52	80.57	21.47
Trichloroethylene	g	-1.40	4.75	77.63	19.17
Trichlorofluoromethane	g	-68.10	-58.68	74.06	18.66
Trichloromethyl	g	19	22	70.9	15.21
1,2,3-Trichloropropane	g	-44.40	-23.37	91.52	26.82
1,1,1-Tricyanoethane	c	83.9			
Tricyanoethylene	c	105.0			
Tridecane	g	-74.45	13.97	158.09	72.47
Tridecanoic acid	c	-192.8			
1-Tridecene	g	-44.45	34.96	157.09	69.89
Triethylaluminum	liq	-56.6			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Triethylamine	g	-23.80	26.36	96.90	38.46
Triethylaminoborane	liq	-47.47			
Triethyl arsenite	liq	-168.9			
Triethylarsine	liq	3.1			
Triethyl borate	liq	-250.4			
Triethylenediamine	c	-3.4	57.28	37.67	
Triethylene glycol	liq	-192.2			
Triethyl phosphate	liq	-297			
Triethylphosphine	liq	-21.3			
Triethyl phosphite	liq	-205.9			
Triethylstibine	liq	1.2			
Triethylsuccinic acid	c	-254.9			
Triethyl thionophosphate	liq	-232.5			
Trifluoroacetic acid	liq	-255.4			
Trifluoroacetonitrile	g	-118.4	-110.4	71.3	18.70
1,1,1-Trifluoroethane	g	-178.20	-162.11	68.67	18.76
2,2,2-Trifluoroethanol	liq	-207.4			
Trifluoroethylene	g	-118.50	-112.22	69.94	16.54
Trifluoroiodomethane	g	-141.0	-136.70	73.50	
Trifluoromethane	g	-165.71	-157.48	62.04	12.22
Trifluoromethyl					
CF ₃ ·	g	-112.4	-109.2	63.3	11.90
CF ₃ ⁺	g	100.6	103.1	60.8	11.87
Trifluoromethylbenzene	liq	-152.40	-123.98	64.89	
	g	-143.42	-122.20	89.05	31.17
Trifluoromethylhypo- fluorite (CF ₃ OF)	g	-183	-169	77.06	18.97
DL-Trihydroxyglutaric acid	c	-356			
Triiodomethane	g	50.40	42.54	84.97	17.94
Trimethylacetic acid	liq	-134.9			
Trimethylacetic anhydride	liq	-186.4			
2,4,5-Trimethylaceto- phenone	liq	-60.3			
2,4,6-Trimethylaceto- phenone	liq	-63.9			
Trimethylaluminum	liq	-36.1		50.05	37.19
Trimethylamine	g	-5.70	23.64	69.02	21.93
Std state, molarity = 1	aq	-18.17	22.22	31.9	
Trimethylamine aluminum chloride adduct	c	-210.1			
Trimethylammonium ion	aq	-26.99	8.90	47.0	
Std state, molarity = 1					
Trimethyl arsenite	liq	-141.2			
Trimethylarsine	liq	-3.9			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
1,2,3-Trimethylbenzene	liq	-14.01	25.68	66.40	
1,2,4-Trimethylbenzene	liq	-14.79	24.46	67.93	
1,3,5-Trimethylbenzene	liq	-15.18	24.83	65.38	
Trimethyl borate	liq	-222.9			
Trimethylboron	liq	-34.1			
2,2,3-Trimethylbutane	g	-48.95	1.02	91.61	39.33
Trimethylchlorosilane	liq	-91.8			
<i>cis,cis</i> -1,3,5-Trimethyl- cyclohexane	g	-51.48	8.10	93.30	42.93
2,2,3-Trimethylpentane	liq	-61.44	2.21	78.30	
	g	-52.61	4.09	101.62	
2,2,4-Trimethylpentane	liq	-61.97	1.65	78.40	
	g	-53.57	3.27	101.15	
2,3,3-Trimethylpentane	liq	-60.63	2.54	79.93	
	g	-51.73	4.52	103.14	
2,3,4-Trimethylpentane	liq	-60.98	2.55	78.71	
	g	-51.97	4.52	102.31	
2,4,4-Trimethyl-1-pentene	liq	-35.21	20.66	73.2	
2,4,4-Trimethyl-2-pentene	liq	-34.44	21.04	74.5	
Trimethylphosphine	liq	-29.2			
Trimethylphosphine- <i>N</i> -ethylimine	liq	-35.8			
Trimethylphosphine oxide	c	-114.2			
Trimethyl phosphite	liq	-177.1			
Trimethylsilanol	liq	-130.3			
Trimethylstibine	liq	0.2			
Trimethylsuccinic acid	c	-239.2			
Trimethylsuccinic anhydride	c	-164.5			
Trimethylthiacyclopropane	liq	-14.47			
Trimethylurea	c	-79.0			
2,4,6-Trinitroanisole	c	-37.6			
1,3,5-Trinitrobenzene	c	-10.40			
Trinitromethane	c	-11.50			
1,4,5-Trinitronaphthalene	c	8.7			
1,3,8-Trinitronaphthalene	c	5.8			
2,4,6-Trinitrophenetole	c	-48.9			
2,4,6-Trinitrophenol	c	-51.23			
2,4,6-Trinitrophenyl- hydrazine	c	8.8			
2,4,6-Trinitrotoluene	c	-16.0			
2,4,6-Trinitro- <i>m</i> -xylene	c	-24.5			
Triphenylamine	c	58.70 ^{18°C}	120.50		
Triphenylarsine	c	74.1			
Triphenylcarbinol	c	-0.80	65.2	78.7	

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
Triphenylene	c	33.72	78.68	60.87	
1,1,1-Triphenylethane	c	37.56			
1,1,2-Triphenylethane	c	31.11			
Triphenylethylene	c	55.8	123.00		
Triphenylmethane	c	38.71	98.60	74.6	70.5
Triphenyl phosphate	c	-181			
Triphenylphosphine	c	55.5			
Triphenylphosphine oxide	c	-14.4			
Tripropylamine	liq	-49.51			
Tris(acetylacetonato)- chromium	c	-366.4			
1,1,1-Tris(hydroxymethyl)- ethane	c	-177.96			
Tropolone	c	-57.18			
L-Tryptophan	c	-99.8	-28.54	60.00	56.92
L-Tyrosine	c	-163.4	-92.18	51.15	51.73
Undecane	liq	-78.05	5.44	109.49	
	g	-64.60	9.94	139.48	61.53
1-Undecene	g	-34.60	30.94	138.48	58.96
Urea	c	-79.71	-47.19	25.00	22.26
Std state, $m = 1$	aq	-75.95			
Urea nitrate	c	-134.8			
Urea oxalate	c	-365.3			
Uric acid	c	-147.73	-85.75	41.4	
Valeric acid	liq	-133.71	-89.10	62.10	50.48
Valine, L and DL-	c	-148.2	-85.80	42.75	40.35
Valylphenylalanine	c	-183.5			
Veronal	c	-178.7			
Vinyl radical	g	63			
Vinyl bromide	g	18.7	19.3	65.90	13.27
Vinyl chloride	g	8.5	12.4	63.07	12.84
Vinylcyclohexane	liq	-21.19			
Vinylcyclopropane	liq	29.3			
2-Vinylpyridine	liq	37.2			
Xanthine	c	-90.49	-39.64	38.5	
<i>o</i> -Xylene	liq	-5.84	26.37	58.91	44.9
	g	4.54	29.18	84.31	31.85
<i>m</i> -Xylene	liq	-6.08	25.73	60.27	43.8
	g	4.12	28.41	85.49	30.49
<i>p</i> -Xylene	liq	-5.84	26.31	59.12	
	g	4.29	28.95	84.23	30.32
2,3-Xylenol	g	-37.57			
2,4-Xylenol	g	-38.93			
2,5-Xylenol	g	-38.63			

TABLE 5.1 Enthalpies and Gibbs (Free) Energies of Formation, Entropies, and Heat Capacities of Organic Compounds (*continued*)

Substance	State	ΔH_f° , kcal · mol ⁻¹	ΔG_f° , kcal · mol ⁻¹	S° , cal · deg ⁻¹ · mol ⁻¹	C_p° , cal · deg ⁻¹ · mol ⁻¹
2,6-Xylenol	g	-38.66			
3,4-Xylenol	g	-37.42			
3,5-Xylenol	g	-38.61			
Xylitol	c	-267.32			
D-Xylose	c	-252.8			

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds*Abbreviations Used in the Table* ΔH_m , enthalpy of melting (at the melting point) in $\text{kcal} \cdot \text{mol}^{-1}$ ΔH_v , enthalpy of vaporization (at the boiling point) in $\text{kcal} \cdot \text{mol}^{-1}$ ΔH_s , enthalpy of sublimation (at 298 K) in $\text{kcal} \cdot \text{mol}^{-1}$ C_p , specific heat (at temperature specified, measured on the Kelvin scale) for physical state in existence at that temperature, expressed in $\text{cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ ΔH_t , enthalpy of transition (at temperature specified, measured in degrees Celsius) in $\text{kcal} \cdot \text{mol}^{-1}$

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Acenaphthene			20.6				
Acenaphthylene			17.0				
Acetaldehyde	0.770	6.24		15.73	20.52	24.20	29.96
Acetanilide			19.3				
Acetic acid	2.80	5.663		19.52	25.15	29.08	31.99
Acetic anhydride	2.51	9.85	11.54	30.86	41.62	48.91	54.11
Acetone	1.366	6.952		22.00	29.34	34.93	39.15
Acetonitrile	1.952	7.3	7.94	14.62	18.35	21.26	23.50
(ΔH_t , 0.215 at -56°C)							
Acetophenone		9.275	13.4				
Acetyl bromide			7.9				
Acetyl chloride			7.2	18.86	23.18	26.30	28.60
Acetylene	0.900	4.05	5.1	11.97	13.73	14.93	15.92
Acetylenedicarbonitrile			6.88	22.66	25.37	27.26	28.62
Acetyl fluoride			6.0				
Acetyl iodide			7.9				
Acrylic acid		11.21	12.98	22.94	29.50	33.93	37.12
Acrylonitrile		7.8		18.36	23.11	26.43	28.88
Adenine			25.8				

Adipic acid			30.8				
α -Alanine			33.0				
Allyl ethyl sulfoxide			17.1				
Allyl trichloroacetate			12.5				
1-Aminobutane			8.50	35.44	47.30	56.01	62.54
2-Aminobutane			7.5	35.40	47.55	56.42	62.54
Aniline	2.519	10.643	13.325	34.17	46.09	53.79	69.18
Anthracene		13.5	24.7				
9,10-Anthracenedione			26.8				
Azoisopropane			8.5				
Azulene	2.89	13.26	22.8	42.15	59.32	70.59	78.24
Benzaldehyde			12				
1,2-Benzanthra-9,10-quinone			19.8				
Benzene	2.358	7.352	8.090	26.74	37.73	45.06	50.16
Benzenethiol	2.736	9.53	11.64	32.76	44.13	51.59	56.79
Benzil			23.5				
Benzoic acid	4.32	12.10	22.70				
Benzoic anhydride			23				
Benzonitrile	2.60	11.0	13.26	33.65	44.80	52.08	57.08
Benzophenone			22.5				
1,4-Benzoquinone			15.00				
Benzoyl bromide			14.0				
Benzoyl chloride			13.1				
Benzoyl iodide			14.8				
3,4-Benzophenanthrene			25.4				
Benzyl bromide			11.3				
Benzyl chloride			12.3				
Benzyl ethyl sulfide			13.6				
Benzyl iodide			11.3				
Benzyl methyl ketone			12.78				
Benzyl methyl sulfide			12.8				
Bicyclo[4.1.0]heptane			9.14				
Bicyclo[3.1.0]hexane			7.85				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Bicyclo[4.2.0]octane			9.85				
Bicyclo[5.1.0]octane			10.42				
Bicyclopropyl			8.0				
Biphenyl	4.44	10.9		52.83	73.54	86.92	96.00
Biphenylene			30.8				
Bromobenzene	2.54	9.05	10.62	30.44	40.99	47.78	52.40
4-Bromobenzoic acid			21.0				
1-Bromobutane	1.6	7.78		32.64	43.00	50.48	56.03
2-Bromobutane			8.45	33.09	43.76	51.31	56.93
Bromoethane	1.4	6.41	6.57	18.93	24.56	28.58	31.59
Bromoethene				15.91	19.83	22.50	24.46
1-Bromoheptane			12.05				
1-Bromohexane			10.91				
Bromomethane ΔH_f , 0.113 at -99.4°C	1.429	5.715		11.94	14.98	17.26	19.01
2-Bromo-2-methylpropane	0.47		7.4	34.93	45.58	52.65	57.74
ΔH_f , 1.35 at -64.5°C ; 0.25 at -41.6°C							
1-Bromooctane			13.14				
1-Bromopentane	2.74	8.24		39.58	52.34	61.55	68.36
1-Bromopropane	1.56	7.14		25.70	33.66	39.41	43.70
2-Bromopropane		6.79		26.34	34.42	40.09	44.26
1,2-Butadiene	1.665	5.82	5.71	23.54	30.72	36.01	40.02
1,3-Butadiene	1.908	5.42	5.03	24.29	31.84	36.84	40.52
<i>n</i> -Butadiene sulfone			14.7				
Butadiyne				20.17	23.14	25.11	26.61
Butane ΔH_f , 0.494 at -165.60°C	1.114	5.352	5.035	29.60	40.30	48.23	54.22
2,3-Butanedione			9.25				
1,4-Butanedithiol			13.22				
1-Butanethiol	2.500	7.702	8.73	34.95	46.54	55.68	62.95

2-Butanethiol	1.548	7.312	8.14	35.38	46.42	54.29	60.02
1-Butanol	2.24	10.31	12.52	32.80	43.90	52.11	58.26
2-Butanol		9.75	11.87	33.70	44.72	52.68	58.62
2-Butanone	2.017	7.475	8.34	29.81	39.09	46.08	51.33
1-Butene	0.920	5.238	4.81	26.04	35.14	41.80	46.82
2-Butene							
<i>cis</i>	1.747		5.29	24.33	33.80	40.87	46.15
<i>trans</i>	2.332	5.580	5.10	26.02	34.80	44.20	46.58
1-Buten-3-yne		5.439		21.26	26.67	30.40	33.16
<i>N</i> -Butylacetamide			18.2				
Butyl acetate			10.42				
<i>tert</i> -Butylamine		8.58	7.10	36.46	48.87	57.49	63.79
Butylbenzene							
stable(I)	2.682(I)		11.98	54.75	75.20	89.37	99.49
metastable(II)	2.691(11)	9.38					
<i>sec</i> -Butylbenzene			11.72				
<i>tert</i> -Butylbenzene			11.50				
<i>sec</i> -Butyl butyrate			11.3				
Butyl chloroacetate			12.2				
Butyl 2-chlorobutyrate			12.6				
Butyl 3-chlorobutyrate			12.7				
Butyl 4-chlorobutyrate			13.0				
Butyl 2-chloropropionate			13.0				
Butyl 3-chloropropionate			13.3				
Butyl crotonate			12.4				
<i>sec</i> -Butyl crotonate			11.8				
Butylcyclohexane	3.384		11.96	66.00	93.10	112.30	125.70
Butylcyclopentane	2.704	9.20	11.00	57.77	80.38	97.35	114.80
<i>N</i> - Butyldiacetimide		8.69	15.4				
Butyl dichloroacetate			12.5				
<i>tert</i> - Butyl hydroperoxide			11.41				
Butylisobutylamine			10.73				
Butyl lithium			25.6				
Butyl trichloroacetate			12.8				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
1-Butyne	1.441		5.67	23.87	30.83	35.95	39.84
2-Butyne	2.207	5.861	6.38	22.62	29.68	35.14	39.29
Butyraldehyde	2.654	6.340	8.05	30.20	39.60	46.60	51.70
Butyric acid	2.50		15.2				
Butyronitrile	1.2	10.04	9.53	28.39	37.07	43.48	48.22
D-Camphor	1.635	8.13					
ϵ -Caprolactam		14.22	19.9				
Carbazole			20.2				
Carbon disulfide	1.049	6.401					
Chloroacetic acid			18				
Chloroacetyl chloride			9.3				
2-Chlorobenzaldehyde			13.3				
Chlorobenzene	2.28	8.73	9.81	30.62	41.16	47.89	52.48
2-Chlorobenzoic acid			19.0				
3-Chlorobenzoic acid			19.6				
4-Chlorobenzoic acid			21.0				
Chlorobenzoquinone			16.5				
1-Chlorobutane		7.38	8.0	32.30	42.77	50.31	55.92
2-Chlorobutane		6.98	7.60	32.52	43.18	50.84	56.60
Chlorocyclohexane			10.4				
Chlorodifluoromethane	0.985	4.833		15.63	18.87	20.84	22.10
Chloroethane	1.064	5.892		18.54	24.28	28.39	31.48
1-Chloro-2-ethylbenzene			11.3				
1-Chloro-4-ethylbenzene			11.5				
Chloroethylene				15.56	19.61	22.35	24.35
Chloroethyne				14.39	15.97	16.98	17.75
Chlorofluoromethane				13.29	16.57	18.81	20.39

Chloroform	2.28	7.08	7.48	17.75	20.38	21.87	22.83
Chloromethane	1.537	5.147		11.52	14.66	17.04	18.86
Chloromethyloxirane			9.7				
1-Chloro-2-methylpropane			7.57	32.52	43.18	50.84	56.60
2-Chloro-2-methylpropane ΔH_f , 0.41 at -90.1°C ; 1.39 at -53.6°C	0.48	6.6		34.00	44.20	51.50	57.00
1-Chloronaphthalene			15.6				
2-Chloronaphthalene			19.6				
1-Chloropentane		7.93	9.1	39.24	52.11	61.38	68.25
3-Chlorophenol			12.7				
4-Chlorophenol			12.4				
1-Chloropropane		6.62	6.9	25.36	33.43	39.24	43.59
2-Chloropropane		6.34	6.47	25.99	34.20	39.94	44.16
3-Chloro-1-propene				22.12	28.43	32.93	36.30
Chlorotrifluoromethane				18.53	21.60	23.17	24.03
Chlorotrinitromethane			10.86				
Chrysene			28.1				
<i>o</i> -Cresol		10.20	18.17	39.74	52.77	61.55	68.82
<i>m</i> -Cresol		10.32	14.75	38.74	52.26	61.27	68.50
<i>p</i> -Cresol		10.32	17.67	38.65	52.10	61.11	68.48
<i>m</i> -Cresyl acetate			14.51				
Cubane			19.2				
4-Cyanothiazole			17.67				
Cyclobutane ΔH_f , 1.38 at -126.79°C	0.260	5.781	5.65	23.89	34.76	42.42	47.96
Cyclobutene				21.59	30.30	36.26	40.53
Cyclododecane			18.26				
Cycloheptane ΔH_f , 1.187 at -138.4°C ; 0.069 at -75.0°C ; 0.108 at -60.8°C	0.450	7.93	9.21	41.82	62.42	77.03	87.40
Cycloheptanone			12.4				
1,3,5-Cycloheptatriene ΔH_f , 0.561 at -118.19°C	0.277	9.250		37.13	50.07	58.58	64.58
Cyclohexane ΔH_f , 1.611 at -87°C	0.640	7.160	7.896	35.82	53.83	66.76	75.80
Cyclohexanol ΔH_f , 1.96 at -9.7°C	0.406	10.875	12.820	41.14	59.29	72.18	81.13
Cyclohexanone		9.00	10.77	36.00	52.90	65.00	73.00
Cyclohexene ΔH_f , 1.016 at -134.4°C	0.787	7.285	8.00	34.64	49.45	59.49	66.62

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Cyclooctane ΔH_t , 1.507 at -106.7°C ; 0.114 at -89.35°C	0.576	8.58	10.36	47.82	71.00	87.30	99.01
Cyclooctanone			13.0				
1,3,5,7-cyclooctatetraene	2.695	8.700	10.30	38.45	52.77	62.23	68.88
Cyclopentadiene			6.78				
Cyclopentane ΔH_t , 1.167 at -150.76°C ; 0.823 at -135.08°C	0.1455	6.524	6.818	28.38	42.57	52.60	59.84
Cyclopentanethiol	1.872	8.443	9.93	34.53	48.65	58.61	65.84
Cyclopentanol			13.74				
Cyclopentanone			10.21				
Cyclopentene ΔH_t , 0.115 at -186.08°C	0.804		6.71	25.08	37.19	45.78	51.94
Cyclopropane	1.301	4.793		18.31	26.15	33.57	35.39
Decahydronaphthalene							
<i>cis</i> ΔH_t , 0.511 at -57.1°C	2.268	9.940	12.0	56.64	84.14	103.36	116.91
<i>trans</i>	3.455	9.260	11.6	56.78	84.20	103.40	116.93
Decanal				71.80	95.70	113.00	125.70
Decane	6.863	9.388	12.277	71.24	96.36	114.92	128.20
1-Decanethiol	7.4	11.1	15.5	76.63	102.63	122.10	136.98
Decanoic acid	7.0		28.4				
1-Decanol	9.0	11.9	18.6	74.44	99.94	118.53	132.24
1-Decene ΔH_t , 1.90 at -74.8°C	3.300	9.24	12.06	67.79	91.27	108.28	120.90
1-Decyne				65.64	86.96	102.42	113.90
Deoxybenzoin			22.3				
Dibenzilidene azine			22.3				
Dibenzyl ketone			21.3				
Dibenzyl sulfide			22.3				
Dibenzyl sulfone			27.8				

1,2-Dibromobutane			10.8	36.77	46.70	53.60	58.50
1,2-Dibromocycloheptane			12.43				
1,2-Dibromocyclohexane			12.07				
1,2-Dibromocyclooctane			13.04				
1,2-Dibromoethane	2.62	8.69	9.86	23.83	29.24	32.94	35.80
1,2-Dibromoheptane			13.01				
1,2-Dibromopropane				29.74	37.63	42.91	46.74
Dibutylborinic acid			15				
Dibutyl ether		8.83	10.5	60.78	81.29	96.52	107.86
Dibutyl mercury			15.6				
Di- <i>tert</i> -butyl peroxide			7.6				
Dibutyl <i>o</i> -phthalate			21.9				
Dibutyl sulfate			18.1				
Dibutyl sulfite			16.2				
Dibutyl sulfone			24.0				
Dichloroacetyl chloride			9.4				
1,2-Dichlorobenzene	3.19	9.7	11.56	34.12	44.07	50.28	54.42
1,3-Dichlorobenzene			11.44	34.18	44.09	50.29	54.42
1,4-Dichlorobenzene	4.34	9.5	15.5	34.24	44.16	50.35	54.46
2,6-Dichlorobenzoquinone			16.7				
2,2'-Dichlorobiphenyl			23.0				
4,4'-Dichlorobiphenyl			24.8				
Dichlorodifluoromethane				19.69	22.37	23.69	24.39
1,1-Dichloroethane	1.881	6.97	7.36	21.85	27.18	30.79	33.40
1,2-Dichloroethane	2.112	7.65	8.47	22.00	26.90	30.40	33.00
1,1-Dichloroethylene	1.557	6.26	6.328	18.80	22.44	24.71	26.29
1,2-Dichloroethylene							
<i>cis</i>	1.72	7.08	7.43	18.41	22.23	24.60	26.23
<i>trans</i>	1.72	6.65	6.92	18.58	22.28	24.62	26.24
Dichlorofluoromethane				16.78	19.70	21.41	22.51
Dichloromethane	1.1	6.74	6.94	14.24	17.30	19.32	20.76
1,2-Dichloropropane		7.59	8.68	28.60	36.47	41.97	46.08
1,3-Dichloropropane		8.10	9.66	28.69	36.22	41.56	45.50
2,2-Dichloropropane		7.0	7.8	30.56	38.06	43.00	46.56

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Dicyanoacetylene			6.88				
2,2-Diethoxypropane			7.61				
Diethylamine			7.6	34.88	47.14	56.16	62.91
1,2-Diethylbenzene	4.01	9.42	12.61	56.01	75.66	89.54	99.49
1,3-Diethylbenzene	2.62	9.41	12.55	55.01	75.19	89.31	99.37
1,4-Diethylbenzene	2.53	9.41	12.54	54.68	74.84	89.04	99.16
Diethylene glycol		12.50	13.7				
Diethyl ether	1.745	6.38	6.516	33.01	43.92	52.26	58.51
Diethylmercury			10.7				
Diethylmethyl phosphonate			13.5				
Diethylnitramine			12.7				
Diethyl oxalate		10.04	15.2				
Diethyl peroxide			7.3				
Diethyl <i>o</i> -phthalate			21.1				
Diethyl selenide			9.3				
Diethyl sulfate			13.6				
Diethyl sulfite			11.6				
Diethyl sulfone			20.6				
Diethyl sulfoxide			14.9				
1,2-Difluorobenzene	2.640	7.699	8.65	32.76	43.33	50.12	54.72
1,3-Difluorobenzene			8.29	32.72	43.13	49.67	53.93
1,4-Difluorobenzene			8.51	32.84	43.20	49.68	53.99
2,2'-Difluorobiphenyl			22.7				
4,4'-Difluorobiphenyl			21.8				
1,1-Difluoroethane		5.1		19.93	25.70	29.70	32.57
1,1-Difluoroethylene				17.16	21.32	23.95	25.74
Difluoromethane				12.22	15.72	18.22	19.98

9,10-Dihydroanthracene			22.3				
4 <i>H</i> -Dihydropyran			7.7				
5,12-Dihydrotetracene			27.7				
2,3-Dihydrothiophene			9.02				
2,5-Dihydrothiophene			9.55				
1,2-Diiodobenzene			15.5				
1,2-Diiodoethane			15.7	22.94	27.92	31.37	33.84
Diiodomethane	3.02(I) 2.88(II)		12.2	15.74	18.37	20.06	21.29
Diisopropyl ether	2.635	6.95	7.75	46.90	62.61	74.39	83.17
Diisopropyl ketone			9.93				
Diisopropylmercury			12.8				
1,2-Dimethoxybenzene			16.0				
Dimethoxyborane			6.14				
2,2-Dimethoxypropane			7.03				
Dimethylamine	1.420	6.330	6.07	20.89	28.41	33.94	38.19
Dimethylaminotrimethylsilane			7.6				
2,2-Dimethylbutane ΔH_f , 1.289 at –147.34°C; 0.068 at –132.28°C	0.138	6.287	6.618	43.70	60.00	71.40	79.70
2,3-Dimethylbutane ΔH_f , 1.552 at –137.08°C	0.194	6.519	6.96	43.30	59.20	75.20	79.10
2,3-Dimethyl-1-butene		6.55	6.97	42.60	55.40	65.00	72.20
2,3-Dimethyl-2-butene a. ΔH_f , b. 0.844 at –76.34°C	1.542	7.083	7.776	37.48	51.78	62.78	71.14
3,3-Dimethyl-1-butene ΔH_f , 1.037 at –148.3°C	0.261	6.13	6.36	38.90	53.40	63.60	71.00
Dimethylcadmium			9.07				
1,1-Dimethylcyclohexane ΔH_f , 1.430 at –120.01°C	0.495	7.79	9.043	50.70	74.10	90.70	102.20
1,2-Dimethylcyclohexane <i>cis</i> ΔH_f , 1.974 at –100.6°C	0.393	8.04	9.492	51.10	74.00	90.10	101.40
<i>trans</i>	2.491(I) 2.508(II)	7.86	9.168	51.90	74.60	90.50	101.70
1,3-Dimethylcyclohexane <i>cis</i>	2.586	7.84	9.137	51.20	74.20	90.50	102.00
<i>trans</i>	2.358	8.09	9.369	51.10	73.80	89.80	101.10

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
1,4-Dimethylcyclohexane							
<i>cis</i>	2.225	8.07	9.329	51.10	73.80	89.80	101.10
<i>trans</i>	2.947	7.79	9.053	51.60	74.60	90.60	101.90
1,1-Dimethylcyclopentane	0.258	7.239	8.079	43.55	62.78	76.18	85.83
ΔH_t , 1.551 at -126.36°C							
1,2-Dimethylcyclopentane							
<i>cis</i> ΔH_t , 1.594 at -131.66°C	0.396	7.576	8.549	43.67	62.72	75.98	85.57
<i>trans</i>	1.713	7.375	8.259	43.71	62.66	75.84	85.43
1,3-Dimethylcyclopentane							
<i>cis</i>	1.761	7.265	8.200	43.71	62.66	75.84	85.43
<i>trans</i>	1.738	7.361	8.248	43.71	62.66	75.84	85.43
Dimethyldichlorosilane			8.2				
<i>cis</i> -2,4-Dimethyl-1,3-dioxane			9.53				
4,5-Dimethyl-1,3-dioxane			10.16				
5,5-Dimethyl-1,3-dioxane			9.86				
Dimethyl ether	1.180	5.141		19.02	25.16	30.04	33.79
<i>N,N</i> -Dimethylformamide			11.4				
Dimethylfulvene			10.6				
Dimethylglyoxime			23.2				
2,2-Dimethylhexane	1.62	7.71	8.91				
2,3-Dimethylhexane		7.94	9.27				
2,4-Dimethylhexane		7.79	9.03				
2,5-Dimethylhexane	3.096	7.80	9.05				
3,3-Dimethylhexane	1.7	7.76	8.97				
3,4-Dimethylhexane		7.95	9.32				
2,2-Dimethyl-3-hexene							
<i>cis</i>			8.88				
<i>trans</i>			8.91				

1,1-Dimethylhydrazine			8.37				
1,2-Dimethylhydrazine			9.40				
Dimethylmercury			8.26				
Dimethylnitramine			16.7				
2,2-Dimethylpentane	1.392	6.97	7.75	50.42	68.33	81.43	91.20
2,3-Dimethylpentane		7.26	8.19	50.42	68.33	81.43	91.20
2,4-Dimethylpentane	1.636	7.05	7.86	50.42	68.33	81.43	91.20
3,3-Dimethylpentane	1.689	7.09	7.89	50.42	68.33	81.43	91.20
2,7-Dimethylphenanthrene			25.5				
4,5-Dimethylphenanthrene			25.0				
9,10-Dimethylphenanthrene			28.6				
2,2-Dimethylpropane ΔH_f , 0.616 at -133.14°C	0.752	5.438	5.205	37.55	51.21	60.78	67.80
2,3-Dimethylpyridine			11.70				
2,4-Dimethylpyridine			11.42				
2,5-Dimethylpyridine			11.43				
2,6-Dimethylpyridine			11.01				
3,4-Dimethylpyridine			12.38				
3,5-Dimethylpyridine			12.04				
Dimethyl sulfate			11.6				
Dimethyl sulfite			9.6				
Dimethyl sulfone			18.4				
Dimethyl sulfoxide	1.56	12.66	12.64				
3,3-Dimethyl-2-thiabutane	2.011(I) 1.83(II)	7.523	8.57				
2,2-Dimethylthiacyclopropane			8.55				
2,2-Dimethyl-3-thiapentane	1.69	8.00	9.4				
2,4-Dimethyl-3-thiapentane	2.49	8.04	9.44	50.64	66.22	77.12	85.24
1,3-Dinitrobenzene			14.3				
2,4-Dinitrophenol			25				
2,6-Dinitrophenol			26.8				
1,1-Dinitropropane			14.93				
1,4-Dioxane ΔH_f , 0.562 at -0.3°C	3.07		9.20	30.23	43.44	52.15	58.05
1,3-Dioxolan			8.5				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Dipentene			11.5				
Diphenylamine			23.1				
Diphenylchlorosilane			16.6				
Diphenyl disulfide			22.7				
Diphenyl disulfone			38.7				
1,2-Diphenylethane		12.3	20.1				
1,1-Diphenylethene			17.5				
Diphenyl ether	4.115	15.5 ²⁵	19.6				
Diphenylfulvene			25				
Diphenylmercury			26.95				
Diphenylmethane			19.7				
Diphenyl sulfide			16.2				
Diphenyl sulfone			25.4				
Diphenyl sulfoxide			23.2				
Dipropyl ether			8.6	46.90	62.61	74.39	83.17
Dipropylmercury			13.2				
Dipropyl sulfate			16.0				
Dipropyl sulfite			14.0				
Dipropyl sulfone			19.1				
Dipropyl sulfoxide			17.8				
2,3-Dithiabutane	2.197	8.05	9.17	26.36	32.83	37.66	41.31
5,6-Dithiadecane		11.2	15.2	68.38	89.98	105.83	117.86
3,4-Dithiahexane	2.248	9.01	10.89	40.90	52.24	60.19	65.97
1,3-Dithian-2-thione			21.85				
4,5-Dithiaoctane	3.30	10.02	12.55	44.50	71.30	83.70	93.20
<i>N,N</i> -Dithiodiethylamine			12.6				
1,3-Diothiolan-2-thione			19.56				
Di- <i>p</i> -tolyl sulfone			26.2				

Divinyl ether			6.26				
Divinyl sulfone			13.5				
Dodecane	8.57	10.43	14.65	85.13	115.04	136.76	152.90
Dodecanedioic acid			36.6				
1-Dodecene	4.76	10.27	14.42	8.68	109.95	130.41	145.50
ΔH_f , 1.088 at -60.2°C							
Eicosane	16.70	13.74	24.1	140.65	189.78	225.28	251.60
Eicosanoic acid	17.2		48				
1-Eicosene	8.2	13.35	23.86	137.20	184.69	218.93	244.20
<i>meso</i> -Erythritol			32.3				
Ethane	0.683	3.517	1.200	15.65	21.35	25.81	29.30
1,2-Ethanedithiol			10.68				
Ethanethiol	1.189	6.401	6.526	21.08	27.21	31.83	35.38
Ethanol	1.198	9.255	10.11	19.36	25.69	30.33	33.83
Ethyl acetate	2.505	7.720	8.63	32.84	43.65	51.01	56.05
Ethyl allyl sulfone			20.0				
Ethylamine		6.7	6.7	21.65	28.68	33.89	37.88
<i>N</i> -Ethylaniline			12.5				
Ethylbenzene	2.195	8.50	10.10	40.76	56.44	67.15	74.77
3-Ethyl-1-butene		6.88	7.41	40.70	54.50	64.40	71.90
Ethyl crotonate			10.6				
Ethylcyclohexane	1.992	8.20	9.67	51.60	74.10	90.10	101.30
1-Ethylcyclohexene			10.34				
Ethylcyclopentane	1.642(I) 1.889(II)	7.715	8.72	43.89	61.70	75.22	85.16
Ethylene	0.801	3.237		12.67	17.87	20.03	22.43
Ethylene carbonate	2.41		17.5				
Ethylene glycol	2.78	11.86	15.68	27.06	32.72	36.90	39.88
Ethyleneimine		7.24	7.55	16.83	23.56	28.14	31.45
Ethylene oxide	1.236	6.101	5.96	14.95	20.62	24.60	27.47
Ethyl formate	2.20	7.201					
2-Ethyl-1-hexanal			11.70				
3-Ethylhexane		8.03	9.48				
Ethylisovalerate			10.5				
Ethyllithium			27.9				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Ethylmercury bromide			18.3				
Ethylmercury chloride			18.2				
Ethylmercury iodide			19.0				
Ethyl methyl ether				26.08	34.58	41.19	46.18
Ethyl nitrate	2.04	7.92	8.67	28.73	37.07	42.72	46.69
3-Ethylpentane	2.282	7.40	8.42	50.42	68.33	81.43	91.20
Ethyl pentanoate			11.0				
2-Ethylphenol			15.20				
3-Ethylphenol			16.30				
4-Ethylphenol			19.20				
Ethylphosphonic acid			12.1				
Ethyl propanoate		8.178	9.0				
Ethyl β -vinylacrylate			11.6				
Ethyl vinyl ether			6.35				
Ethynylbenzene				35.95	48.01	55.79	61.17
Fluoranthrene			24.65				
Fluorobenzene	2.702	7.457	8.27	29.99	40.86	47.83	52.58
4-Fluorobenzoic acid			21.8				
Fluoroethane				17.71	23.56	27.82	31.00
Fluoromethane				10.56	13.83	16.45	18.44
1-Fluoropropane				24.55	32.82	38.88	43.37
2-Fluoropropane				24.72	33.14	39.14	43.55
4-Fluorotoluene	2.235	8.144	9.42	36.43	49.70	58.60	64.84
Fluorotrinitromethane			8.3				
Formaldehyde		5.85		9.38	11.52	13.37	14.81
Formic acid	3.035	5.24	11.03	12.85	16.02	18.35	19.95
Formyl							
HCO·				8.73	9.79	10.75	11.49
HCO ⁺				9.39	10.39	11.14	11.78

Fumaric acid			32.5				
Fumaronitrile			17.2				
Furan ΔH_f , 0.489 at -123.2°C	0.909	6.474	6.61	21.20	29.31	34.41	37.89
Furfuryl alcohol	3.12		15.4				
2-Furoic acid			25.92				
Furylethylene			9.1				
Glycerol	4.416		20.5				
Glyceryl triacetate			19.6				
Glyceryl trinitrate			23.9				
Heptadecane ΔH_f , 2.62 at 11.1°C	9.67	12.64	20.6	119.83	161.75	192.08	214.60
Heptadecanoic acid	12.3						
1-Heptadecene	7.5	12.39	20.32	116.38	156.66	185.74	207.20
1-Heptanal	5.637		11.40	51.00	67.70	79.80	88.70
Heptane	3.359	7.575	8.74	50.42	68.33	81.43	91.20
1-Heptanethiol	6.067	9.5	12.06	55.81	74.60	88.91	99.98
Heptanoic acid			18.0				
1-Heptanol	3.16	11.5	16.5	53.62	71.92	85.32	95.25
1-Heptene ΔH_f , 0.07 at 1.36°C	2.964(I)	7.43	8.52	46.97	63.24	75.09	83.90
	3.021(II)						
Hexachlorobenzene	6.1		23.2	48.08	55.78	59.96	62.34
Hexachloroethane ΔH_f , 1.9 at 71.3°C	2.33	12.2	16.5	36.21	39.82	41.48	42.38
Hexadecafluoroethylcyclohexane			9.20				
Hexadecafluoroheptane			8.7				
Hexadecane	12.39	12.24	19.38	112.89	152.41	181.02	202.20
Hexadecanoic acid	12.8		36.9				
1-Hexadecanol	7.8		40.5	116.09	156.00	184.90	206.30
ΔH_f , 4.8 at 44.0°C ; 5.7 at 49.1°C							
1-Hexadecene	7.216	12.05	19.14	109.44	147.32	174.67	194.80
Hexafluorobenzene	2.770	7.571	8.61	43.88	52.55	57.62	60.63
Hexafluoroethane	0.642	3.860		30.01	35.60	38.40	39.87
ΔH_f , 0.893 at -169.17°C							
Hexahydroindane							
<i>cis</i>			11.0				
<i>trans</i>			10.7				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Hexamethylbenzene ΔH_f , 0.269 at -156.67°C ; 0.422 at 110.7°C	4.93		17.9	74.18	97.13	113.51	125.55
Hexmethylidisiloxane			8.9				
Hexanal				44.00	58.30	68.70	76.40
Hexanamide			22.72				
Hexane	3.126	6.896	7.54	43.47	58.99	70.36	78.89
1-Hexanethiol	4.305	8.9	11.14	48.87	65.26	77.84	87.65
Hexanoic acid	6.98	15.45	17.3				
1-Hexanol	3.68	11.6	14.8	46.68	62.58	74.25	82.92
1-Hexene	2.234	6.76	7.32	40.03	53.90	64.02	71.54
2-Hexene							
<i>cis</i>		6.96	7.52	38.60	53.00	63.40	71.20
<i>trans</i>		6.91	7.54	39.70	53.40	63.60	71.20
3-Hexene							
<i>cis</i>		6.86	7.47	38.50	53.20	63.50	71.20
<i>trans</i>		6.92	7.54	40.20	53.90	63.90	71.40
1-Hexyne				37.87	49.59	58.16	64.56
Hydroquinone			23.7				
8-Hydroxyquinoline			26.0				
Indane			11.8				
Indene			12.64				
Indole			16.7				
Iodobenzene	2.33	9.44	11.85	31.10	41.43	48.07	52.60
4-Iodobenzoic acid			21.0				
Iodocyclohexane			11.3				
Iodoethane		7.115	7.7	19.18	24.64	28.65	31.65
Iodomethane		6.52	6.63	12.33	15.28	17.47	19.17

2-Iodo-2-methylpropane	3.47		8.46	35.27	45.82	52.85	57.91
1-Iodonaphthalene			17.3				
2-Iodonaphthalene			21.7				
1-Iodopropane			8.6	26.27	34.11	39.80	44.03
2-Iodopropane			8.14	26.59	34.58	40.21	44.34
3-Iodopropene			9.1				
Iodotoluene, 3- and 4-			13.0				
Isobutylbenzene			11.54				
Isobutyl dichloroacetate			12.5				
Isobutyl phenyl ketone			14.22				
Isobutyl trichloroacetate			12.7				
Isobutyronitrile	7.754	8.99	28.56	37.39	43.74	48.40	
Isopropyl acetate			8.89				
Isopropylbenzene	1.86	8.97	10.79	48.00	66.20	78.60	87.30
Isopropyl nitrate		8.35	9.27	35.96	46.81	54.13	59.26
Isopropyl trichloroacetate			12.4				
Isothiocyanic acid				12.71	14.57	15.74	16.57
Ketene			4.18	14.22	16.89	18.80	20.25
Lauric acid	8.8		31.7				
Leucine			36.0				
(+)-Limonene			11.5				
Maleic acid			26.3				
Maleic anhydride			17.1				
Malononitrile			18.9				
D-Mannitol	5.39						
Melamine			29.7				
2,2-Metacyclophane			22.0				
Methane ΔH_f , 0.0187 at -248 to -252.7°C	0.225	1.953		9.71	12.55	15.18	17.40
Methanethiol ΔH_f , 0.0525 at -135.6°C	1.411	5.872	5.7	14.04	17.57	20.32	22.48
Methanol ΔH_f , 0.152 at -115.8°C	0.768	8.24	8.94	12.29	16.02	19.04	21.38
4-Methoxybenzaldehyde			15.42				
Methoxybenzene			11.18				
2-Methoxytetrahydropyran			10.2				
Methyl (CH_3)				10.05	11.54	12.89	14.09

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Methyl allyl sulfone			19.0				
Methylamine	1.466	6.169	5.80	14.38	18.86	22.44	25.26
Methyl benzyl sulfone			23.7				
2-Methyl-1,3-butadiene	1.155	6.191	6.32	31.80	41.40	48.00	52.90
3-Methyl-1,2-butadiene		6.51	6.68	31.00	40.30	47.20	52.40
2-Methylbutane	1.231	5.901	5.94	36.49	49.89	59.71	67.12
2-Methyl-1-butanethiol		8.0					
3-Methyl-1-butanethiol	1.78						
2-Methyl-2-butanethiol	0.1454	7.50	8.51	42.79	56.58	66.28	73.30
ΔH_t , 1.907 at -114.0°C							
3-Methylbutanoic acid	1.750	10.32					
2-Methyl-1-butanol		10.5	12.9				
3-Methyl-1-butanol		10.54	13.0				
2-Methyl-2-butanol	1.06	9.6	11.9				
ΔH_t , 0.47 at -127.2°C							
3-Methyl-2-butanol		9.9	12.4				
2-Methyl-1-butene	1.891	6.094	6.181	33.20	44.72	53.15	59.43
3-Methyl-1-butene	1.281	5.750	5.70	35.26	45.90	53.85	59.83
2-Methyl-2-butene	1.816	6.287	6.468	31.93	43.42	52.05	58.55
Methyl butyl sulfone			18.2				
Methyl <i>tert</i> -butyl sulfone			19.7				
3-Methyl-1-butyne		6.25	6.16	31.10	40.60	47.40	52.40
Methyl crotonate			9.8				
Methylcyclohexane	1.614	7.44	8.45	44.35	64.46	78.74	88.79
2-Methylcyclohexanol, <i>cis</i> - and <i>trans</i> -			15.1				
3-Methylcyclohexanol							
<i>cis</i>			15.6				
<i>trans</i>			15.7				

4-Methylcyclohexanol			15.7				
<i>cis</i>			15.8				
<i>trans</i>			7.55	36.11	52.43	64.00	72.44
Methylcyclopentane	1.656	6.95	7.55	32.50	46.80	57.00	64.30
1-Methylcyclopentene			7.7	32.60	47.10	57.20	64.50
3-Methylcyclopentene			7.7	32.60	47.00	57.10	64.40
4-Methylcyclopentene			6.7				
Methyldichlorosilane			9.23				
2-Methyl-1,3-dioxane			9.36				
4-Methyl-1,3-dioxane							
Methylene (CH ₂)				8.64	9.37	10.14	10.89
1-Methyl-2-ethylbenzene	2.38	9.29	11.40	48.50	65.80	78.10	86.90
	2.28						
1-Methyl-3-ethylbenzene	1.82	9.21	11.21	47.50	65.40	77.80	86.80
	1.79						
1-Methyl-4-ethylbenzene	3.19	9.18	11.14	47.20	65.00	77.60	86.60
2-Methyl-3-ethylpentane	2.71	7.88	9.20				
3-Methyl-3-ethylpentane	2.59	7.84	9.08				
2-Methyl-3-ethyl-1-pentene			8.98				
Methyl ethyl sulfite			10.4				
Methyl ethyl sulfone			18.6				
Methyl formate	1.800	6.75		19.50	25.20	29.10	32.00
Methylglyoxal			9.1				
2-Methylheptane	2.839	8.08	9.48				
3-Methylheptane	2.779	8.10	9.52				
4-Methylheptane	2.59	8.10	9.48				
Methyl heptanoate			12.0				
2-Methylhexane	2.195	7.33	8.32	50.42	68.33	81.43	91.20
3-Methylhexane		7.36	8.39	50.42	68.33	81.43	91.20
Methyl hexanoate			11.1				
Methylhydrazine			9.65				
Methylidyne							
CH				6.98	7.11	7.40	7.78
CH ⁺				6.98	7.10	7.36	7.65
1-Methyl-2-isopropylbenzene	2.39	9.17	12.10				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
1-Methyl-3-isopropylbenzene	3.27	9.11	11.94				
1-Methyl-4-isopropylbenzene	2.31	9.12	12.02				
Methyl isopropyl ether			6.27	32.97	44.17	52.67	59.08
Methyl isopropyl ketone			8.82				
Methyl isopropyl sulfone			16.8				
3-Methylisoxazole			9.8				
5-Methylisoxazole			10.0				
Methylmercury bromide			16.2				
Methylmercury chloride			15.5				
Methylmercury iodide			15.6				
1-Methylnaphthalene	1.160	11.0		50.74	69.79	82.48	91.21
ΔH_t , 1.190 at -32.37°C							
2-Methylnaphthalene	2.808	11.0		50.50	69.31	82.03	90.86
ΔH_t , 1.34 at 15.4°C							
Methyl nitrate	1.97	7.54	8.1	21.87	27.54	31.47	34.19
Methyl nitrite		5.0	5.4	18.24	23.35	26.97	29.52
2-Methylpentane	1.498	6.643	7.138	44.00	59.60	70.80	79.20
3-Methylpentane		6.711	7.236	43.47	59.00	70.40	78.90
Methyl pentanoate			10.2				
2-Methyl-1-pentene		6.71	7.29	40.80	54.40	64.40	71.80
3-Methyl-1-pentene		6.43	6.83	42.50	55.60	65.20	72.30
4-Methyl-1-pentene		6.47	6.86	38.90	52.90	63.10	70.70
2-Methyl-2-pentene		6.93	7.55	39.00	53.20	58.60	71.10
3-Methyl-2-pentene							
<i>cis</i>		6.89	7.49	39.00	53.20	63.40	71.10
<i>trans</i>		7.00	7.67	39.00	53.20	63.40	71.10
4-Methyl-2-pentene							
<i>cis</i>		6.59	7.04	40.05	54.10	64.00	71.50
<i>trans</i>		6.68	7.16	41.90	54.80	64.50	71.80

Methyl phenyl sulfone			22.0				
Methylphosphonic acid			11.5				
2-Methylpropanal			7.5				
2-Methylpropane	1.085	5.089	4.57	29.77	40.62	48.49	54.40
2-Methyl-1-propanethiol	1.191	7.412	8.28	35.31	46.26	53.77	59.17
2-Methyl-2-propanethiol							
ΔH_f , 0.972 at -121.6°C ; 0.155 at -116.2°C ; 0.232 at -73.8°C	0.593	6.80	7.36	36.13	47.60	55.53	61.24
2-Methyl-1-propanol		9.80	12.04				
2-Methyl-2-propanol	1.602	9.33	12.73	34.16	45.37	53.28	59.16
ΔH_f , 0.20 at 12.99°C							
2-Methylpropene	1.418	5.286	4.92	26.57	35.30	41.86	46.85
Methyl propyl ether			6.6	33.01	43.92	52.26	58.51
2-Methylpyridine	2.324	8.654	10.15	31.92	44.55	53.21	59.34
3-Methylpyridine	3.389	8.932	10.62	31.82	44.47	53.12	59.23
α -Methylstyrene				44.80	60.70	71.80	79.80
β -Methylstyrene							
<i>cis</i>				44.80	60.70	71.80	79.80
<i>trans</i>				45.20	61.20	72.20	80.00
3-Methyl-2-thiabutane	2.236	7.338	8.15	34.69	46.01	54.95	62.29
2-Methylthiacyclopentane		8.7	10.1				
2-Methyl-3-thiapentane	2.08		9.2				
4-Methylthiazole			10.48				
2-Methylthiophene	2.263	8.103	9.26	29.43	39.57	46.43	51.30
3-Methylthiophene	2.518	8.186	9.44	29.38	39.34	45.95	50.59
Naphthalene	4.536	10.34	17.6	42.83	59.67	70.77	78.38
1-Naphthol			21.9				
2-Naphthol			19.8				
1,4-Naphthoquinone			17.3				
1-Naphthylamine			21.5				
2-Naphthylamine			21.1				
<i>p</i> -Nitroaniline	5.04		26				
Nitrobenzene	2.78	9.744					
1-Nitrobutane		9.3	11.6	37.65	50.21	59.03	65.39
2-Nitrobutane		8.8	10.48	37.61	50.46	59.44	65.96

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Nitroethane		8.4	9.9	23.66	31.45	36.81	40.67
Nitromethane	2.319	8.12	9.17	16.80	21.92	25.56	28.17
1-Nitronaphthalene			25.6				
1-Nitropropane		8.8	10.37	30.72	40.87	47.96	53.06
2-Nitropropane		8.4	9.88	30.89	41.19	48.22	53.24
Nonadecane ΔH_t , 3.30 at 22.8°C	10.95	13.39	22.9	133.71	180.43	214.21	239.20
1-Nonadecene	8.0	13.06	22.68	130.26	175.35	207.86	231.80
1-Nonanal			17.28	64.80	86.40	101.90	113.40
Nonane ΔH_t , 1.50 at -55.97°C	3.72	8.82	11.10	64.30	87.01	103.56	115.90
1-Nonanethiol	8.0	10.6		69.69	93.28	111.04	124.65
Nonanoic acid			19.7				
1-Nonanol		13.0	18.6	67.50	90.60	107.46	119.91
1-Nonene	4.3	8.68	10.88	60.85	81.93	97.22	108.50
Octadecane	14.81	13.02	21.7	126.77	171.09	203.15	226.90
Octadecanoic acid	15.1		39.8				
1-Octadecene	7.8	12.74	21.50	123.32	166.00	196.80	219.50
Octafluorocyclobutane	0.662	5.58		44.50	53.85	58.65	61.50
1-Octanal			16.28	57.90	77.00	90.90	101.00
Octanamide			26.4				
Octane	4.957	8.225	9.916	57.35	77.67	92.50	103.60
1-Octanethiol	58	10.1		62.75	83.94	99.97	112.31
Octanoic acid	3.30	16.73	19.2				
1-Octanol	10.1	11.2	15.6	60.56	81.26	96.39	107.58
1-Octene	3.660	8.07	9.70	53.91	72.58	86.15	96.20
1-Octyne				51.75	68.28	80.30	89.20
Oxalic acid ΔH_t , 0.3($\alpha \rightarrow \beta$)			23.4				
Oxalyl chloride			7.6				
Oxamide			26.8				

Palmitic acid	10.30		37				
[1.8]-Paracyclophane			26.5				
[2.2]-Paracyclophane			23.0				
[6.6]-Paracyclophane			27.5				
Paraldehyde			9.9				
Pentachloroethane	2.7	8.9	10.9	31.96	36.35	38.71	40.17
Pentachlorofluoroethane	0.449						
Pentachlorophenol			16.1				
Pentadecane ΔH_f , 2.19 at -2.25°C	8.31	11.82	18.20	105.95	143.07	169.95	189.90
1-Pentadecene	6.9	11.63	17.96	102.50	137.98	163.60	182.50
1,2-Pentadiene		6.59	6.85	31.40	40.80	47.70	52.80
1,3-Pentadiene							
<i>cis</i>		6.60	6.77	29.50	39.90	47.00	52.20
<i>trans</i>		6.46	6.64	31.20	40.90	47.70	52.60
1,4-Pentadiene	1.468	6.01	6.01	31.30	40.80	47.60	52.70
2,3-Pentadiene		6.75	7.05	29.90	39.40	46.60	52.00
Pentaerythritol			34.4				
Pentaerythritol tetranitrate			36.3				
Pentafluorobenzoic acid			21.9				
Pentafluoroethane				27.20	32.94	36.12	37.98
Pentafluorophenol			16.1				
Pentamethylbenzene	2.95			65.00	86.08	101.29	112.33
ΔH_f , 0.473 at 23.7°C							
1-Pentanal				37.10	49.00	57.70	64.00
Pentanamide			21.34				
Pentan-2,4-dione			10.82				
Pentane	2.008	6.16	6.32	36.53	49.64	59.30	66.55
Pentan-1,5-dithiol			14.17				
Pentanenitrile	1.130	7.98					
1-Pentanethiol	4.19	8.34	9.83	41.93	55.92	66.78	75.32
Pentanoic acid	3.850	10.53	16.6				
1-Pentanol	2.34	10.6	13.61	39.74	53.24	63.18	70.59
2-Pentanol		10.3	12.7				
3-Pentanol		10.1	12.8				
2-Pentanone		7.98	9.89	36.42	48.32	57.13	63.61

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
1-Pentene	1.388	6.02	6.09	33.10	44.56	52.95	59.21
2-Pentene							
<i>cis</i>	1.700	6.24	6.41	31.57	43.62	52.29	58.78
<i>trans</i>	1.996	6.23	6.38	32.67	44.02	52.45	58.81
1-Pentyne		6.63	6.79	31.10	40.40	47.10	52.20
2-Pentyne		6.99	7.35	29.20	38.70	45.90	51.40
Perylene			30.0				
α -Phellandrene			12.1				
9,10-Phenanthraquinone			21.9				
Phenanthrene		13.3	21.1				
Phenol	2.752	9.73	16.41	32.45	43.54	50.62	55.49
Phenyl acetate			13.0				
β -Phenyl-1-alanine, DL- and L-			36.8				
Phenyl benzoate			23.0				
N-Phenyldiacetamide			21.5				
Phenyl ethyl sulfide			13.2				
Phenyldiazine			14.69				
1-Phenyl-2-methylpropane	2.99	9.04	11.82				
Phenyl methyl sulfide			12.1				
Phenyl salicylate			22.0				
Phosgene	1.372	5.832		15.28	16.98	17.92	18.49
	1.335						
	1.131						
<i>m</i> -Phthalic acid			25.5				
<i>p</i> -Phthalic acid			23.5				
Phthalic anhydride			21.19				
α -Pinene			10.7				

β -Pinene			11.1				
Propadiene		4.45		17.21	22.00	25.42	28.00
1-Propanal			7.09	23.09	30.22	35.45	39.27
Propane	0.842	4.487	3.605	22.47	30.76	36.99	41.73
Propane-2,3-dithiol			11.87				
1-Propanethiol ΔH_f , 0.949 at -131.06°C	1.309	7.059	7.62	27.86	36.72	43.60	49.01
2-Propanethiol ΔH_f , 0.013 at -160.6°C	1.371	6.670	7.039	28.35	37.02	43.26	47.92
1-Propanol	1.242	9.982	11.36	25.86	34.56	41.04	45.93
2-Propanol	1.293	9.510	10.85	26.78	35.76	42.13	46.82
2-Propen-1-ol			11.3	22.81	30.11	35.28	39.06
Propionic acid	1.800	7.716	13.7				
Propionic anhydride			12.6				
Propionitrile ΔH_f , 0.408 at -96.19°C	1.202	7.353	8.632	21.18	27.42	32.14	35.70
1-Propylamine			7.46	28.51	37.99	44.94	50.21
Propylbenzene	2.215	9.14	11.05	47.82	65.86	78.30	87.16
	2.03						
Propyl carbamate			19.4				
Propyl chloroacetate			11.6				
Propylcyclohexane	2.479	8.62	10.78	59.10	83.80	101.20	113.40
Propylcyclopentane	2.398	8.15	9.82	50.83	71.04	86.28	97.50
Propylene	0.718	4.40		19.23	25.81	30.77	34.52
Propylene oxide	1.561	6.87	6.67	22.16	30.07	35.68	39.79
Propyl nitrate		8.58	9.70	35.79	46.49	53.87	59.08
Propyl phenyl ketone			14.51				
Propyl trichloroacetate			12.7				
Propyne		5.29		17.33	21.80	25.14	27.71
Pyrazine			13.45				
Pyrene			22.5				
Pyridazine			12.78				
Pyridine	1.979	8.39	9.61	25.42	35.72	42.49	47.17
Pyrimidine			11.95				
Pyrrole			10.80				
Pyrrolidine ΔH_f , 0.129 at -66.01°C	2.050	7.89	8.98	27.33	40.31	49.35	55.84
Salicyclic acid			22.74				
Sebacic acid			38.4				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
5,5'-Spirobis(1,3-dioxane)			17.4				
Spiropentane	1.538	6.39	6.58	28.55	40.10	47.91	53.51
<i>cis</i> -Stilbene			16.5				
Styrene	2.617	8.85	10.50	38.32	52.14	61.40	67.92
Suberic acid			34.2				
Succinic acid			28.1				
Tetrabromomethane				23.20	24.51	25.51	25.32
Tetracene			30				
Tetrachlorobenzoquinone			23.6				
1,1,1,2-Tetrachloroethane				28.36	33.28	36.24	38.17
1,1,2,2-Tetrachloroethane		9.24	10.7	27.90	32.91	35.85	37.76
Tetrachloroethylene	2.5	8.3	9.4	25.10	27.86	29.29	30.07
Tetrachloromethane							
ΔH_f , 1.095 at -47.9°C	0.601	7.16	7.79	21.92	23.82	24.64	25.05
Tetracyanoethylene			19.4				
Tetradecane	10.90	11.38	17.01	99.01	133.72	158.89	177.60
Tetradecanoic acid			33.4				
1-Tetradecene	6.6	11.21	16.78	95.56	128.64	152.54	170.20
Tetraethylene glycol			24				
Tetraethyllead			13.6				
1,1,1,2-Tetrafluoroethane				24.90	30.76	34.20	36.36
Tetrafluoroethylene	1.844	4.02		21.97	25.53	27.61	28.86
Tetrafluoromethane							
ΔH_f , 0.353 at -196.92°C	0.167			17.30	20.74	22.58	23.61
Tetrahydrofuran			7.65				
Tetrahydrofurfuryl alcohol			15.9				
1,2,3,4-Tetrahydronaphthalene			13.4				
Tetrahydropyran			8.35				

Tetraiodomethane				24.00	24.94	25.31	25.49
1,2,3,4-Tetramethylbenzene	2.684	10.76	13.66	56.81	75.68	89.42	99.47
1,2,3,5-Tetramethylbenzene	2.561	10.47	13.34	55.76	74.81	88.79	99.01
1,2,4,5-Tetramethylbenzene	5.02	10.88	18	55.50	74.38	88.41	98.71
2,2,3,3-Tetramethylbutane	1.802	7.51	10.24				
ΔH_f , 0.478 at -120.66°C							
Tetramethyllead			9.1				
Tetranitromethane			10.3				
Tetrazole			23				
2-Thiabutane	2.333	7.06	7.61	27.81	36.41	42.93	47.94
Thiacyclobutane							
ΔH_f , 0.160 at -96.45°C	1.971	7.7	8.56	21.89	30.45	36.40	40.67
Thiacycloheptane			11.30	42.0	65.0	79.0	88.0
Thiacyclohexane							
ΔH_f , 0.262 at -71.75°C ; 1.858 at -33.14°C	0.585	8.60	10.22	35.71	52.37	64.00	72.34
Thiacyclopentane	1.757	8.28	9.28	28.95	40.04	47.66	53.14
Thiacyclopropane		6.98	7.24	16.53	21.99	25.61	28.21
4-Thia-5,5'-dimethyl-1-hexene			10.6				
2-Thiaheptane			10.88	48.67	65.02	77.59	87.41
3-Thiaheptane	2.96	8.78	10.74	48.37	64.96	77.74	87.75
4-Thiaheptane	2.90	8.76	10.64	48.21	65.13	78.45	89.05
2-Thiahexane	2.976	8.2	9.8	41.73	55.68	66.53	75.08
3-Thiahexane	2.529	8.3	9.58	41.43	55.62	66.68	75.42
5-Thianonane	4.64		12.75	62.09	83.81	100.58	113.71
2-Thiapentane	2.369	7.62	8.65	34.64	45.86	54.45	61.14
3-Thiapentane	2.845	7.59	8.55	34.65	46.11	54.91	61.79
2-Thiapropane	1.908	6.45	6.61	21.12	27.01	31.58	35.17
6-Thiaundecane			14.7				
Thioacetic acid				22.25	26.72	30.41	32.62
Thiophene ΔH_f , 0.152 at -101.6°C	1.216	7.52	8.27	23.02	30.95	36.01	39.54
Thymol			21.8				
Toluene	1.586	7.93	9.08	33.48	47.20	56.61	63.32
2-Toluenethiol			12.3				
2,4,6-Triamino-1,3,5-triazine			29.5				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Tribromomethane				18.80	21.03	22.29	23.12
Tributyl phosphate			17.2				
Trichloroacetyl chloride			9.8				
Trichlorobenzoquinone			21.2				
1,1,1-Trichloroethane							
ΔH_t , 1.79 at -48.95°C	0.45	7.96	7.76	25.72	30.68	33.73	35.81
1,1,2-Trichloroethane	2.7	8.3	9.4	25.03	30.13	33.28	35.42
Trichloroethylene		7.52	8.2	21.80	25.06	26.94	28.15
Trichlorofluoromethane				20.84	23.13	24.19	24.74
Trichloromethyl (CCl_3)				16.66	18.16	18.83	19.18
1,2,3-Trichloropropane		8.87	11.22	31.71	38.87	43.79	47.34
Tricyanoethylene			19.4				
Tridecane ΔH_t , 1.831 at -18.2°C	6.81	10.91	15.83	92.07	124.38	147.82	165.20
Tridecanoic acid	8.2		35.0				
1-Tridecene	6.2	10.75	15.60	88.62	119.29	141.48	157.80
Trimethylaluminum			17.5				
Triethylamine			8.29	48.70	66.10	78.56	87.80
Triethylaminoborane			14.5				
Triethyl arsenite			12.1				
Triethylarsine			10.3				
Triethyl borate			10.5				
Triethylenediamine							
ΔH_t , 2.30 at 79.8°C	1.45		14.8				
Triethylene glycol		17.07	18.9				
Triethyl phosphate			13.7				
Triethylphosphine			9.5				
Triethyl phosphite			10.0				
Triethylstibine			10.4				

1,1,1-Trifluoroethane	1.480	4.58		22.75	28.38	31.98	34.44
Trifluoroethylene				19.39	23.30	25.69	27.23
Trifluoromethane	0.970	3.99		14.61	18.16	20.35	21.76
Trifluoromethyl							
CF ₂				13.74	16.17	17.50	18.25
CF ₃ ⁺				13.62	16.00	17.35	18.13
Trifluoromethylbenzene	3.29	7.80	8.98	40.59	54.20	62.75	68.45
Triodomethane	3.9		16.7	19.60	21.52	22.64	23.38
2,4,5-Trimethylacetophenone			15.1				
2,4,6-Trimethylacetophenone			14.9				
Trimethylaluminum			15.1				
Trimethylamine	1.564	5.48	5.26	28.08	38.34	45.62	50.98
Trimethyl arsenite			10.1				
Trimethylarsine			6.9				
1,2,3-Trimethylbenzene	1.955	9.57	11.73	46.90	64.00	76.70	85.90
Δ <i>H</i> _t , 0.157 at −54.46 °C;							
0.319 at −42.89 °C							
1,2,4-Trimethylbenzene	3.153	9.38	11.46	46.96	64.29	76.93	86.10
1,3,5-Trimethylbenzene	2.274	9.33	11.35	46.41	64.08	76.84	86.07
	1.932						
	1.892						
Trimethyl borate			8.3				
Trimethylboron			4.83				
2,2,3-Trimethylbutane							
Δ <i>H</i> _t , 0.586 at −157.8 °C	0.540	6.92	7.65	50.83	69.61	82.73	92.32
Trimethylchlorosilane			7.2				
<i>cis,cis</i> -1,3,5-Trimethylcyclohexane				58.05	83.94	102.20	115.21
2,2,3-Trimethylpentane	2.06	7.65	8.82				
2,2,4-Trimethylpentane	2.20	7.41	8.40				
2,3,3-Trimethylpentane	0.205	7.73	8.90				
Δ <i>H</i> _t , 1.850 at −109.01 °C							
2,3,4-Trimethylpentane	2.215	7.82	9.01				
2,4,4-Trimethyl-1-pentene		7.5	8.5				
2,4,4-Trimethyl-2-pentene		7.8	8.9				
Trimethylphosphine			6.7				
Trimethylphosphine oxide			12.0				

TABLE 5.2 Heats of Melting and Vaporization (or Sublimation) and Specific Heat at Various Temperatures of Organic Compounds (*continued*)

Substance	ΔH_m	ΔH_v	ΔH_s	C_p			
				400 K	600 K	800 K	1000 K
Trimethyl phosphite			8.8				
Trimethylsilanol			10.9				
Trimethylstibine			7.5				
Trimethylsuccinic anhydride			17.7				
Trimethylthiacyclopropane			9.40				
2,4,6-Trinitroanisole			31.8				
1,3,5-Trinitrobenzene			23.8				
Trinitromethane			11.15				
2,4,6-Trinitrophenetole			28.8				
2,4,6-Trinitrotoluene			28.3				
Triphenylarsine			23.5				
Triphenylene			28.2				
Triphenylmethane			23.9				
Triphenylphosphine			23				
Tropolone			20.0				
Undecane ΔH_t , 1.64 at -36.55°C	5.28	9.92	13.47	78.18	105.80	125.69	140.60
Undecanoic acid	6.2		29.0				
1-Undecene ΔH_t , 2.202 at -55.8°C	4.06	9.77	13.24	74.74	100.61	119.34	133.20
Urea			21.0				
<i>o</i> -Xylene	3.25	8.80	10.38	41.03	55.98	66.64	74.35
<i>m</i> -Xylene	2.765	8.69	10.20	40.03	55.51	66.41	74.23
<i>p</i> -Xylene	4.09	8.60	10.13	39.70	55.16	66.14	74.02
2,3-Xylenol			20.1				
2,4-Xylenol			15.74				
2,5-Xylenol			20.31				
2,6-Xylenol			18.07				
3,4-Xylenol			20.49				
3,5-Xylenol			19.80				

CRITICAL PHENOMENA

The *critical temperature* T_c of a gas is the temperature above which the gas cannot be liquefied no matter how high the pressure.

The *critical pressure* P_c is the lowest pressure which will liquefy the gas at its critical temperature.

The *critical molar volume* V_c is the volume of 1 mol at the critical temperature and the critical pressure. It can be computed from the critical density ρ_c as follows:

$$\frac{\text{Molecular weight in g} \cdot \text{mol}^{-1}}{\rho_c \text{ in g} \cdot \text{cm}^{-3}} = V_c \text{ in cm}^3 \cdot \text{mol}^{-1}$$

The critical pressure, critical molar volume, and critical temperature are the values of the pressure, molar volume, and thermodynamic temperature at which the densities of coexisting liquid and gaseous phases just become identical. At this critical point the *critical compressibility factor* Z_c is

$$Z_c = \frac{P_c V_c}{RT_c}$$

Since pressure, volume, and temperature are related to the corresponding critical properties, the function connecting the reduced properties becomes the same for each substance. The reduced property is expressed as a fraction of the critical property.

$$P_r = \frac{P}{P_c} \quad V_r = \frac{V}{V_c} \quad T_r = \frac{T}{T_c}$$

TABLE 5.3 Critical Properties

Substance	T_c , K	P_c , atm	V_c , $\text{cm}^3 \cdot \text{mol}^{-1}$
Acetaldehyde	461	55	154
Acetic acid	594.4	57.1	171.3
Acetic anhydride	569	46.2	290
Acetone	508.1	46.4	209
Acetonitrile	548	47.7	173
Acetophenone	701	38	376
Acetyl chloride	508	58	204
Acetylene	308.3	60.6	113
Acrylic acid	615	56	210
Acrylonitrile	536	45	210
Air	132.5	37.2	92.7
Allene	393		
Allyl alcohol	545	56.4	203
Allyl sulfide	653		
Aluminum trichloride	629	26	261
Aminoethanol	614	44	196
Ammonia	405.6	111.3	72.5
Aniline	699	52.4	270
Anisole	368	41.2	
Anthracene	883		
Antimony tribromide	904.5	56	
Antimony trichloride	794		270

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Argon	150.8	48.1	74.9
Arsine	373.0		
Benzaldehyde	695	46	
Benzene	562.1	48.3	259
Benzoic acid	752	45	341
Benzonitrile	699.4	41.6	
Benzyl alcohol	677	46	334
Biphenyl	789	38	502
Bismuth tribromide	1219		301
Bismuth trichloride	1179	118	261
Boron pentafluoride	470		
Boron tribromide	573		280
Boron trichloride	451.9	38.2	
Boron trifluoride	260.8	49.2	
Bromine	584	102	127
Bromobenzene	670	44.6	324
Bromoethane	503.8	61.5	215
Bromomethane	464	85	
Bromopentafluorobenzene	670	44.6	
Bromotrifluoromethane	340.2	39.2	200
1,2-Butadiene	443.7	44.4	219
1,3-Butadiene	425	42.7	221
Butane	425.2	37.5	255
1-Butanol	562.9	43.6	274
2-Butanol	536.0	41.4	268
2-Butanone	535.5	41.0	267
1-Butene	419.6	39.7	240
<i>cis</i> -2-Butene	435.6	41.5	234
<i>trans</i> -2-Butene	428.6	40.5	238
3-Butenenitrile	585	39	265
1-Buten-3-yne	455	49	202
Butyl acetate	579	31	400
1-Butylamine	524	41	288
<i>N</i> -Butylaniline	72	28	518
Butylbenzene	660.5	28.5	497
<i>sec</i> -Butylbenzene	664	29.1	
<i>tert</i> -Butylbenzene	660	29.3	
Butyl benzoate	723	26	561
Butylcyclohexane	667	31.1	
<i>sec</i> -Butylcyclohexane	669	26.4	
<i>tert</i> -Butylcyclohexane	659	26.3	
Butyl ethyl ether	531	30	390
1-Butyne	463.7	46.5	220
2-Butyne	488.6	502	221
Butyraldehyde	524	40	278
Butyric acid	628	52.0	292
Butyronitrile	582.2	37.4	285
Carbon dioxide	304.2	72.8	94.0
Carbon disulfide	552	78.0	170

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Carbon monoxide	132.9	34.5	93.1
Carbon tetrachloride	556.4	45.0	276
Carbon tetrafluoride	227.6	36.9	140
Carbonyl chloride (phosgene)	455	56	190
Carbonyl sulfide	375	58	140
Chlorine	417	76.1	124
Chlorine pentafluoride	415.7	51.9	230.9
Chlorine trifluoride	426.6		
Chlorobenzene	632.4	44.6	308
1-Chlorobutane	542	36.4	312
2-Chlorobutane	520.6	39	305
1-Chloro-1, 1-difluoroethane	410.2	40.7	231
2-Chloro-1,1-difluoroethylene	400.5	44.0	197
Chlorodifluoromethane	369.2	49.1	165
Chloroethane	460.4	52.0	199
Chloroform	536.4	54.0	239
Chloromethane	416.3	65.9	139
2-Chloro-2-methylpropane	507	39	295
Chloropentafluoroacetone	410.7	28.4	
Chloropentafluoroethane	353.2	31.2	252
1-Chloropropane	503	45.2	254
2-Chloropropane	485	46.6	230
3-Chloropropene	514	47	234
Chlorotrifluoromethane	302.0	38.7	180
Chlorotrifluorosilane	308.5	34.2	
<i>o</i> -Cresol	697.6	49.4	282
<i>m</i> -Cresol	705.8	45.0	310
<i>p</i> -Cresol	704.6	50.8	277
Cyanogen	400	59	
Cyclobutane	459.9	49.2	210
Cycloheptane	589	36.7	390
Cyclohexane	553.4	40.2	308
Cyclohexanol	625	37	327
Cyclohexanone	629	38	312
Cyclohexene	560.4	42.9	292
Cyclopentane	511.6	44.5	260
Cyclopentanone	626	53	268
Cyclopentene	506.0		
Cyclopropane	397.8	54.2	170
Cymene	658		
<i>cis</i> -Decalin	702.2	31	
<i>trans</i> -Decalin	690.0	31	
Decane	617.6	20.8	603
Decanenitrile	621.9	32.1	
1-Decanol	700	22	600
1-Decene	615	21.8	650
Decylcyclohexane	750	13.4	
Decylcyclopentane	723.8	15.0	

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Deuterium			
(equilibrium)	38.3	16.28	60.4
(normal)	38.4	16.43	60.3
Deuterium bromide	361.9		
Deuterium chloride	328.4		
Deuterium hydride	35.8	14.64	62.8
Deuterium iodide	421.7		
Deuterium oxide	644.0	213.8	55.6
Diborane	289.0	39.5	
1,2-Dibromoethane	582.9	70.6	
Dibromomethane	583	71	
Dibromotetrafluoroethane	487.6	34	329
Dibutylamine	596	25	517
Dibutyl ether	580	25	500
1,2-Dichlorobenzene	697.3	40.5	360
1,3-Dichlorobenzene	684	38	359
1,4-Dichlorobenzene	685	39	372
Dichlorodifluoromethane	385.0	40.7	217
1,1-Dichloroethane	523	50	240
1,2-Dichloroethane	561	53	220
1,1-Dichloroethylene	544		
1,2-Dichloroethylene	516.5	54.4	
Dichlorofluoromethane	451.6	51.0	197
Dichloromethane	510	60.0	193
1,2-Dichloropropane	577	44	226
Dichlorosilane	449	46.1	
1,1-Dichloro-1,2,2,2-tetrafluoroethane	418.6	32.6	294
1,2-Dichloro-1,1,2,2-tetrafluoroethane	418.9	32.6	293
Diethylamine	496.6	36.6	301
1,4-Diethylbenzene	657.9	27.7	480
Diethyl disulfide	642		
Diethylene glycol	681	46	316
Diethyl ether	466.7	35.9	280
3,3-Diethylpentane	610	26.4	
Diethyl sulfide	557	39.1	318
Difluoroamine (HNF ₂)	403	93	
<i>cis</i> -Difluorodiazine (N ₂ F ₂)	272	70	
<i>trans</i> -Difluorodiazine	260	55	
1,1-Difluoroethane	386.6	44.4	181
1,1-Difluoroethylene	302.8	44.0	154
Dihexyl ether	657	18	720
Dihydrogen disulfide	572	58.3	
Dihydrogen heptasulfide	1015	33	
Dihydrogen hexasulfide	980	36	
Dihydrogen octasulfide	1040	32	
Dihydrogen pentasulfide	930	38.4	
Dihydrogen tetrasulfide	855	43.1	
Dihydrogen trisulfide	738	50.6	
Diisopropyl ether	500	28.4	385

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
1,2-Dimethoxyethane	536	38.2	271
Dimethoxymethane	497		
Dimethylamine	437.6	52.4	187
<i>N,N</i> -Dimethylaniline	687	35.8	
2,2-Dimethylbutane	488.7	30.4	359
2,3-Dimethylbutane	499.9	30.9	358
2,3-Dimethyl-1-butene	501	32.0	343
2,3-Dimethyl-2-butene	524	33.2	351
3,3-Dimethyl-1-butene	490	32.1	340
1,1-Dimethylcyclohexane	591	29.3	416
<i>cis</i> -1,2-Dimethylcyclohexane	606	29.3	
<i>trans</i> -1,2-Dimethylcyclohexane	596	29.3	
<i>cis</i> -1,3-Dimethylcyclohexane	591	29.3	
<i>trans</i> -1,3-Dimethylcyclohexane	598	29.3	
1,1-Dimethylcyclopentane	547	34.0	360
<i>cis</i> -1,2-Dimethylcyclopentane	564.8	34.0	368
<i>trans</i> -1,2-Dimethylcyclopentane	553.2	34.0	362
Dimethyl ether	400.0	53.0	178
2,2-Dimethylhexane	549.8	25.0	478
2,3-Dimethylhexane	563.4	25.9	468
2,4-Dimethylhexane	553.5	25.2	472
2,5-Dimethylhexane	550.0	24.5	482
3,3-Dimethylhexane	562.0	26.2	443
3,4-Dimethylhexane	568.8	26.6	466
Dimethyl oxalate	628	39.2	
2,2-Dimethylpentane	520.4	27.4	416
2,3-Dimethylpentane	537.3	28.7	393
2,4-Dimethylpentane	519.7	27.0	418
3,3-Dimethylpentane	536.3	29.1	414
2,2-Dimethylpropane	433.8	31.6	303
2,2-Dimethyl-1-propanol	549	39	319
2,3-Dimethylpyridine	655.4		
2,4-Dimethylpyridine	644.2		
2,5-Dimethylpyridine	644		
2,6-Dimethylpyridine	623.7		
3,4-Dimethylpyridine	683.8		
3,5-Dimethylpyridine	667.2		
<i>N,N</i> -Dimethyl- <i>o</i> -toluidine	668	30.8	
1,4-Dioxane	587	51.4	238
Diphenyl ether	766	31	
Diphenylmethane	767	29.4	
Dipropylamine	550	31	407
Dodecane	658.3	18.0	713
1-Dodecanol	679	19	718
1-Dodecene	657	18.3	
Dodecylcyclopentane	750	12.8	
Ethane	305.4	48.2	148
Ethanethiol	498.6	54.2	207

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Ethanol	516.2	63.0	167
Ethoxybenzene	647.1	33.8	
Ethyl acetate	523.2	37.8	286
Ethyl acetoacetate	673		
Ethyl acrylate	552	37.0	320
Ethylamine	456	55.5	178
Ethylbenzene	617.1	35.6	374
Ethyl benzoate	697	32	451
2-Ethyl-1-butanol	418.8		
Ethyl butyrate	565.9	30.2	395
Ethyl crotonate	599		
Ethylcyclohexane	609	29.9	450
Ethylcyclopentane	369.5	33.5	375
Ethylene	282.4	49.7	129
Ethylenediamine	592.9	62.1	206
Ethylene glycol	645	76	186
Ethylene oxide	469	71.0	140
Ethyl formate	508.4	46.8	229
3-Ethylhexane	565.4	25.7	455
2-Ethylhexanol	613	27.2	494
2-Ethyl-1-methylbenzene	651	30.0	460
3-Ethyl-1-methylbenzene	637	28.0	490
4-Ethyl-1-methylbenzene	640	29.0	470
Ethyl 3-methylbutyrate	588.0		
1-Ethyl-1-methylcyclopentane	592	29.5	
Ethyl methyl ether	437.8	43.4	221
Ethyl methyl ketone	535.6	41.0	267
3-Ethyl-2-methylpentane	567.0	26.7	443
3-Ethyl-2-methylpentane	576.5	27.7	455
3-Ethyl-3-methylpentane	576.4	27.7	455
Ethyl-2-methylpropanoate	553	30	410
Ethyl methyl sulfide	533	42	
3-Ethylpentane	540.6	28.5	416
<i>o</i> -Ethylphenol	703.0		
<i>m</i> -Ethylphenol	716.4		
<i>p</i> -Ethylphenol	716.4		
Ethylpropanoate	546.0	33.2	345
Ethyl propyl ether	500.6	32.1	244
<i>o</i> -Ethyltoluene	653	31	461
<i>m</i> -Ethyltoluene	636	31	461
<i>p</i> -Ethyltoluene	636	31	461
Ethyl vinyl ether	475	40.2	260
Fluorine	144.3	51.5	66.2
Fluorobenzene	560.1	44.9	271
Fluoroethane	375.3	49.6	169
Fluoromethane	317.8	58.0	124
Fluorotrichloromethane	471.1	43.2	248
Formaldehyde	408	65	

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Formic acid	580		
Furan	490.2	54.3	218
Germanium tetrachloride	550.0	38	330
Glycerol	726	66	255
Hafnium tetrabromide	746		415
Hafnium tetrachloride	723	57.0	304
Hafnium tetraiodide	916		528
Helium-3	3.30	1.167	73.2
Helium-4	5.19	2.24	57.3
Heptadecane	733	13	1000
1-Heptadecanol	736	14	
Heptane	540.2	27.0	432
1-Heptanol	633	30	435
1-Heptene	537.2	28	440
Heptylcyclopentane	679	19.2	
Hexadecane	717	14	
1-Hexadecene	717	13.2	
Hexadecylcyclopentane	791	9.6	
1,5-Hexadiene	507	34	328
Hexafluoroethane	292.8	29.4	223.7
Hexamethylbenzene	767		
Hexane	507.4	29.3	370
1-Hexanol	610	40	381
1-Hexene	504.3	31.3	350
<i>cis</i> -2-Hexene	518	32.4	351
<i>trans</i> -2-Hexene	516	32.3	351
<i>cis</i> -3-Hexene	517	32.4	350
<i>trans</i> -3-Hexene	519.9	32.1	350
Hexylcyclopentane	660.1	21.1	
Hydrazine	653	145	96.1
Hydrogen (equilibrium)	32.9	12.77	65.4
(normal)	33.2	12.8	65.0
Hydrogen bromide	363.2	84.4	100.0
Hydrogen chloride	324.6	82.0	81.0
Hydrogen cyanide	456.8	53.2	139
Hydrogen deuteride, <i>see</i> Deuterium hydride			
Hydrogen fluoride	461	64	69
Hydrogen iodide	424.0	82.0	131
Hydrogen selenide	411	88	
Hydrogen sulfide	373.2	88.2	98.5
Icosane	767	11.0	
1-Icosanol	770	12.0	
Iodine	819	115	155
Iodobenzene	721	44.6	351
Iodomethane	528	65	190

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Isobutyl acetate	561	30	414
Isobutylamine	516	42	284
Isobutylbenzene	650	31	480
Isobutyl butyrate	611		
Isobutylcyclohexane	659	30.8	
Isobutyl formate	551	38.3	350
Isobutyl 3-methylbutyrate	621		
Isobutyl propanoate	592		
Isobutyric acid	609	40	292
Isopropylamine	476	50	229
Isopropylbenzene	631.0	31.7	428
Isopropylcyclohexane	640	28	
Isopropylcyclopentane	601	29.6	
2-Isopropyl-1-methylbenzene	670	28.6	
3-Isopropyl-1-methylbenzene	666	290	
4-Isopropyl-1-methylbenzene	653	27.9	
Isoquinoline	803		
Isoxazole	552.0		
Ketene	380	64	145
Krypton	209.4	54.3	91.2
Mercury	1173	180	
Methane	190.6	45.4	99.0
Methanethiol	470.0	71.4	145
Methanol	512.6	79.9	118
Methoxybenzene (anisole)	641	41.2	
Methyl acetate	506.8	46.3	228
Methyl acrylate	536	42	265
Methylamine	430	73.6	140
<i>N</i> -Methylaniline	701	51.3	
Methyl benzoate	692	36	396
2-Methyl-1,3-butadiene	484	38.0	276
3-Methyl-1,2-butadiene	496	40.6	267
2-Methylbutane	460.4	33.3	306
2-Methyl-1-butanol	571	38	322
3-Methyl-1-butanol	579.5	38	329
2-Methyl-2-butanol	545	39	319
3-Methyl-2-butanone	553.4	38.0	310
2-Methyl-1-butene	465	34.0	294
2-Methyl-2-butene	470	34.0	318
3-Methyl-1-butene	450	34.7	300
Methyl butyrate	554.4	34.3	340
3-Methylbutyric acid	634		
Methylcyclohexane	572.1	34.3	368
Methylcyclopentane	532.7	37.4	319
<i>N</i> -Methylethylamine	496.6	36.6	243
Methyl formate	487.2	59.2	172
2-Methylheptane	559.6	24.5	488

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
3-Methylheptane	563.6	25.1	464
4-Methylheptane	561.7	25.1	476
2-Methylhexane	530.3	27.0	421
3-Methylhexane	535.2	27.8	404
Methylhydrazine	567	79.3	271
Methyl isobutyrate	540.8	33.9	339
Methyl isocyanate	491	55	
1-Methylnaphthalene	772	35.2	445
2-Methylnaphthalene	761	34.6	462
2-Methylpentane	497.5	29.7	367
3-Methylpentane	504.4	30.8	367
2-Methyl-2,4-pentanediol	678	33.9	
4-Methyl-2-pentanone	571	32.3	371
2-Methyl-2-pentene	518	32.4	351
<i>cis</i> -3-Methyl-2-pentene	518	32.4	351
<i>trans</i> -3-Methyl-2-pentene	521	32.3	350
<i>cis</i> -4-Methyl-2-pentene	490	30	360
<i>trans</i> -4-Methyl-2-pentene	493	30	360
Methyl phenyl ether	641	41.2	
2-Methylpropanal	513	41	274
2-Methylpropane	408.1	36.0	263
Methyl propanoate	530.6	39.5	282
2-Methyl-1-propanol (isobutyl alcohol)	547.7	42.4	273
2-Methyl-2-propanol	506.2	39.2	275
2-Methylpropene	417.9	39.5	239
2-Methylpyridine	621		
3-Methylpyridine	645		
4-Methylpyridine	646	44	311
α -Methylstyrene	654	33.6	397
Methyl vinyl ether	436	47	205
Morpholine	618	54	253
Naphthalene	748.4	40.0	410
Neon	44.4	27.2	41.7
Niobium pentabromide	1010		469
Niobium pentachloride	807		400
Niobium pentafluoride	737	62	155
Nitric oxide	180	64	58
Nitrobenzene	732		
Nitrogen-14	126.2	33.5	89.5
Nitrogen-15	126.3	33.5	90.4
Nitrogen dioxide (equilibrium)	431.4	100	170
Nitrogen trifluoride	234.0	44.7	
Nitromethane	588	62.3	173
Nitrosyl chloride	440	90	139
Nitrous oxide	309.6	71.5	97.4
Nitryl fluoride	349.4		
Nonadecane	756	11.0	
Nonane	594.6	22.8	548
1-Nonanol	677		546

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
1-Nonene	592	23.1	580
Nonylcyclopentane	710.5	16.3	
Octadecane	745	11.9	
1-Octadecanol	747	14	
1-Octadecene	739	11.2	
Octane	568.8	24.5	492
1-Octanol	658	34	490
2-Octanol	637	27	494
1-Octene	566.6	25.9	464
<i>trans</i> -2-Octene	580	27.3	
Octylcyclopentane	694	17.7	
Oxygen	154.6	49.8	73.4
Oxygen difluoride	215.2	48.9	97.7
Ozone	161.3	55.0	88.9
Paraldehyde	563		
Pentachloroethane	646.1		
Pentadecane	707	15	880
1-Pentadecene	704	14.4	
Pentadecylcyclopentane	780	10.1	
1,2-Pentadiene	503	40.2	276
<i>trans</i> -1,3-Pentadiene	496	39.4	275
1,4-Pentadiene	478	37.4	276
Pentafluorobenzene	532.0	34.7	
1,1,2 <i>H</i> -Pentafluoropropane	380.11	31.0	273
Pentanal	554	35	333
Pentane	469.6	33.3	304
Pentanoic acid	651	38	340
1-Pentanol	586	38	326
2-Pentanone	564.0	38.4	301
3-Pentanone	561.0	36.9	336
1-Pentene	464.7	40.0	300
<i>cis</i> -2-Pentene	476	36.0	300
<i>trans</i> -2-Pentene	475	36.1	300
Pentyl formate	576		
1-Pentyne	493.4	40	278
Perchloryl fluoride	368.4	53.0	161
Perfluoroacetone	357.3	28.0	
Perfluorobenzene	516.7	32.6	
Perfluorobutane	386.4	22.9	378
Perfluoro-(2-butyltetrahydrofuran)	500.3	15.9	588
Perfluorocyclobutane	388.4	27.41	260
Perfluorocyclohexane	457.2	24	
Perfluorocyclohexene	461.8		
Perfluorodecene	542.3	14.3	
Perfluoroethane	292.8	29.4	223.7
Perfluoroheptane	474.8	16.0	664
Perfluoroheptene	478.1		
Perfluorohexane	451.7	18.8	442

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Perfluorohexene	454.3		
Perfluoromethylcyclohexane	486.8	23	
Perfluoronaphthalene	673.1		
Perfluorononane	524.0	15.4	
Perfluorooctane	502	16.4	
Perfluoropentane	422	20.1	
Perfluoropropane	345.1	26.5	299
Phenanthrene	878		
Phenetole	647	33.8	
Phenol	694.2	60.5	229
Phosgene	455	56	190
Phosphine	324.4	64.5	
Phosphonium chloride	322.2	72.7	
Phosphorus bromide difluoride	386		
Phosphorus chloride difluoride	362.32	44.6	
Phosphorus dibromide fluoride	527		
Phosphorus dichloride fluoride	463.0	49.3	
Phosphorus pentachloride	645		
Phosphorus trichloride	563		260
Phosphorus trifluoride	271.2	42.7	
Phosphoryl chloride difluoride	423.8	43.4	
Phosphoryl trichloride	602		
Phosphoryl trifluoride	346.5	41.8	
Phthalic anhydride	810	47	368
Piperidine	594.0	47	289
Propadiene	393	54.0	162
Propane	369.8	41.9	203
1,2-Propanediol	625	60	237
1,3-Propanediol	658	59	241
Propanoic acid	612	53.0	230
1-Propanol	536.7	51.0	218.5
2-Propanol	508.3	47.0	220
2-Propenal	506	51	
Propionaldehyde	496	47	223
Propionitrile	564.4	41.3	230
Propyl acetate	549.4	23.9	345
Propylamine	497.0	46.8	233
Propylbenzene	638.3	31.6	440
Propylcyclopentane	603	29.6	425
Propylcyclohexane	639	27.7	
Propylene	365.0	45.6	181
Propylene oxide	482.2	48.6	186
Propyl formate	538.0	40.1	285
Propyl propanoate	578		
1-Propyne	402.4	55.5	164
Pyridine	620.0	55.6	254
Pyrrole	639.6	56	
Pyrrolidine	568.6	55.4	249

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Quinoline	794.4		
Radon	376.9	62	139
Rhenium(VII) oxide	942		334
Selenium	1766		
Silane	269.6	47.8	
Silicon chloride trifluoride	307.6	34.2	
Silicon tetrachloride	507	37	326
Silicon tetrafluoride	259.1	36.7	
Silicon trichlorofluoride	438.5	35.3	
Styrene	647	39.4	
Sulfur	1314		
Sulfur dioxide	430.8	77.8	122
Sulfur hexafluoride	318.7	37.1	198
Sulfur tetrafluoride	364.0		
Sulfur trioxide	491.0	81	130
Tantalum pentabromide	974		461
Tantalum pentachloride	767		400
<i>o</i> -Terphenyl	891.0	38.5	769
<i>m</i> -Terphenyl	924.8	34.6	784
<i>p</i> -Terphenyl	926.0	32.8	779
1,1,2,2-Tetrachloro-1,2-difluoroethane	551	34	370
1,1,2,2-Tetrachloroethane	661.1		
Tetrachloroethylene	620	44	290
Tetradecane	694	16	830
1-Tetradecene	689	15.4	
Tetradecylcyclopentane	772	11.1	
Tetrafluoroethylene	306.4	38.9	175
Tetrafluorohydrazine	309.4	37	
Tetrahydrofuran	540.2	51.2	224
1,2,3,4-Tetrahydronaphthalene	719	34.7	
Tetrahydrothiophene	631.9		
1,2,4,5-Tetramethylbenzene	675	29	480
2,2,3,3-Tetramethylbutane	567.8	28.3	461
2,2,3,3-Tetramethylhexane	623.1	24.8	
2,2,5,5-Tetramethylhexane	581.5	21.6	
2,2,3,3-Tetramethylpentane	607.6	27.0	
2,2,3,4-Tetramethylpentane	592.7	25.7	
2,2,4,4-Tetramethylpentane	574.7	24.5	
2,3,3,4-Tetramethylpentane	607.6	26.8	
2-Thiapropane	503.1	54.6	201
Thiophene	579.4	56.2	219
Thymol	698		
Tin(IV) chloride	591.8	37.0	351
Titanium tetrachloride	638	46	340
Toluene	591.7	40.6	316
<i>o</i> -Toluidine	694	37	343
<i>m</i> -Toluidine	709	41	343
<i>p</i> -Toluidine	667		
Toluenitrile	723		

TABLE 5.3 Critical Properties (*continued*)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
Tributylamine	643	18	
1,1,2-Trichloroethane	602	41	294
Trichloroethylene	571	48.5	256
Trichlorofluoromethane	471.2	43.5	248
1,2,3-Trichloropropane	651	39	348
1,2,2-Trichloro-1,1,2-trifluoroethane	487.2	33.7	304
Tridecane	675.8	17.0	780
1-Tridecene	674	16.8	
Tridecylcyclopentane	761	11.9	
Triethanolamine	787.4	24.2	
Triethylamine	535	30	390
Trifluoroacetic acid	491.3	32.2	204
1,1,1-Trifluoroethane	346.2	37.1	221
Trifluoromethane	298.89	47.7	133.3
Trimethylamine	433.2	40.2	254
1,2,3-Trimethylbenzene	664.5	34.1	430
1,2,4-Trimethylbenzene	649.1	31.9	430
1,3,5-Trimethylbenzene	637.3	30.9	433
2,2,3-Trimethylbutane	531.1	29.2	398
2,2,3-Trimethyl-1-butene	533	28.6	400
Trimethylchlorosilane	497.7	31.6	
1,1,2-Trimethylcyclopentane	579.5	29.0	
1,1,3-Trimethylcyclopentane	569.5	27.9	
<i>cis,cis,trans</i> - 1,2,4-Trimethylcyclopentane	579	28.4	
<i>cis,trans,cis</i> - 1,2,4-Trimethylcyclopentane	571	27.7	
3,3,5-Trimethylheptane	609.6	22.9	
2,2,3-Trimethylhexane	588	24.6	
2,2,4-Trimethylhexane	573.7	23.4	
2,2,5-Trimethylhexane	567.9	23.0	519
2,2,3-Trimethylpentane	563.4	26.9	436
2,2,4-Trimethylpentane	543.9	25.3	468
2,3,3-Trimethylpentane	573.5	27.8	455
2,3,4-Trimethylpentane	566.3	26.9	461
2,2,4-Trimethyl-1,3-pentanediol	671	25.6	364.6
1 <i>H</i> -Undecafluoropentane	443.9		
Undecane	638.8	19.4	660
1-Undecene	637	19.7	
Uranium hexafluoride	505.8	45.5	250
Vinyl acetate	525	43	265
Vinyl chloride	429.7	55.3	169
Vinyl fluoride	327.8	51.7	114
Vinyl formate	475	57	210
Water	647.3	217.6	56.0
Xenon	289.7	57.6	118
<i>o</i> -Xylene	630.2	36.8	369

TABLE 5.3 Critical Properties (continued)

Substance	T_c , K	P_c , atm	V_c , cm ³ ·mol ⁻¹
<i>m</i> -Xylene	617.0	35.0	376
<i>p</i> -Xylene	616.2	347	379
2,3-Xylenol	722.6	48	470
2,4-Xylenol	707.6	43	509
2,5-Xylenol	723.0	48	470
2,6-Xylenol	700.9	42	509
3,4-Xylenol	729.8	49	552
3,5-Xylenol	715.6	36	611
Zirconium tetrabromide	805		415
Zirconium tetrachloride	778	56.9	319
Zirconium tetraiodide	960		528
Zirconium tetraiodide	960		528

Estimation of Critical Properties

When the critical properties are unavailable, they may be estimated employing structural contributions to estimate T_c , P_c , and V_c . Lydersen's critical-property increments* provide good estimates for T_c and P_c ; Vetere's group contributions† yield reasonable estimates for V_c . The units employed are kelvins, atmospheres, and cubic centimeters per mole. Typical errors in estimated values are less than 2% for T_c but may rise up to 5% for higher-molecular-weight (greater than 100) nonpolar materials; errors are uncertain for molecules with multifunctional polar groups. Errors for estimated values of P_c and V_c are about double those for T_c .

The relations are

$$T_c = T_b \left[0.567 + \sum \Delta_T - \left(\sum \Delta_T \right)^2 \right]^{-1}$$
$$P_c = M \left(0.34 + \sum \Delta \right)^{-2}$$
$$V_c = 33 + \left[\sum_i \left(M_i \Delta_v \right) \right]^{1.029}$$

where T_b is the normal boiling point and M is the molular weight. Group contributions are listed in Table 5.4.

TABLE 5.4 Group Contributions for the Estimation of Critical Properties

There are no increments for hydrogen. All bonds shown as free are connected with atoms other than hydrogen. Values in parentheses are based upon very few experimental values.

Group	Δ_T , K	Δ_P , atm	Δ_V , cm ³ ·mol ⁻¹
Nonring increments			
—CH ₃ , —CH ₂ —	0.020	0.227	3.360 (linear chain) 2.888 (side chain)

* A. L. Lydersen, Univ. Wisconsin Coll. Eng., Eng. Exp. Stn, Rep 3, Madison, April 1955.
† A Vetere, cited in R. C. Reid, J. M. Prausnitz, and T. K Sherwood, *The Properties of Gases and Liquids*, 3d ed., McGraw-Hill, New York, 1977, p. 17.

TABLE 5.4 Group Contributions for the Estimation of Critical Properties (*continued*)

Group	Δ_T , K	Δ_p , atm	v , $\text{cm}^3 \cdot \text{mol}^{-1}$
$\begin{array}{c} \\ -\text{CH} \\ \end{array}$	0.012	0.210	3.360 (linear chain) 2.888 (side chain)
$\begin{array}{c} \\ -\text{C}- \\ \end{array}$	0.0	0.210	3.360 (linear chain) 2.888 (side chain)
$=\text{CH}_2, \begin{array}{c} \\ =\text{CH} \end{array}$	0.018	0.198	2.940
$\begin{array}{c} \\ =\text{C}- \end{array}$	0.0	0.198	2.940
$=\text{C}=\text{C}=\text{C}=\text{C}-$	0.0	0.198	2.908
$\equiv\text{CH}, \equiv\text{C}-$	0.005	0.153	2.648
$-\text{O}-$	0.021	0.16	1.075
$>\text{C}=\text{O}$	0.040	0.29	1.765
$>\text{NH}$	0.031	0.135	2.333
$>\text{N}-$	0.014	0.17	1.793
$-\text{S}-$	0.015	0.27	0.591
Ring increments			
$-\text{CH}_2-$	0.013	0.184	2.813
$\begin{array}{c} \\ -\text{CH}- \\ \end{array}$	0.012	0.192	2.813
$\begin{array}{c} \\ -\text{C}- \\ \end{array}$	(-0.007)	(0.154)	2.813
$=\text{CH}, =\text{C}, =\text{C}=\text{C}=\text{C}-$	0.011	0.154	2.538
$-\text{O}-$	(0.014)	(0.12)	0.790
$>\text{C}=\text{O}$	(0.033)	(0.2)	1.500
$>\text{NH}$	(0.024)	(0.09)	1.736
$>\text{N}-$	(0.007)	(0.13)	1.883
$-\text{S}-$	(0.008)	(0.24)	0.911
General substituents			
$-\text{F}$	0.018	0.224	0.770
$-\text{Cl}$	0.017	0.320	1.237
$-\text{Br}$	0.010	(0.50)	0.899
$-\text{I}$	0.012	(0.83)	0.702
$-\text{OH}$			
Alcohols	0.082	0.06	0.704
Phenols	0.031	(-0.02)	1.553
$\text{HC}=\text{O}$ (aldehyde)	0.048	0.33	2.333
$-\text{COOH}$	0.085	(0.4)	1.652
$-\text{COO}-$ (ester)	0.047	0.47	1.607
$-\text{NH}_2$	0.031	0.095	2.184
$-\text{CN}$	(0.060)	(0.36)	2.784
$-\text{NO}_2$	(0.055)	(0.42)	1.559
$-\text{SH}$	0.015	0.27	1.537
$\begin{array}{c} \\ -\text{Si}- \\ \end{array}$	0.03	(0.54)	

SECTION 6

SPECTROSCOPY

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For more than half a century, spectroscopy has been the key structural tool for organic chemistry and biochemistry. This remains the case today although the availability of enhanced methods of X-ray analysis has somewhat altered the balance in both disciplines. A vast array of specialized texts are available that survey spectroscopic techniques in general or individual methods in particular. It would be folly to try to duplicate those efforts here. A brief overview of the methods may prove helpful and serve as a reminder for the practitioner who consults this handbook.

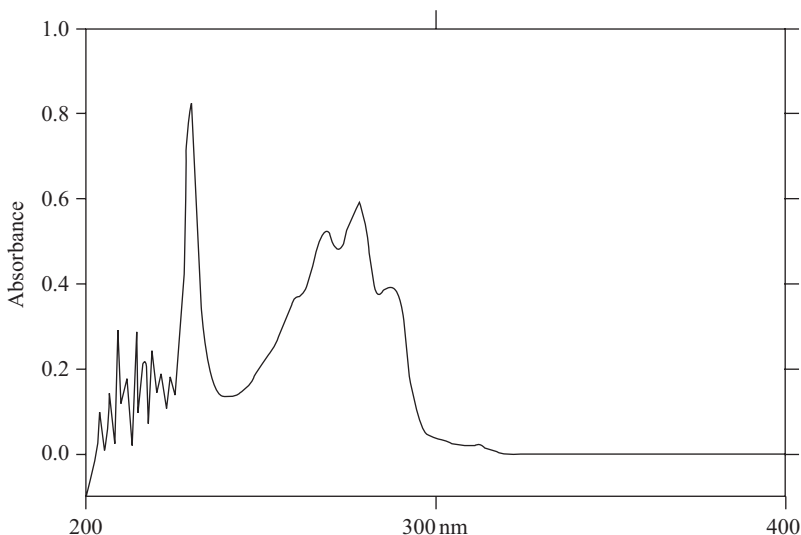
ULTRAVIOLET-VISIBLE SPECTROSCOPY

Generally, spectroscopic methods involve the absorption of radiation at certain wavelengths (and therefore certain energies) by molecules. For the techniques of ultraviolet-visible (UV-VIS) and infrared spectroscopy, there is an inverse proportionality between the amount of energy absorbed and the structural information that is revealed. The UV-VIS wavelength range is generally considered to be 200–800 nm. At the lower end, oxygen absorbs energy and the lowest end of the range is called the “vacuum UV.” Relatively limited structural information may be obtained from the typically broad bands that are observed. Even so, the electronic transitions that are observed are sensitive to structure. Individual absorbing groups or chromophores absorb light at a characteristic wavelength. The absorption usually shifts when two or more chromophores are linked or in conjugation.

The UV-VIS technique may be used quantitatively by application of Beer’s law:

$$\varepsilon = abc.$$

In this relationship, ε is the extinction coefficient that is characteristic of a given compound. The values a and c represent absorption and concentration, respectively. The



UV Spectrum of Naphthalene.

variable b is the pathlength of light through the sample, usually 1 cm. If the extinction coefficient is known, the measured absorption will give the compound's concentration.

The spectrum of naphthalene is shown above. Its broad bands reflect the absorption of energy by the extended pi-electron system.

The tables in this section present the essential data required for interpretation of UV-VIS spectra. Table 6.1 lists representative chromophores. These are identified by λ_{\max} , the maximum height of any given peak, and by ϵ_{\max} , the extinction coefficient at the maximum wavelength. Both the wavelength and absorption intensity are characteristic of individual chromophores.

Table 6.2 lists the ultraviolet cutoff for a variety of solvents commonly used in UV-VIS spectroscopy. The solvent chosen must dissolve the sample, yet be relatively transparent in the spectral region of interest. Typically, very low concentrations of sample will be present in the solvent. It is therefore important to avoid solvents that have even weak absorptions near the solute's bands of interest. Methanol and ethanol are two of the most commonly used solvents. Care must be exercised when using the latter that no benzene (an azeotropic drying agent) is present as this will alter the solvent's transparency. Normally, this will not be a problem in spectral grade solvents.

Tables 6.3–6.5 record data developed to undertake structural analysis in systems possessing chromophores that are conjugated or otherwise interact with each other. Chromophores within a molecule interact when linked directly to each other or when they are forced into proximity owing to structural constraints. Certain combinations of functional groups comprise chromophoric systems that exhibit characteristic absorption bands. In the era when UV-VIS was one of the principal spectral methods available to the organic chemist, sets of empirical rules were developed to extract as much information as possible from the spectra. The correlations referred to as Woodward's rules or the Woodward-Fieser rules, enable the absorption maxima of dienes (Table 6.3) and enones and dienones (Table 6.4) to be predicted. When this method is applied, wavelength increments correlated to structural features are added to the respective base values (absorption wavelength of parent compound). The data refer to spectra determined in methanol or ethanol. When other solvents are used, a numerical correction must be applied. These corrections are recorded in Table 6.5.

The benzene ring is a common structural element in organic chemistry. It is rigid and substituents are arranged in a fixed orientation. Shifts in the wavelength are expected for substituents that can interact electronically with the aromatic ring. Typically, shifts to longer wavelength (and intensification of the absorption band) are observed for any ring substitution. In the absence of conjugation, the shifts are small. Also, interposition of a single methylene group, or *meta* orientation within the aromatic ring, is sufficient to insulate chromophores almost completely from each other. With electron-withdrawing substituents, practically no change in the maximum position is observed. Directly conjugated groups may produce quite large spectral shifts. Examples include double and triple bonds and carbonyl groups. The spectra of heteroaromatics are related to their isocyclic analogs, but only in a general way. As with benzene, the magnitude of substituent shifts can be estimated, but tautomeric possibilities may invalidate the empirical method. Table 6.6 records data for substituents bonded directly to a benzene ring.

When electronically complementary groups are situated *para* to each other in disubstituted benzenes, there is a more pronounced shift to a longer wavelength than would be expected from the additive effect due to the extension of the chromophore from the electron-donating group through the ring to the electron-withdrawing group. When the *para* groups are not complementary, or when the groups are situated *ortho* or *meta* to each other, disubstituted benzenes show a more or less additive effect of the two substituents on the wavelength maximum. Calculation of the principal band of selected substituted benzenes is illustrated in Table 6.7.

TABLE 6.1 Electronic Absorption Bands for Representative Chromophores

Chromophore	System	λ_{\max}	ϵ_{\max}
Acetylene (ethynyl)	$-\text{C}\equiv\text{C}-$	175–180	6000
Aldehyde	$-\text{CHO}$	210 280–300	strong 11–18
Amine	$-\text{NH}_2$	195	2800
Azido	$>\text{C}=\text{N}-$	190	5000
Azo	$-\text{N}=\text{N}-$	285–400	3–25
Bromide	$-\text{Br}$	208	300
Carbonyl	$>\text{C}=\text{O}$	195 270–285	1000 18–30
Carboxyl	$-\text{COOH}$	200–210	50–70
Disulfide	$-\text{S}-\text{S}-$	194 255	5500 400
Ester	$-\text{COOR}$	205	50
Ether	$-\text{O}-$	185	1000
Ethylene	$-\text{C}=\text{C}-$	190	8000
Iodide	$-\text{I}$	260	400
Nitrate ester	$-\text{ONO}_2$	270 (shoulder)	12
Nitrile	$-\text{C}\equiv\text{N}$	160	—
Nitrite ester	$-\text{ONO}$	220–230 300–400	1 000–2000 10
Nitro	$-\text{NO}_2$	210	strong
Nitroso	$-\text{NO}$	302	100
Oxime	$-\text{NOH}$	190	5000
Sulfone	$-\text{SO}_2-$	180	—
Sulfoxide	$>\text{S}=\text{O} (>\text{S}\rightarrow\text{O})$	210	1 500
Thiocarbonyl	$>\text{C}=\text{S}$	205	strong
Thioether	$-\text{S}-$	194 215	4600 1 600
Thiol	$-\text{SH}$	195	1 400
	$-(\text{C}=\text{C})_2-$ (acyclic)	210–230	21 000
	$-(\text{C}=\text{C})_3-$	260	35 000
	$-(\text{C}=\text{C})_4-$	300	52 000
	$-(\text{C}=\text{C})_5-$	330	118 000
	$-(\text{C}=\text{C})_2-$ (alicyclic)	230–260	3 000–8 000
	$\text{C}=\text{C}-\text{C}\equiv\text{C}$	219	6 500
	$\text{C}=\text{C}-\text{C}=\text{N}$	220	23 000
	$\text{C}=\text{C}-\text{C}=\text{O}$	210–250 300–350	10 000–20 000 weak
	$\text{C}=\text{C}-\text{NO}_2$	229	9 500
Benzene		184 204 255	46 700 6 900 170
Diphenyl		246	20 000
Naphthalene		222 275 312	112 000 5 600 175
Anthracene		252 375	199 000 7 900
Phenanthrene		251 292	66 000 14 000

TABLE 6.1 Electronic Absorption Bands for Representative Chromophores (*continued*)

Chromophore	System	λ_{\max}	ϵ_{\max}
Naphthacene		272	180 000
		473	12 500
Pentacene		310	300 000
		585	12 000
Pyridine		174	80 000
		195	6 000
		257	1 700
Quinoline		227	37 000
		270	3 600
		314	2 750
Isoquinoline		218	80 000
		266	4 000
		317	3 500

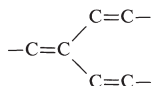
TABLE 6.2 Ultraviolet Cutoffs of Spectrograde Solvents*Absorbance of 1.00 in a 10.0 mm cell vs. distilled water*

Solvent	Wavelength, nm	Solvent	Wavelength, nm
Acetic acid	260	Hexadecane	200
Acetone	330	Hexane	210
Acetonitrile	190	Isobutyl alcohol	230
Benzene	280	Methanol	210
1-Butanol	210	2-Methoxyethanol	210
2-Butanol	260	Methylcyclohexane	210
Butyl acetate	254	Methylene chloride	235
Carbon disulfide	380	Methyl ethyl ketone	330
Carbon tetrachloride	265	Methyl isobutyl ketone	335
1-Chlorobutane	220	2-Methyl-1-propanol	230
Chloroform (stabilized with ethanol)	245	<i>N</i> -Methylpyrrolidone	285
Cyclohexane	210	Nitromethane	380
1,2-Dichloroethane	226	Pentane	210
Diethyl ether	218	Pentyl acetate	212
1,2-Dimethoxyethane	240	1-Propanol	210
<i>N,N</i> -Dimethylacetamide	268	2-Propanol	210
<i>N,N</i> -Dimethylformamide	270	Pyridine	330
Dimethylsulfoxide	265	Tetrachloroethylene	
1,4-Dioxane	215	(stabilized with thymol)	290
Ethanol	210	Tetrahydrofuran	220
2-Ethoxyethanol	210	Toluene	286
Ethyl acetate	255	1,1,2-Trichloro-1,2,2- trifluoroethane	231
Ethylene chloride	228	2,2,4-Trimethylpentane	215
Glycerol	207	<i>o</i> -Xylene	290
Heptane	197	Water	191

TABLE 6.3 Absorption Wavelength of Dienes

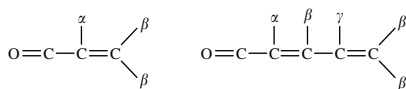
Heteroannular and acyclic dienes usually display molar absorptivities in the 8000–20000 range, whereas homoannular dienes are in the 5000–8000 range.

Poor correlations are obtained for cross-conjugated polyene systems such as



The correlations presented here are sometimes referred to as Woodward's rules or the Woodward-Fieser rules.

Base value for heteroannular or open chain diene, nm	214
Base value for homoannular diene, nm	253
Increment (in nm) for	
double bond extending conjugation	30
Alkyl substituent or ring residue	5
Exocyclic double bond	5
Polar groupings:	
-O-acyl	0
-O-alkyl	6
-S-alkyl	30
-Cl, -Br	5
-N(alkyl) ₂	60
Solvent correction (see Table 6.5)	
Calculated wavelength =	total

TABLE 6.4 Absorption Wavelength of Enones and Dienones

Base values, nm	
Acyclic α,β -unsaturated ketones	215
Acyclic α,β -unsaturated aldehyde	210
Six-membered cyclic α,β -unsaturated ketones	215
Five-membered cyclic α,β -unsaturated ketones	214
α,β -Unsaturated carboxylic acids and esters	195
Increments (in nm) for	
Double bond extending conjugation:	
Heteroannular	30
Homoannular	69
Alkyl group or ring residue:	
α	10
β	12
γ, δ	18

TABLE 6.4 Absorption Wavelength of Enones and Dienones (*continued*)

Polar groups:	
—OH	
α	35
β	30
γ	50
—O—CO—CH ₃ and —O—CO—C ₆ H ₅ : $\alpha, \beta, \gamma, \delta$	6
—OCH ₃	
α	35
β	30
γ	17
δ	31
—S—alkyl, β	85
—Cl	
α	15
β	12
—Br	
α	25
β	30
—N(alkyl) ₂ , β	95
Exocyclic double bond	5
Solvent correction (see Table 6.5)	
Calculated wavelength = total	

TABLE 6.5 Solvent Correction for UV–VIS spectroscopy

Solvent	Correction, nm
Chloroform	+1
Diethyl ether	+11
1,4-Dioxane	+5
Ethanol	0
Hexane	+11
Methanol	0
Water	−8

TABLE 6.6 Primary Band of Substituted Benzene and Heteroaromatics*In methanol*

Base value: 203.5 nm

Substituent	Wavelength shift, nm	Substituent	Wavelength shift, nm
—CH ₃	3.0	—COOH	25.5
—CH=CH ₂	44.5	—COO [−]	20.5
—C≡CH	44	—CN	20.5
—C ₆ H ₅	48	—NH ₂	26.5
—F	0	—NH ₃ ⁺	−0.5
—Cl	6.0	—N(CH ₃) ₂	47.0
—Br	6.5	—NH—CO—CH ₃	38.5
—I	3.5	—NO ₂	57
—OH	7.0	—SH	32
—O [−]	31.5	—SO—C ₆ H ₅	28
—OCH ₃	13.5	—SO ₂ CH ₃	13
—OC ₆ H ₅	51.5	—SO ₂ NH ₂	14.0
—CHO	46.0	—CH=CH—C ₆ H ₅	
—CO—CH ₃	42.0	<i>cis</i> (Z)	79
—CO—C ₆ H ₅	48	<i>trans</i> (E)	92.0
		—CH=CH—COOH, <i>trans</i>	69.5
Heteroaromatic	Base value, nm	Heteroaromatic	Base value, nm
Furan	200	Pyridine	257
Pyrazine	257	Pyrimidine	ca 235
Pyrazole	214	Pyrrole	209
Pyridazine	ca 240	Thiophene	231

TABLE 6.7 Wavelength Calculation of the Principal Band of Substituted Benzene Derivatives*In ethanol*

Base value of parent chromophore, nm

C₆H₅COOH or C₆H₅COO—alkyl 230C₆H₅—CO—alkyl (or aryl) 246C₆H₅CHO 250

Increment (in nm) for each substituent on phenyl ring

—Alkyl or ring residue

o-, *m*- 3*p*- 10

—OH and —O— alkyl

o-, *m*- 7*p*- 25—O[−]*o*- 11*m*- 20*p*- 78*

* Value may be decreased markedly by steric hindrance to coplanarity.

TABLE 6.7 Wavelength Calculation of the Principal Band of Substituted Benzene Derivatives
(continued)

—Cl	
<i>o</i> -, <i>m</i> -	0
<i>p</i> -	10
—Br	
<i>o</i> -, <i>m</i> -	2
<i>p</i> -	15
—NH ₂	
<i>o</i> -, <i>m</i> -	13
<i>p</i> -	58
—NHCO—CH ₃	
<i>o</i> -, <i>m</i> -	20
<i>p</i> -	45
—NHCH ₃	
<i>p</i> -	73
—N(CH ₃) ₂	
<i>o</i> -, <i>m</i> -	20
<i>p</i> -	85

PHOTOLUMINESCENCE

Luminescence processes may be categorized by the excitation method used with any particular luminescent molecule. Photoluminescence is the excitation process that involves the interaction of electromagnetic radiation with photons. The process is termed chemiluminescence when the exciting energy results from a chemical reaction. Any luminescence arising from an organism is referred to as bioluminescence.

The most common application of photoluminescence is found in fluorescence spectroscopy. Fluorescence is the immediate release of electromagnetic energy from an excited molecule or release of the energy from the singlet state. If the emitted energy arises from the triplet state or is delayed, the process is referred to as phosphorescence.

A fluorescence spectrum is characteristic of a given compound. It is observed as a result of radiative emission of the energy absorbed by the molecule. The observed spectrum does not depend on the wavelength of the exciting light, except that the spectrum will be more intense if irradiation occurs at the absorption maximum. The spectral intensity is called the quantum efficiency and is usually abbreviated as Φ . The quantum yield or quantum efficiency, Φ , which is solvent dependent, is the ratio: Φ = number of quanta emitted/number of quanta absorbed. Approximate values of quantum efficiencies are as follows: naphthalene, ~0.1; anthracene, ~0.3; indole, ~0.5; and fluorescein, ~0.9.

An equation similar to Beer’s law applies to fluorescence spectroscopy at dilute concentrations. In its most general form, it is given as

$$F = \Phi I_0(1 - e^{-\epsilon bc}).$$

In this equation, F is the observed fluorescence, Φ is the quantum efficiency (see above), I_0 is the intensity of the incident radiation, ϵ is the molar absorptivity, b is the cell’s path length, and c is the compound’s molar concentration.

The appearance of a fluorescence spectrum is reminiscent of a UV–VIS spectrum. The fluorescence spectrum for a 3-substituted indole derivative is shown in Figure 6.1. The

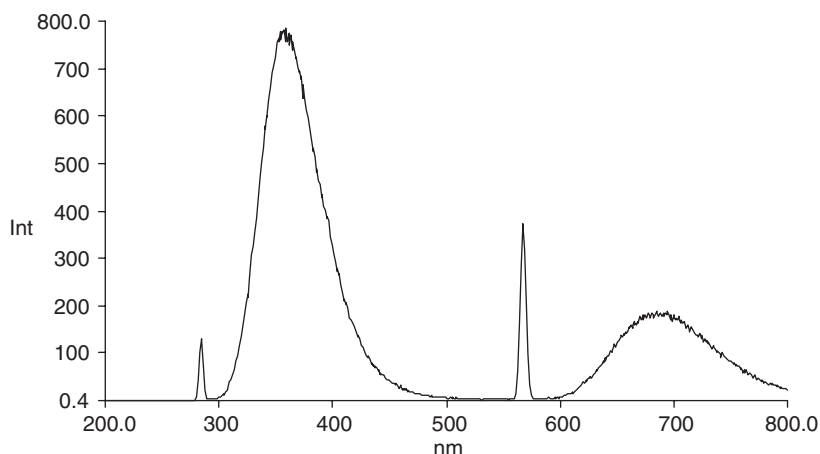


FIGURE 6.1 Fluorescence Spectrum for a 3-substituted indole derivative.

compound concentration was approximately 10^{-5} M in acetonitrile (CH_3CN). The sample was irradiated at a wavelength of 283 nm. The abscissa shows the wavelength in nanometers (nm) and the intensity ("int") is recorded on the ordinate. The maximum emission intensity is observed at 356 nm. The longest wavelength peak (λ_{max}) is observed at approximately 680 nm.

TABLE 6.8 Fluorescence Spectroscopy Data for Selected Organic Compounds


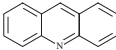
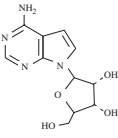
Compound	Solvent	pH	Excitation wavelength, nm	Emission wavelength, nm
Acenaphthene 	Pentane		291	341
Acridine 	CF_3COOH		358	475
Adenine	Water	1	280	375
Adenosine 	Water	1	285	395
Adenosine triphosphate	Water	1	285	395
Adrenalin			295	335
<i>p</i> -Aminobenzoic acid	Water	8	295	345

TABLE 6.8 Fluorescence Spectroscopy Data for Selected Organic Compounds (*continued*)

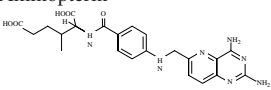
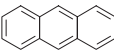
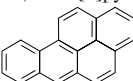
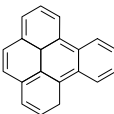
Compound	Solvent	pH	Excitation wavelength, nm	Emission wavelength, nm
Aminopterin 	Water	7	280, 370	460
1-Aminopyrene	CF ₃ COOH		330, 342	415
<i>p</i> -Aminosalicylic acid	Water	11	300	405
Amobarbital	Water	14	265	410
Anilines (aminobenzenes)	Water	7	280, 291	344, 361
Anthracene 	Pentane		420	430
Anthranilic acid (2-aminobenzoic acid)	Water	7	300	405
Azaindoles	Water	10	290, 299	310, 347
Benz[<i>c</i>]acridine	CF ₃ COOH		295, 380	480
Benz[<i>a</i>]anthracene	Pentane		284	382
1,2-Benzanthracene			280, 340	390, 410
Benzanthrone	CF ₃ COOH		370, 420	550
Benzo[<i>b</i>]chrysene	Pentane		283	398
11- <i>H</i> -Benzo[<i>a</i>]fluorene	Pentane		317	340
Benzoic acid	70% H ₂ SO ₄		285	385
3,4-Benzopyrene (benzo[<i>a</i>]pyrene) 	Benzene		365	390, 480
4,5-Benzopyrene (benzo[<i>e</i>]pyrene) 	Pentane		329	389
Benzoquinoline	CF ₃ COOH		280	425
Benzoxanthane	Pentane		363	418
Bromolysergic acid diethylamide	Water	1	315	460
Brucine	Water	7	305	500

TABLE 6.8 Fluorescence Spectroscopy Data for Selected Organic Compounds (*continued*)

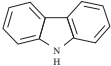
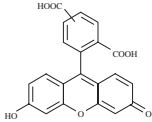
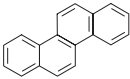

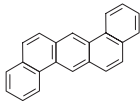

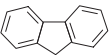
Compound	Solvent	pH	Excitation wavelength, nm	Emission wavelength, nm
Carbazole 	<i>N,N</i> -Dimethyl-formamide		291	359
Carboxyfluorescein 	Solvent		000	000
Chlortetracycline			355	445
Chrysene 	Pentane		250, 300, 310	260, 380
Cinchonine	Water	1	320	420
Coumarin 	Ethanol		280	352
Dibenzo[<i>a,c</i>]anthracene 	Pentane		280	381
Dibenzo[<i>b,k</i>]chrysene	Pentane		308	428
Dibenzo[<i>a,e</i>]pyrene	Pentane		370	401
3,4,8,9-Dibenzopyrene			370, 335, 390, 410	480, 510
5,12-Dihydronaphthacene	Pentane		282	340
1,4-Diphenylbutadiene	Pentane		328	370
Epinephrine	Water	7	295	335
Ethacridine	Water	2	370, 425	515
Fluoranthrene 	Pentane		354	464
Fluorene 	Pentane		300	321

TABLE 6.8 Fluorescence Spectroscopy Data for Selected Organic Compounds (*continued*)

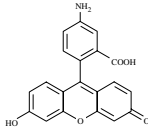
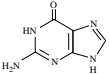
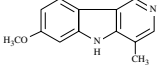
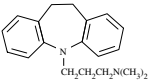

Compound	Solvent	pH	Excitation wavelength, nm	Emission wavelength, nm
Fluorescein 	Water	7–11	490	515
Folic acid	Water	7	365	450
Gentisic acid	Water	7	315	440
Griseofulvin	Water	7	295, 335	450
Guanine	Water	1	285	365
				
Harmine 	Water	1	300, 365	400
Hippuric acid	70% H ₂ SO ₄		270	370
Homovanillic acid	Water	7	270	315
<i>m</i> -Hydroxybenzoic acid	Water	12	314	430
<i>p</i> -Hydroxycinnamic acid	Water	7	350	440
7-Hydroxycoumarin	Ethanol		325	441
5-Hydroxyindole	Water	1	290	355
5-Hydroxyindoleacetic acid	Water	7	300	355
3-Hydroxykynurenine	Water	11	365	460
<i>p</i> -Hydroxymandelic acid	Water	7	300	380
<i>p</i> -Hydroxyphenylacetic acid	Water	7	280	310
<i>p</i> -Hydroxyphenylpyruvic acid	Water	7	290	345
<i>p</i> -Hydroxyphenylserine	Water	1	290	320
5-Hydroxytryptophan	Water	7	295	340
Imipramine 	Water	14	295	415
Indoleacetic acid	Water	8	285	360
Indoles 	Water	7	269, 315	355

TABLE 6.8 Fluorescence Spectroscopy Data for Selected Organic Compounds (*continued*)

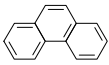
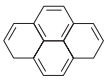
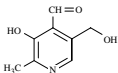
Compound	Solvent	pH	Excitation wavelength, nm	Emission wavelength, nm
Indomethacin	Water	13	300	410
Kynurenic acid	Water	7	325	405
		11	325	440
Lysergic acid diethylamide	Water	1	325	445
Menadione	Ethanol		335	480
9-Methylanthracene	Pentane		382	410
3-Methylcholanthrene	Pentane		297	392
7-Methyldibenzopyrene	Pentane		460	467
2-Methylphenanthrene	Pentane		257	357
3-Methylphenanthrene	Pentane		292	368
1-Methylpyrene	Pentane		336	394
4-Methylpyrene	Pentane		338	386
Naphthacene (2,3-benzanthracene)			290, 310	480, 515
1-Naphthol	0.1 M NaOH 20% ethanol		365	480
2-Naphthol	0.1 M NaOH 20% ethanol		356	426
Oxytetracycline			390	520
Phenanthrene	Pentane		252	362
				
Phenylalanine	Water		215, 260	282
<i>o</i> -Phenylenepyrene	Pentane		360	506
Phenylephrine			270	305
Picene	Pentane		281	398
Procaine	Water	11	275	345
Pyrene	Pentane		330	382
				
Pyridoxal	Water	12	310	365
				
Quinacrine	Water	11	285	420
Quinidine	Water	1	350	450
Quinine	Water	1	250, 350	450

TABLE 6.8 Fluorescence Spectroscopy Data for Selected Organic Compounds (*continued*)


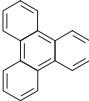

Compound	Solvent	pH	Excitation wavelength, nm	Emission wavelength, nm
Reserpine	Water	1	300	375
Resorcinol	Water		265	315
Riboflavin	Water	7	270, 370, 445	520
Rutin	Water	1	430	520
Salicylic acid	Water	11	310	435
Scoparone	Water	10	350, 365	430
Scopoletin	Water	10	365, 390	460
Serotonin	3 M HCl		295	550
Skatole	Water		290	370
Streptomycin	Water	13	366	445
<i>p</i> -Terphenyl	Pentane		284	338
				
Thiopental			315	530
Thymol	Water	7	265	300
Tocopherol	Hexane– ethanol		295	340
Tribenzo[<i>a,e,i</i>]pyrene	Pentane		384	448
Triphenylene	Pentane		288	357
				
Tryptamine	Water	7	290	360
Tryptophan	Water	11	285	365
Tyramine	Water	1	275	310
Tyrosine	Water	7	275	310
Uric acid	Water	1	325	370
Vitamin A	1-Butanol		340	490
Vitamin B ₁₂	Water	7	275	305
Warfarin	Methanol		290, 342	385
Xanthine	Water	1	315	435
				
2,6-Xylenol			275	305
3,4-Xylenol			280	310
Yohimbine	Water	1	270	360
Zoxazolamine	Water	11	280	320

TABLE 6.9 Fluorescence Quantum Yield Values

Compound	Solvent	Q_F value vs. Q_F standard	
Q_F standard			
9-Aminoacridine	Water	0.99	
Anthracene	Ethanol	0.30	
POPOP*	Toluene	0.85	
Quinine sulfate dihydrate	1 N H ₂ SO ₄	0.55	
Secondary standards			
Acridine orange hydrochloride	Ethanol	0.54	Quinine sulfate
		0.58	Anthracene
1,8-ANS [†] (free acid)	Ethanol	0.38	Anthracene
		0.39	POPOP
1,8-ANS (magnesium salt)	Ethanol	0.29	Anthracene
		0.31	POPOP
Fluorescein	0.1 N NaOH	0.91	Quinine sulfate
		0.94	POPOP
Fluorescein, ethyl ester	0.1 N NaOH	0.99	Quinine sulfate
		0.99	POPOP
Rhodamine B	Ethanol	0.69	Quinine sulfate
		0.70	Anthracene
2,6-TNS [‡] (potassium salt)	Ethanol	0.48	Anthracene
		0.51	POPOP

* POPOP *p*-bis[2-(5-phenyloxazolyl)]benzene.

† ANS, anilino-8-naphthalenesulfonic acid.

‡ TNS, 2-*p*-toluidinylnaphthalene-6-sulfonate.**TABLE 6.10** Phosphorescence Spectroscopy of Some Organic Compounds**Abbreviation Used in the Table**

EPA: diethyl ether, isopentane, and ethanol (5:5:2) volume ratio

Compound	Solvent	Lifetime, s	Excitation wavelength, nm	Emission wavelength, nm
Acenaphthene	Ethanol		300	515
3-Acetylpyridine	Ethanol	0.5	395	525
Adenine	Water-methanol (9:1)	2.9	278	406
Adenosine	Ethanol	0.8	280	422
<i>p</i> -Aminobenzoic acid	Ethanol		305	425
2-Aminofluorene	Ethanol	4.6	380	590
6-Amino-6-methylmercapto- purine	Water-methanol (9:1)	0.66	321	456
2-Amino-4-methylpyrimidine	Ethanol	2.1	302	438

TABLE 6.10 Phosphorescence Spectroscopy of Some Organic Compounds (*continued*)

Compound	Solvent	Lifetime, s	Excitation wavelength, nm	Emission wavelength, nm
2-Amino-5-nitrobenzothiazole	EPA	0.41	375	515
2-Amino-5-nitrobiphenyl	EPA	0.56	380	520
3-L-Aminotyrosine · 2HCl	Ethanol	0.8	286	398
Anthracene	Ethanol		300	462
Aspirin	EPA	2.1	240	380
Atropine	Ethanol	1.4		410
8-Azaguanine	Ethanol	1.8	282	442
Benzaldehyde	Ethanol	3.4	254	433
1,2-Benzanthracene	Ethanol	2.2	310	510
Benzimidazole	Ethanol	2.3	280	406
Benzocaine	Ethanol	3.4	310	430
1,2-Benzofluorene	Ethanol		315	502
Benzoic acid	EPA	2.4	240	400
3,4-Benzopyrene	Ethanol		325	508
Benzyl alcohol	Ethanol		219	393
6-Benzylaminopurine	Water-methanol (9:1)	2.8	286	413
Biphenyl	Ethanol	1.0	270	385
6-Bromopurine	Water-methanol (9:1)	0.5	273	420
Brucine	Ethanol	0.9	305	435
Caffeine	Ethanol	2.0	285	440
Carbazole	Ethanol	7.8	341	436
2-Chloro-4-aminobenzoic acid	Ethanol	1.0	312	337
<i>p</i> -Chlorophenol	Ethanol	< 0.2	290	505
<i>o</i> -Chlorophenoxyacetic acid	Ethanol	0.7	280	518
<i>p</i> -Chlorophenoxyacetic acid	Ethanol	< 0.5	283	396
6-Chloropurine	Water-methanol (9:1)	0.64	273	419
Chlorpromazine · HCl	Ethanol	0.3	320	490
Chlorotetracycline	Ethanol	2.7	280	410
Cocaine · HCl	Ethanol	2.7	240	400
Codeine	Ethanol	0.3	270	505
Cytidine	Water-methanol (9:1)		290	420
Desoxypyridoxine · HCl	Ethanol	1.4	290	442
Diacetylsulfanilamide	Ethanol	1.3	280	405
2,6-Diaminopurine	Water-methanol (9:1)	2.7	288	410
2,6-Diaminopurine sulfate	Ethanol	1.7	294	424
1,2,5,6-Dibenzanthracene	Ethanol	1.3	340	550
2,6-Dichloro-4-nitroaniline	EPA	0.5	368	525
2,4-Dichlorophenoxyacetic acid	Ethanol	< 0.5	289	490
2,6-Diethyl-4-nitroaniline	EPA	0.66	388	525
3,4-Dihydroxymandelic acid	Ethanol	1.1	294	412
3,4-Dihydroxyphenylacetic acid	Ethanol	0.9	295	430

TABLE 6.10 Phosphorescence Spectroscopy of Some Organic Compounds (*continued*)

Compound	Solvent	Lifetime, s	Excitation wavelength, nm	Emission wavelength, nm
2,5-Dimethoxy-4-methyl- amphetamine	Water-methanol (9:1)	3.9	289	411
5,7-Dimethyl-1,2-benzacridine	Ethanol	0.6	310	555
<i>N,N</i> -Dimethyl-4-nitroaniline	EPA	0.54	398	525
<i>N,N</i> -Dimethyltryptamine	Water-methanol (9:1)	6.9	286	434
Dopamine	Ethanol	0.9	285	430
Ephedrine	Ethanol	3.6	225	390
Epinephrine	Ethanol	1.0	283	425
<i>N</i> -Ethylcarbazole	Ethanol	7.8	340	437
Ethyl 3-indoleacetate	Ethanol	3.3	290	440
Folic acid	Ethanol		367	425
Hippuric acid	EPA	4.9	311	450
Homovanillic acid	Ethanol	0.8	289	435
DL-5-Hydroxytryptophan	Ethanol	6.3	315	435
Indole-3-acetic acid	Ethanol	< 0.5	290	438
3-Indoleacetonitrile	Ethanol	7.1	285	438
Indole-3-butyonic acid	Ethanol	0.6	284	510
Indolecarboxylic acid	Ethanol	5.5	290	429
Indole-2-propanoic acid	Ethanol	0.6	290	440
D-Lysergic acid	Water-methanol (9:1)	0.1	310	518
2-Methylcarbazole	Ethanol	8.1	333	442
<i>N</i> -Methylcarbazole	Ethanol	8.4	336	437
6-Methylmercaptapurine	Water-methanol (9:1)	0.6	291	420
<i>N</i> -Methyl-4-nitroaniline	EPA	0.5	390	522
6-Methylpurine	Water-methanol (9:1)	3.2	272	405
Morphine	Ethanol	0.3	285	500
Naphthacene	Ethanol		300	518
Naphthalene	EPA	1.8	310	475
1-Naphthaleneacetic acid	Ethanol	2.8	295	510
1-Naphthol	Ethanol	1.1	320	475
2-Naphthoxyacetic acid	Ethanol	2.6	328	497
2-Naphthylamine	Ethanol	2.3	270	303
Niacinamide	Ethanol		270	410
Nicotine	Ethanol	5.2	270	390
5-Nitroacenaphthene	EPA		380	540
4-Nitroaniline	EPA	0.6	380	510
9-Nitroanthracene	EPA		248	488
1-Nitroanthraquinone	EPA	0.3	250	490
4-Nitrobiphenyl	EPA		330	480
3-Nitro- <i>N</i> -ethylcarbazole	EPA	0.4	315	475
2-Nitrofluorene	EPA	0.4	340	517
6-Nitroindole	EPA	0.4	372	520
1-Nitronaphthalene	EPA		340	520

TABLE 6.10 Phosphorescence Spectroscopy of Some Organic Compounds (*continued*)

Compound	Solvent	Lifetime, s	Excitation wavelength, nm	Emission wavelength, nm
2-Nitronaphthalene	EPA	0.4	260	500
4-Nitro-1-naphthylamine	EPA		400	578
4-Nitrophenol	Ethanol	< 0.2	355	520
4-Nitrophenylhydrazine	EPA	0.5	390	520
4-Nitro-2-toluidine	EPA	0.5	375	520
Papaverine · HCl	Ethanal	1.5	260	480
Phenacetin	EPA			410
Phenanthrene	EPA	2.6	340	465
Phenobarbital	Ethanol	1.8	240	380
Phenylalanine	Ethanol		270	385
DL-2-Phenyllactic acid	Ethanol	5.4	262	383
Phthalylsulfathiazole	Ethanol	0.9	305	405
Procaine · HCl	Ethanol	3.5	310	430
Purine	Water-methanol (9:1)	2.2	272	405
Pyrene	Ethanol		330	515
Pyridine	Ethanol	1.4	310	440
Pyridine-3-sulfonic acid	Ethanol	1.2	272	408
Pyridoxine · HCl	Ethanol		290	425
Quercetin	Ethanol	2.1	345	480
Quinidine sulfate	Ethanol	1.3	340	500
Quinine · HCl	Ethanol	1.3	340	500
Salicylic acid	Ethanol	6.2	315	430
Strychnine phosphate	Ethanol	1.2	290	440
Sulfabenzamide	Ethanol	0.7	305	405
Sulfadiazine	Ethanol	0.7	275	410
Sulfanilamide	Ethanol	2.9	300	410
Sulfapyridine	Ethanol	1.4	310	440
Sulfathiazole	Ethanol	0.9	310	420
1,2,4,5-Tetramethylbenzene	EPA	4.5	275	390
2-Thiouracil	Ethanol	< 0.5	310	430
2,4,5-Trichlorophenol	Ethanol	< 0.2	305	485
2,4,5-Trichlorophenoxyacetic acid	Ethanol	1.1	295	475
Triphenylene	Ethanol	15	290	460
Tryptophan	Ethanol	1.5	295	440
Tyrosine	Ethanol	2.8	290	390
Vitamin K ₁	Hexane	0.4	345	570
Vitamin K ₃	Hexane	0.5	335	510
Vitamin K ₅	Water-methanol (9:1)	1.3	310	535
Warfarin	Ethanol	0.8	305	460
Yohimbine · HCl	Ethanol	7.4	290	410

INFRARED SPECTROSCOPY

Infrared (IR) and Raman spectroscopy rely on the interaction of a bond between two elements and IR radiation in the $400\text{--}4000\text{cm}^{-1}$ range. The two techniques are distinct but closely related. Historically, infrared analysis has been the more widely used in organic chemistry but much of the brief discussion that follows applies equally to both methods.

A chemical bond may be considered as a spring to which two weights are attached. The weights are atoms of different atomic masses. The length and strength of the spring may be correlated to the length and strength of the chemical bond. Each bond will vibrate at a frequency that is characteristic of the attached atoms and the type of bond (*i.e.*, single, double, or triple) between them. Radiation of an appropriate frequency will be absorbed by the bond and the wavelength at which this occurs will be detected and recorded by the instrument in the spectrum. Indeed, most molecules have many bonds so multiple peaks are observed in an IR spectrum.

An electrical dipole is required for IR energy to be efficiently absorbed by a molecule. Thus, bonds between different elements will give more prominent absorption peaks than will symmetrical bonds. This is because the bond's dipole moment changes as the bond stretches and contracts. Symmetrical bonds do not change dipole moment even if the bond distance changes. Usually, the most prominent peaks are observed when the electronegativity difference between the bound elements is greatest. Thus, a C—O bond will usually be more prominent than a C—H bond.

The position (frequency) of the absorption depends on the strength of the bond linking them. Thus, single, double, and triple bonds are observed in characteristic ranges. In addition, the frequency is related to the masses of the attached atoms. The largest mass differences occur when an element is attached to hydrogen. Such bonds as C—H, O—H, and N—H typically are observed in the $2900\text{--}3600\text{cm}^{-1}$ range.

The remarkable versatility of NMR as an analytical method has diminished the importance of IR analysis in modern laboratories but it remains a very useful technique. The very small amount of sample required and the prominence of functional group absorption means that the progress of a reaction can be monitored very conveniently. For example, the reduction of an aldehyde to an alcohol will be accompanied by the disappearance of the prominent C=O peak and the appearance of a C—OH absorption. Because both peaks are so readily identifiable in a small sample, the reaction is easy to follow and its completeness can be assayed.

TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen

<i>Abbreviations Used in the Table</i>		
	m, moderately strong	var, of variable strength
	m-s, moderate to strong	w, weak
	s, strong	w-m, weak to moderately strong
Group	Band, cm^{-1}	Remarks
Saturated C—H		
$\begin{array}{c} \text{H} \\ \\ -\text{C}-\text{H} \\ \\ \text{H} \end{array}$	2975–2950 (s) 2885–2865 (w)	Two or three bands usually; asymmetrical and symmetrical CH stretching, respectively. In

TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm^{-1}	Remarks
Saturated C—H (<i>continued</i>)		
	1 450–1 260 (m)	presence of double bond adjacent to CH_3 group symmetrical band splits into two. Sensitive to adjacent negative substituents
$\begin{array}{c} \text{H} \\ \\ -\text{C}- \\ \\ \text{H} \end{array} \quad \text{acyclic}$	ca 2 930 (s) 2 870–2 840 (w) 1 480–1 440 (m) ca 720 (w)	Frequency increased in strained systems. Symmetrical band splits into two bands when double bond adjacent. Scissoring mode Rocking mode
Alkane residues attached to carbon		
Cyclopropane	ca 3 050 (w) 540–500 470–460 (s)	CH stretching Aliphatic cyclopropanes
Cyclobutanes Cyclopentanes	580–490 (s) 595–490 (s)	Alkyl derivatives: $550\text{--}530\text{ cm}^{-1}$ Alkyl derivatives: $585\text{--}530\text{ cm}^{-1}$
$\text{>C}(\text{CH}_3)_2$	ca 1 380 (m) 1 175–1 165 (m) 1 150–1 130 (m)	A roughly symmetrical doublet If no H on central carbon, then one band at $\text{ca } 1\,190\text{ cm}^{-1}$
$\text{—C}(\text{CH}_3)_3$	1 395–1 385 (m) 1 365 (s)	Split into two bands
Aryl- CH_3 Aryl- C_2H_5 Aryl- C_3H_7 (or C_4H_9) $\text{—}(\text{CH}_2)_n\text{—}$ $n = 1$ $n = 2$ $n = 3$ $n \geq 4$	390–260 (m) 565–540 (m–s) 585–565 (m) 785–770 (w–m) 745–735 (w–m) 735–725 (w–m) 725–720 (w–m)	Two bands Rocking vibrations
Alkane residues attached to miscellaneous atoms		
Epoxide C—H $\begin{array}{c} \text{NH} \\ \diagup \quad \diagdown \\ \text{>C} \text{—} \text{CH}_2 \end{array}$	ca 3 050 (m–s) ca 3 050 (m–s)	
$\text{—CH}_2\text{—halogen}$	ca 3 050 (m–s) 1 435–1 385 (m) 1 300–1 240 (s)	Halogens except fluorine

TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm^{-1}	Remarks
Alkane residues attached to miscellaneous atoms (<i>continued</i>)		
—CHO	2900–2800 (w) 2775–2700 (w) 1420–1370 (m)	
—CO—CH ₃	3100–2900 (w) 1450–1400 (s) 1360–1355 (s)	
—O—CH ₃ ethers	2835–2810 (s) 1470–1430 (m–s) ca 1030 (w–m)	Two bands
—O—C(CH ₃) ₃	1200–1155 (s)	
—O—CH ₂ —O—	2790–2770 (m)	
—O—CH ₂ — esters	1475–1460 (m–s) 1470–1435 (m–s)	Acyclic esters. Frequency increased ca 30cm^{-1} for cyclic and small ring systems.
—O—CO—CH ₃	1450–1400 (s) 1385–1365 (s) 1360–1355 (s)	Acetate esters The high intensity of these bands often dominates this region of the spectrum.
—CH ₂ — $\overset{ }{\text{C}}=\text{C}<$	1445–1430 (m)	
—CH ₂ —SO ₂ —	ca 1250 (m)	
P—CH ₃ Se—CH ₃ B—CH ₃ Si—CH ₃ Sn—CH ₃ Pb—CH ₃ As—CH ₃ Ge—CH ₃ Sb—CH ₃ Bi—CH ₃ —CH ₂ —(Cd, Hg, Zn, Sn)	1320–1280 (s) ca 1280 (m) 1460–1405 (m) 1320–1280 (m) 1265–1250 (m–s) 1200–1180 (m) 1170–1155 (m) 1265–1240 (m) 1240–1230 (m) 1215–1195 (m) 1165–1145 (m) 1430–1415 (m)	
N—CH ₃ and N—CH ₂ —	2820–2780 (s) 1440–1390 (m)	Ethylenediamine complexes Ethylenediamine complexes
N—CH ₂ —CH ₂ —N	1480–1450 (s)	

TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

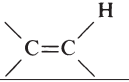
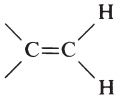
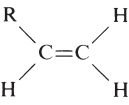
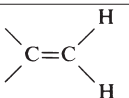
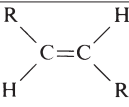
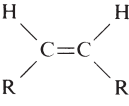
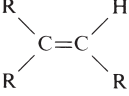
Group	Band, cm^{-1}	Remarks
Alkane residues attached to miscellaneous atoms (<i>continued</i>)		
$\text{N}-\text{CH}_3$ Amine $\cdot \text{HCl}$ Amino acid $\cdot \text{HCl}$ Amides $\text{N}-\text{CH}_2-$ amides	1475–1395 (m) 1490–1480 (m) 1420–1405 (s) ca 1440 (m)	
$\text{S}-\text{CH}_3$	2990–2955 (m–s) 2900–2865 (m–s) 1440–1415 (m) 1325–1290 (m) 1030–960 (m) 710–685 (w–m)	
$\text{S}-\text{CH}_2-$	2950–2930 (m) 2880–2845 (m) 1440–1415 (m) 1270–1220 (s)	
$-\text{C}\equiv\text{CH}$	ca 3300 (s) 700–600	Sharp Bending
	3040–3010 (m)	
	3095–3075 (m) 2985–2970 (m)	CH stretching sometimes obscured by much stronger bands of saturated CH groups
	995–980 (s) 940–900 (s) ca 635 (s) 485–445 (m–s)	
	895–885 (s) 560–530 (s) 470–435 (m)	
	980–955 (s) 455–370 (m–s)	
	730–655 (m) 670–455 (s)	
	850–790 (m) 570–515 (s) 525–470 (s)	

TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm^{-1}	Remarks
Alkane residues attached to miscellaneous atoms (<i>continued</i>)		
—O—CH=CH_2	965–960 (s) 945–940 (m) 820–810 (s)	
—S—CH=CH_2	ca 965 (s) ca 860 (s)	
—CO—CH=CH_2	995–980 (s) 965–955 (m)	
—CO—OCH=CH_2	950–935 (s) 870–850 (s)	
—CO—C=CH_2	ca 930 (s)	
—CO—OC=CH_2	880–865	
—O—CH=CH— trans	940–920 (s)	
—CO—CH=CH— trans	ca 990 (s)	
Hydroxyl group O—H compounds		
Primary aliphatic alcohols	3 640–3 630 (s) 1 350–1 260 (s) 1 085–1 030 (s)	Only in very dilute solutions in nonpolar solvents OH bending Also broad band at $700\text{--}600\text{ cm}^{-1}$
Secondary aliphatic alcohols	3 625–3 620 (s) 1 350–1 260 (s) 1 125–1 085 (s)	See comments under primary aliphatic alcohols Also for α -unsaturated and cyclic tertiary aliphatic alcohols
Tertiary aliphatic alcohols	3 620–3 610 (s) 1 410–1 310 (s) 1 205–1 125 (s)	See comments under primary aliphatic alcohols
Aryl—OH	ca 3 610 (s) 1 410–1 310 (s) 1 260–1 180 (s) 1 085–1 030 (s)	See comments under primary aliphatic alcohols Also for unsaturated secondary aliphatic alcohols
Carboxylic acids	3 300–2 500 (w–m) 995–915 (s)	Broad Broad diffuse band
Enol form of β -diketones	2 700–2 500 (var)	Broad

TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm^{-1}	Remarks
Hydroxyl group O—H compounds (<i>continued</i>)		
Free oximes	3 600–3 570(w–m)	Shoulder
Free hydroperoxides	3 560–3 530 (m)	
Peroxy acids	ca 3 280 (m)	
Phosphorus acids	2 700–2 560 (m)	Broad
Water in solution	3 710	When solution is damp
Intermolecular H bond Dimeric	3 600–3 500	Rather sharp. Absorptions arising from H bond with polar solvents also appear in this region.
Polymeric	3 400–3 200 (s)	Broad
Intramolecular H bond Polyvalent alcohols Chelation	3 600–3 500 (s) 3 200–2 500	Sharper than dimeric band above Broad and occasionally weak; the lower the frequency, the stronger the intramolecular bond
Water of crystallation (solid state spectra)	3 600–3 100 (w)	Usually a weak band at 1 640–1 615 cm^{-1} also. Water in trace amounts in KBr disks shows a broad band at 3 450 cm^{-1} .
Amine, imine, ammonium, and amide N—H		
Primary amines Aliphatic	3 550–3 300 (m) 1 650–1 560 (m) 1 090–1 020 (w–m) 850–810 (w–m)	Two bands in this range With α -carbon branching at 795 cm^{-1} and strong
	495–445 (m–s) ca 290 (s)	Broad Broad
Aromatic	1 350–1 260 (s) 445–345	Also for secondary aryl amines
Amino acids	3 100–3 030 (m)	Values for solid states; broad bands also (but not always) near 2 500 and 200 cm^{-1}
	2 800–2 400 (m) 1 625–1 560 (m) 1 550–1 550 (m)	Number of sharp bands; dilute solution
Amino salts	3 550–3 100 (m) ca 3 380 ca 3 280	Values for solid state Dilute solutions

TABLE 6.11 Absorption Frequencies of Single Bonds to Hydrogen (*continued*)

Group	Band, cm^{-1}	Remarks
Amine, imine, ammonium, and amide N—H (<i>continued</i>)		
Secondary amines	3 550–3 400 (w) 1 580–1 490 (w) 1 190–1 170 (m) 1 145–1 130 (m) 455–405 (w–m)	Only one band, whereas primary amines show two bands Often too weak to be noticed
Salts	ca 2 500 ca 2 400 1 620–1 560 (m–s)	Sharp; broad values for solid state Sharp; broad values for solid state
Tertiary amines $\text{R}_1\text{R}_2\text{R}_3\text{NH}^+$	2 700–2 250	Group of relatively sharp bands; broad bands in solid state
Ammonium ion	3 300–3 030 (s) 1 430–1 390 (s)	Group of bands
Imines $=\text{N}=\text{H}$	3 350–3 310 (w) 3 490 (s) 3 490 (s)	Aliphatic Aryl Pyrroles, indoles; band sharp
Imine salts	2 700–2 330 (m–s) 2 200–1 800 (m)	Dilute solutions One or more bands; useful to distinguish from protonated tertiary amines
Primary amide $-\text{CONH}_2$	ca 3 500 (m) ca 3 400 (m)	Lowered ca 150 cm^{-1} in the solid state and on H bonding; often several bands $3\,200\text{--}3\,050\text{ cm}^{-1}$
Secondary amide $-\text{CONH}-$	3 460–3 400 (m) 3 100–3 070 (w)	Two bands; lowered on H bonding and in solid state. Only one band with lactams Extra band with bonded and solid-state samples
Miscellaneous R—H		
$-\text{S}-\text{H}$	2 600–2 550 (w)	Weaker than OH and less affected by H bonding
$\text{P}-\text{H}$ $\begin{array}{c} \text{O} \\ \parallel \\ \text{P} \\ \diagdown \\ \text{OH} \end{array}$ $\text{R}-\text{D}$	2 440–2 350 (m) 2 700–2 560 (m) 100/137 times the corresponding RH frequency	Sharp Associated OH Useful when assigning RH bands; deuteration leads to a known shift to lower frequency

TABLE 6.12 Absorption Frequencies of Triple Bonds*Abbreviations Used in the Table*

m, moderately strong

var, of variable strength

m-s, moderate to strong

w-m, weak to moderately strong

s, strong

Group	Band, cm^{-1}	Remarks
Alkynes		
Terminal	3 300 (s) 2 140–2 100 (w-m)* 1 375–1 225 (w-m) 695–575 (m-s)	CH stretching $\text{C}\equiv\text{C}$ stretching Two bands if molecule has axial symmetry
Nonterminal	ca 630 (s) 2 260–2 150 (var)*	Alkyl monosubstituted Symmetrical or nearly symmetrical substitution makes the $\text{C}\equiv\text{C}$ stretching frequency inactive. When more than one $\text{C}\equiv\text{C}$ linkage is present, and sometimes when there is only one, there are frequently more absorption bands in this region than there are triple bonds to account for them.
$\text{R}_1-\text{C}\equiv\text{C}-\text{R}_2$	540–465 (m)	The longer the chain, the lower the frequency
Aryl— $\text{C}\equiv\text{C}$ —	ca 550 (m) ca 350 (var)	
— $\text{C}\equiv\text{C}$ —halogen (Cl, Br, I)	185–160 (var)	
Nitriles — $\text{C}\equiv\text{N}$	2 260–2 200 (var)	Stronger and toward the lower end of the range when conjugated; occasionally very weak or absent
Aliphatic	580–555 (m-s) 560–525 (m-s) 390–350 (s)	
Aromatic	580–540 (s) 430–380 (m)	
Isonitriles $\text{R}-\text{N}^+\equiv\text{C}^-$ or $\text{R}-\text{N}=\text{C}:$	2 175–2 150 (s) 2 150–2 115 (s) 1 595	Very sensitive to changes in substituents Not found for nitriles
Cyanamides $>\text{N}-\text{C}\equiv\text{N}\rightleftharpoons\text{N}^+=\text{C}=\text{N}^-$	2 225–2 210 (s)	

* Conjugation with olefinic or acetylenic groups lowers the frequency and raises the intensity. Conjugation with carbonyl groups usually has little effect on the position of absorption.

TABLE 6.12 Absorption Frequencies of Triple Bonds (*continued*)

Group	Band, cm^{-1}	Remarks
Thiocyanates $\text{R}-\text{S}-\text{C}\equiv\text{N}$	2 175–2 140 (s) 404–400 (s) ca 600 (m–s)	Aryl thiocyanates at the upper end of the range, alkyl at the lower end Aliphatic derivatives
Nitrile <i>N</i> -oxides $-\text{C}\equiv\text{N}\rightarrow\text{O}$	2 305–2 285 (s) 1 395–1 365 (s)	Aryl derivatives
Diazonium salts $\text{R}-\text{N}^+\equiv\text{N}$	2 300–2 230 (m–s)	
Selenocyanates $\text{R}-\text{Se}-\text{C}\equiv\text{N}$	ca 2 160 (m–s) 545–520 ca 390 ca 350	

TABLE 6.13 Absorption Frequencies of Cumulated Double Bonds*Abbreviations Used in the Table*

m–s, moderate to strong

vs, very strong

s, strong

w, weak

Group	Band, cm^{-1}	Remarks
Carbon dioxide $\text{O}=\text{C}=\text{O}$	2 349 (s)	Appears in many spectra as a result of inequalities in path length
Isocyanates $-\text{N}=\text{C}=\text{O}$	2 275–2 250 (vs)	Position unaffected by conjugation
Isoselenocyanates $-\text{N}=\text{C}=\text{Se}$	2 200–2 000 (s) 675–605	Broad; usually two bands
Azides $-\text{N}_3$ or $-\text{N}=\text{N}^+=\text{N}^-$	2 140–2 030 (s) 1 340–1 180 (w)	Not observed for ionic azides
$-\text{N}=\text{C}=\text{N}-$	2 155–2 130 (s)	Split into unsymmetrical doublet by conjugation with aryl groups: 2 145–2 125 (vs) and 2 115–2 105 (vs)

TABLE 6.13 Absorption Frequencies of Cumulated Double Bonds (*continued*)

Group	Band, cm^{-1}	Remarks
Isothiocyanates $\text{—N}=\text{C}=\text{S}$	2 140–1 990 (vs) 649–600 (m–s) 565–510 (m–s) 470–440 (m–s)	Broad; usually a doublet
Ketenes $\text{>C}=\text{C}=\text{O}$	ca 2 150 (s)	
Ketenimines $\text{C}=\text{C}=\text{N}—$	2 050–2 000 (s)	
Allenes $\text{>C}=\text{C}=\text{C}<$	2 000–1 915 (m–s)	Two bands when terminal allene or when bonded to electron-attracting groups
Thionylamines $\text{—N}=\text{S}=\text{O}$	1 300–1 230 (s) 1 180–1 110 (s)	
Diazoalkanes $\text{R}_2\text{C}=\overset{+}{\text{N}}=\overset{-}{\text{N}}$ $\text{—CH}=\overset{+}{\text{N}}=\overset{-}{\text{N}}$	2 030–2 000 (s) 2 050–2 035 (s)	
Diazoketones $\text{—CO}—\text{CH}=\overset{+}{\text{N}}=\overset{-}{\text{N}}$	2 100–2 080 2 075–2 050	Monosubstituted Disubstituted

Position of Carbonyl Absorption

Because the carbonyl absorption is one of the most prominent and identifiable bands in the IR spectrum, it is often used diagnostically. The general trends of structural variation on the position of $\text{C}=\text{O}$ stretching frequencies are summarized in six principles, as follows. Details of carbonyl absorptions are recorded in Table 6.14 and for other double bonds in Table 6.15, for aromatic bonds in Table 6.16 and other miscellaneous bonds in Table 6.17.

1. The more electronegative the group X in the system $\text{R}—\text{CO}—\text{X}—$, the higher is the frequency.
2. α,β -Unsaturation lowers the frequency by $15\text{--}40\text{ cm}^{-1}$, except in amides, where little shift is observed; if present it is usually to higher frequency.
3. Further conjugation has relatively little effect.

4. Ring strain in cyclic compounds causes a relatively large shift to higher frequency. This phenomenon provides a remarkably reliable test of ring size, distinguishing clearly between four-, five-, and larger-membered-ring ketones, lactones, and lactams. Six-membered-ring and larger ketones, lactones, and lactams show the normal frequency found for the open-chain compounds.
5. Hydrogen bonding to a carbonyl group causes a shift to lower frequency of $40\text{--}60\text{ cm}^{-1}$. Acids, amides, enolized β -keto carbonyl systems, and *o*-hydroxyphenol and *o*-aminophenyl carbonyl compounds show this effect. All carbonyl compounds tend to give slightly lower values for the carbonyl stretching frequency in the solid state compared with the value for dilute solutions.
6. Where more than one of the structural influences on a particular carbonyl group is operating, the net effect is usually close to additive.

An especially convenient aspect of IR spectroscopy is its practice. A small amount of sample can be pressed between two NaCl or KBr (Table 6.19) disks and the spectrum can be determined without further preparation. A spectrum so obtained is recorded as “neat” or “between salts.” If the sample is a solid, it may be mixed in a mortar and pestle with KBr and then pressed into a disk. The salt disk may be placed directly in the IR beam. In neither case is there a concern about solvent peaks. Of course, solvents may be used. Carbon tetrachloride and chloroform are the most commonly used solvents when the compound requires dissolution. Alternately, the sample may be intimately mixed (mulled) with mineral oil (a hydrocarbon oil). The thick slurry may then be smeared on a salt disk and placed in the spectrometer. The brand of mineral oil used historically is Nujol and such slurries are still called “Nujol mulls.” The transmission characteristics of potential solvents for IR spectroscopy may be found in Table 6.20.

Traditional analog spectrometers were calibrated by taking a second spectrum of polystyrene. The sharp 1641 cm^{-1} band was recorded on the same sheet as the original spectrum. Modern Fourier transform instruments do not usually require this step but still require calibration.

TABLE 6.14 Absorption Frequencies of Carbonyl Bands

All bands quoted are strong.

Groups	Band, cm^{-1}	Remarks
Acid anhydrides —CO—O—CO—		
Saturated	1 850–1 800 1 790–1 740	Two bands usually separated by about 60 cm^{-1} . The higher-frequency band is more intense in acyclic anhydrides, and the lower-frequency band is more intense in cyclic anhydrides.
Aryl and α,β -unsaturated	1 830–1 780 1 700–1 710	
Saturated five-ring	1 870–1 820 1 800–1 750	
All classes	1 300–1 050	
		One or two strong bands due to CO stretching

TABLE 6.14 Absorption Frequencies of Carbonyl Bands (*continued*)

Groups	Band, cm^{-1}	Remarks
Acid chlorides — COCl		
Saturated	1 815–1 790	Acid fluorides higher, bromides and iodides lower
Aryl and α,β -unsaturated	1 790–1 750	
Acid peroxide		
CO—O—O—CO—		
Saturated	1 820–1 810 1 800–1 780	
Aryl and α,β -unsaturated	1 805–1 780 1 785–1 755	
Esters and lactones		
—CO—O—		
Saturated	1 750–1 735	
Aryl and α,β -unsaturated	1 730–1 715	
Aryl and vinyl esters		
C=C—O—CO—alkyl	1 800–1 750	The C=C stretching band also shifts to higher frequency.
Esters with electronegative α substituents; <i>e.g.</i> , >CCl—CO—O—	1 770–1 745	
α -Keto esters	1 755–1 740	
Six-ring and larger lactones	Similar values to the corresponding open-chain esters	
Five-ring lactone	1 780–1 760	
α,β -Unsaturated five-ring lactone	1 770–1 740	When $\alpha\text{-CH}$ is present, there are two bands, the relative intensity depending on the solvent.
β,γ -Unsaturated five-ring lactone, vinyl ester type	ca 1 800	
Four-ring lactone	ca 1 820	
β -Keto ester in H bonding enol form	ca 1 650	Keto from normal; chelate-type H bond causes shift to lower frequency than the normal ester. The C=C band is strong and is usually near $1\,630\text{ cm}^{-1}$.
All classes	1 300–1 050	Usually two strong bands due to CO stretching
Aldehydes — CHO		
(See also Table 6.39 for C—H .) All values given below are lowered in liquid-film or solid-state spectra by about $10\text{--}20\text{ cm}^{-1}$. Vapor-phase spectra have values raised about 20 cm^{-1} .		

TABLE 6.14 Absorption Frequencies of Carbonyl Bands (*continued*)

Groups	Band, cm^{-1}	Remarks
Aldehydes —CHO (<i>continued</i>)		
Saturated	1 740–1 720	
Aryl	1 715–1 695	<i>o</i> -Hydroxy or amino groups shift this value to 1 655–1 625 cm^{-1} because of intramolecular H bonding.
α,β -Unsaturated	1 705–1 680	
$\alpha,\beta,\gamma,\delta$ -Unsaturated	1 680–1 660	
β -Ketoaldehyde in enol form	1 670–1 645	Lowering caused by chelate-type H bonding
Ketones >C=O		
All values given below are lowered in liquid-film or solid-state spectra by about 10–20 cm^{-1} . Vapor-phase spectra have values raised about 20 cm^{-1} .		
Saturated	1 725–1 705	
Aryl	1 700–1 680	
α,β -Unsaturated	1 685–1 665	
$\alpha,\beta,\alpha',\beta'$ -Unsaturated and diaryl	1 670–1 660	
Cyclopropyl	1 705–1 685	
Six-ring ketones and larger	Similar values to the corresponding open-chain ketones	
Five-ring ketones	1 750–1 740	α,β Unsaturation, $\alpha,\beta,\alpha',\beta'$ unsaturation, etc., have a similar effect on these values as on those of open-chain ketones.
Four-ring ketones	ca 1 780	
α -Halo ketones	1 745–1 725	Affected by conformation; highest values are obtained when both halogens are in the same plane as the C=O.
α,α' -Dihaloketones	1 765–1 745	
1,2-Diketones, <i>syn-trans</i> -open chains	1 730–1 710	Anti-symmetrical stretching frequency of both C=O's. The symmetrical stretching is inactive in the infrared but active in the Raman.
<i>syn-cis</i> -1,2-Diketones, six-ring	1 760 and 1 730	
<i>syn-cis</i> -1,2-Diketones, five ring	1 775 and 1 760	
<i>o</i> -Amino-aryl or <i>o</i> -hydroxy-aryl ketones	1 655–1 635	Low because of intramolecular H bonding. Other substituents and steric hindrance affect the position of the band.

TABLE 6.14 Absorption Frequencies of Carbonyl Bands (*continued*)

Groups	Band, cm^{-1}	Remarks
Ketones $>\text{C}=\text{O}$ (<i>continued</i>)		
Quinones	1 690–1 660	$\text{C}=\text{C}$ band is strong and is usually near $1\,600\text{cm}^{-1}$.
Extended quinones	1 655–1 635	
Tropone	1 650	Near $1\,600\text{cm}^{-1}$ when lowered by H bonding as in tropolones
Carboxylic acids $-\text{CO}_2\text{H}$		
All types	3 000–2 500	OH stretching; a characteristic group of small bands due to combination bands
Saturated	1 725–1 700	The monomer is near $1\,760\text{cm}^{-1}$, but is rarely observed. Occasionally both bands, the free monomer, and the H-bonded dimer can be seen in solution spectra. Ether solvents give one band near $1\,730\text{cm}^{-1}$.
α,β -Unsaturated	1 715–1 690	
Aryl	1 700–1 680	
α -Halo-	1 740–1 720	
Carboxylate ions $-\text{CO}_2^-$		
Most types	1 610–1 550	Anti-symmetrical and symmetrical stretching, respectively
	1 420–1 300	
Amides $-\text{CO}-\text{N}<$ (See also Table 6.39 for NH stretching and bending.)		
Primary $-\text{CONH}_2$		
In solution	ca 1 690	Amide I; $\text{C}=\text{O}$ stretching
Solid state	ca 1 650	
In solution	ca 1 600	Amide II: mostly NH bending
Solid state	ca 1 640	
		Amide I is generally more intense than amide II. (In the solid state, amides I and II may overlap.)
Secondary $-\text{CONH}-$		
In solution	1 700–1 670	Amide I
Solid state	1 680–1 630	
In solution	1 550–1 510	Amide II; found in open-chain amides only
Solid state	1 570–1 515	
		Amide I is generally more intense than amide II.
Tertiary	1 670–1 630	Since H bonding is absent, solid and solution spectra are much the same.
Lactams		
Six-ring and larger rings	ca 1 670	Shifted to higher frequency when the N atom is in a bridged system
Five-ring	ca 1 700	
Four-ring	ca 1 745	

TABLE 6.14 Absorption Frequencies of Carbonyl Bands (*continued*)

Groups	Band, cm^{-1}	Remarks
$\text{R}-\text{CO}-\text{N}=\text{C}=\text{C}$		Shifted $+15\text{ cm}^{-1}$ by the additional double bond
$\text{C}=\text{C}-\text{CO}-\text{N}$		Shifted by up to $+15\text{ cm}^{-1}$ by the additional double bond. This is an unusual effect by α,β unsaturation. It is said to be due to the inductive effect of the $\text{C}=\text{C}$ on the well-conjugated $\text{CO}-\text{N}$ system, the usual conjugation effect being less important in such a system.
Imides $-\text{CO}-\text{N}-\text{CO}-$		
Cyclic six-ring	ca 1710 and ca 1700	
Cyclic five-ring	ca 1770 and ca 1700	Shift of $+15\text{ cm}^{-1}$ with α,β unsaturation
Ureas $\text{N}-\text{CO}-\text{N}$		
RNHCONHR	ca 1660	
Six-ring	ca 1640	
Five-ring	ca 1720	
Urethanes $\text{R}-\text{O}-\text{CO}-\text{N}$	1740–1690	Also shows amide II band when nonsubstituted on N
Thioesters and Acids $\text{RCO}-\text{S}-\text{R}'$		
RCOSH	ca 1720	α,β -Unsaturated or aryl acid or ester shifted about -25 cm^{-1}
$\text{RCOS}-\text{alkyl}$	ca 1690	
$\text{RCOS}-\text{aryl}$	ca 1710	

TABLE 6.15 Absorption Frequencies of Other Double Bonds*Abbreviations Used in the Table*

m, moderately strong

m-s, moderate to strong

var, of variable strength

vs, very strong

w, weak

Group	Band, cm^{-1}	Remarks
Alkenes $>\text{C}=\text{C}<$		
Nonconjugated	1680–1620 (w-m)	May be very weak if symmetrically substituted
Conjugated with aromatic ring	1640–1610 (m)	More intense than with unconjugated double bonds

TABLE 6.15 Absorption Frequencies of Other Double Bonds


Alkenes >C=C< (continued)		
Internal (ring) Carbons: $n = 3$ $n = 4$ $n = 5$ $n \geq 6$	3 060–2 995 (m) ca 1 665 (w-m) ca 1 565 (w-m) ca 1 610 (w-m) 1 370–1 340 (s) 1 650–1 645 (w-m)	Highest frequencies for smallest ring Characteristic
Exocyclic $\text{C=C(CH}_2)_n$ $n = 2$ $n = 3$ $n \geq 4$	1 780–1 730 (m) ca 1 680 (m) 1 655–1 650 (m)	
Fulvene 	1 645–1 630 (m) 1 370–1 340 (s) 790–765 (s)	
Dienes, trienes, etc.	1 650 (s) and 1 600 (s)	Lower-frequency band usually more intense and may hide or overlap the higher-frequency band
α,β -Unsaturated carbonyl compounds	1 640–1 590 (m)	Usually much weaker than the C=O band
Enol esters, enol ethers, and enamines	1 700–1 650 (s)	
Imines, oximes, and amidines >C=N-		
Imines and oximes Aliphatic α,β -Unsaturated and aromatic Conjugated cyclic systems	1 690–1 640 (w) 1 650–1 620 (m) 1 660–1 480 (var) 960–930 (s)	NO stretching of oximes
Imino ethers —O—C=N—	1 690–1 640 (var)	Usually a strong doublet
Imino thioethers —S—C=N=	1 640–1 605 (var)	
Imine oxides $\text{>C=N}^+\text{—}\bar{\text{O}}$	1 620–1 550 (s)	
Amidines >N—C—N—	1 685–1 580 (var)	
Benzamidines Aryl —C=N=N	1 630–1 590	

TABLE 6.15 Absorption Frequencies of Other Double Bonds (continued)

Group	Band, cm^{-1}	Remarks
Imines, oximes, and amidines >C=N— (continued)		
Guanidine $\begin{array}{c} \text{>N—C=N—} \\ \\ \text{N} \end{array}$	1 725–1 625 (s)	
Azines >C=N—N=C<	1 670–1 600	
Hydrazoketones —CO—C=N—N	1 600–1 530 (vs)	
Azo compounds —N=N—		
Azo —N=N— Aliphatic Aromatic <i>cis</i> (Z) <i>trans</i> (E)	ca 1 575 (var) ca 1 510 (w) 1 440–1 410 (w)	Very weak or inactive
Azoxy $\begin{array}{c} \text{—N}^+=\text{N—} \\ \\ \text{O}^- \end{array}$ Aliphatic Aromatic	1 590–1 495 (m-s) 1 345–1 285 (m-s) 1 480–1 450 (m-s) 1 340–1 315 (m-s)	
Azothio $\text{—N}^+=\text{N—}\ddot{\text{S}}\text{—}$	1 465–1 445 (w) 1 070–1 055 (w)	
Nitro compounds N=O		
Nitro C—NO_2 Aliphatic Aromatic	ca 1 560 (s) 1 385–1 350 (s) 1 570–1 485 (s) 1 380–1 320 (s) 865–835 (s)	The two bands are due to asymmetrical and symmetrical stretching of the N=O bond. Electron-withdrawing substituents adjacent to nitro group increase the frequency of the asymmetrical band and decrease that of the symmetrical frequency. See above remark; also bulky orthosubstituents shift band to higher frequencies. Strong H bonding shifts frequency to lower end of range. Strong and sometimes at ca 750 cm^{-1}

TABLE 6.15 Absorption Frequencies of Other Double Bonds

Group	Band, cm ⁻¹	Remarks
Nitro compounds N=O (<i>continued</i>)		
α,β -Unsaturated Nitroalkenes	580–520 (var) 1 530–1 510 (s) 1 360–1 335 (s)	
Nitrates —O—NO ₂	1 650–1 625 (vs) 1 285–1 275 (vs) 870–855 (vs) 760–755 (w-m) 710–695 (w-m)	
Nitrates >N—NO_2	1 630–1 550 (s) 1 300–1 250 (s)	
Nitrates —O—N=O	1 680–1 610 (vs) 815–750 (s) 850–810 (s) 690–615 (s)	Two bands <i>Trans</i> (<i>E</i>) form <i>Cis</i> (<i>Z</i>) form
Thionitrites —S—N=O	730–685 (m-s)	
Nitroso >C—N=O	1 600–1 500 (s)	
N—N ⁺ =O ⁻ Aliphatic Aromatic	1 530–1 495 (m-s) 1 480–1 450 (m-s) 1 335–1 315 (m-s)	
Nitrogen oxides N→O Pyridine Pyrazine	1 320–1 230 (m-s) 1 190–1 150 (m-s) 1 380–1 280 (m-s) 1 040–990 (m-s) ca 850 (m)	Affected by ring substituents

TABLE 6.16 Absorption Frequencies of Aromatic Bands*Abbreviations Used in the Table*

m, moderately strong

var, of variable strength

m-s, moderate to strong

w-m, weak to moderately strong

s, strong

Group	Band, cm^{-1}	Remarks
Aromatic rings	ca 1 600 (m) ca 1 580 (m) ca 1 470 (m) ca 1 510 (m)	Stronger when ring is further conjugated When substituent on ring is electron acceptor When substituent on ring is electron donor
Five adjacent H	900–860 (w-m) 770–730 (s) 720–680 (s) 625–605 (w-m) ca 550 (w-m)	Substituents: $\text{C}=\text{C}$, $\text{C}\equiv\text{C}$, $\text{C}\equiv\text{N}$
1,2-Substitution	770–735 (s) 555–495 (w-m) 470–415 (m-s)	
1,3-Substitution	810–750 (s) 560–505 (m) 460–415 (m-s)	490–460 cm^{-1} when substituents are electron-accepting groups
1,4-Substitution	860–800 (s) 650–615 (w-m) 520–440 (m-s)	520–490 cm^{-1} when substituents are electron-donating groups
1,2,3-Trisubstitution	800–760 (s) 720–685 (s) 570–535 (s) ca 485	
1,2,4-Trisubstitution	900–885 (m) 780–760 (s) 475–425 (m-a)	
1,3,5-Trisubstitution	950–925 (var) 865–810 (s) 730–680 (m-s) 535–495 (s) 470–450 (w-m)	
Pentasubstitution	900–860 (m-s) 580–535 (s)	
Hexasubstitution	415–385 (m-s)	

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands*Abbreviations Used in the Table*

m, moderately strong	vs, very strong
m-s, moderate to strong	w, weak
s, strong	w-m, weak to moderately strong
var, of variable strength	

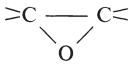
Group	Band, cm^{-1}	Remarks
Ethers		
Saturated aliphatic $\text{>C—O—C<}<$	1 150–1 060 (vs) 1 140–900 (s)	Two peaks may be observed for branched chain, usually 1 140–1 110 cm^{-1} . Usually 930–900 cm^{-1} ; may be absent for symmetric ethers
Alkyl-aryl >C—O—C< $ $	1 270–1 230 (vs) 1 120–1 020 (s)	=CO stretching CO stretching
Vinyl	1 225–1 200 (s)	Usually about 1 205 cm^{-1}
Diaryl >C—O—C= $ \quad $	1 200–1 120 (s) 1 100–1 050 (s)	
Cyclic	1 270–1 030 (s)	
Epoxides 	1 260–1 240 (m-s) 880–805 (m) 950–860 (var) 865–785 (m) 770–750 (m)	Monosubstituted <i>Trans</i> (<i>E</i>) form <i>Cis</i> (<i>Z</i>) form Trisubstituted
Ketals and acetals	1 190–1 140 (s) 1 195–1 125 (s) 1 100–1 000 (s) 1 060–1 035 (s)	Strongest band Sometimes obscured
Phthalanes	915–895 (s)	
Aromatic methylenedioxy	1 265–1 235 (s)	
Peroxides		
—O—O—	900–830 (w) 1 150–1 030 (m-s) ca 1 000 (m)	Alkyl Aryl

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm^{-1}	Remarks
Sulfur compounds		
Thiols —S—H —CO—SH —CS—SH	2 600–2 450 (w) 840–830 (m) ca 860 (s)	Broad
Thiocarbonyl >C=S >N—C=S $\quad \quad $ —S—C=S $\quad \quad $	1 200–1 050 (s) 1 570–1 395 1 420–1 260 1 140–940 ca 580 (s)	Behaves generally in a manner similar to carbonyl band
Sulfoxides >S=O	1 075–1 040 (vs) 730–690 (var) 395–360 (var)	Halogen or oxygen atom bonded to sulfur increases the frequency.
Sulfones >SO_2	1 360–1 290 (vs) 1 170–1 120 (vs) 610–545 (m-s) 525–495 (m-s)	Halogen or oxygen atom bonded to sulfur increases the frequency.
Sulfonamides $\text{—SO}_2\text{—N<}$	1 380–1 330 (vs) 1 170–1 140 (vs) 950–860 (m) 715–700 (w-m)	
Sulfonates $\text{—SO}_2\text{—O—}$	1 420–1 330 (s) 1 200–1 145 (s)	May appear as doublet
Thiosulfonates $\text{—SO}_2\text{—S—}$	ca 1 340 (vs)	
Sulfates $\text{—O—SO}_2\text{—O—}$ Primary alkyl salts	1 415–1 380 (s) 1 200–1 185 (s) 1 315–1 220 (s) 1 140–1 075 (m)	Electronegative substituents increase frequencies. Strongly influenced by metal ion

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm^{-1}	Remarks
Sulfur compounds (<i>continued</i>)		
Sulfates $\text{—O—SO}_2\text{—O}$ (<i>continued</i>) Secondary alkyl salts	1 270–1 210 (vs) 1 075–1 050 (s)	Doublet; both bands strongly influenced by metal ion
Stretching frequencies of C—S and S—S bonds —S—CH ₃ —S—CH ₂ — —S—CH< —S—C≡ —S—aryl R—S—S—R Aryl—S—S—aryl Polysulfides CH ₂ —S—CH ₂ — (R—S) ₂ C=O —CO—S— —CS—S $\begin{array}{c} \text{S—} \\ \diagup \\ \text{=C} \\ \diagdown \\ \text{S—} \end{array}$	710–685 (w-m) 660–630 (w-m) 630–600 (w-m) 600–570 (w-m) 1 110–1 070 (m) 710–685 (w-m) 705–570 (w) 520–500 (w) 500–430 (w-m) 500–470 (w-m) 695–655 (w-m) 880–825 (s) 570–560 (var) 1 035–935 (s) ca 580 (s) 1 050–900 (m-s) 980–850 (m-s) 900–800 (m-s)	CSC stretching Monoionic Ionic 1,1-dithiolates
Phosphorus compounds		
P—H	2 455–2 265 (m) 1 150–965 (w-m)	Sharp. Phosphines lie in the region 2 285–2 265 cm^{-1} .
—PH ₂	1 100–1 085 (m) 1 065–1 040 (w-m) 940–910 (m)	
P—alkyl	795–650 (m-s)	
P—aryl	1 130–1 090 (s) 750–680 (s)	
P—O—alkyl	1 050–970 (s)	Broad
P—O—aryl	1 240–1 190 (s)	
P—O—P	970–910	Broad

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm^{-1}	Remarks
Phosphorus compounds (<i>continued</i>)		
$\text{P}=\text{O}$	1 350–1 150 (s)	May appear as doublet
$\begin{array}{c} \text{O} \\ \parallel \\ \text{P} \\ \diagdown \\ \text{OH} \end{array}$	2 725–2 520 (w-m) 2 350–2 080 (w-m) 1 740–1 600 (w-m) 1 335 (s) 1 090–910 (s) 540–450 (w-m)	H-bonded; broad Broad; may be doublet for aryl acids P=O stretching
$\text{P}=\text{S}$	865–655 (m-s) 595–530 (var)	
$\begin{array}{c} \text{S} \\ \parallel \\ \text{P} \\ \diagdown \\ \text{OH} \end{array}$	3 100–3 000 (w) 2 360–2 200 (w) 935–910 (s) 810–750 (m-s) 655–585 (var)	PO stretching P=S stretching P=S stretching
Silicon compounds		
$\text{Si}-\text{H}$	2 250–2 100 (s) 985–800	SiH_3 has two bands.
$\text{Si}-\text{C}\equiv$	860–760	Accompanied by CH_2 rocking
$\text{Si}-\text{CH}_3$	1 280–1 250 (s)	Sharp
$\text{Si}-\text{C}_2\text{H}_5$	1 250–1 220 (m) 1 020–1 000 (m) 970–945 (m)	
$\text{Si}-\text{Aryl}$	1 125–1 090 (vs)	Splits into two bands when two aryl groups are attached to one silicon atom, but has only one band when three aryl groups attached
$\equiv\text{Si}-\text{OH}$	870–820	OH deformation band
$\equiv\text{Si}-\text{O}-\text{Si}\equiv$	1 100–1 000	
$\equiv\text{Si}-\text{N}-\text{Si}\equiv$	940–870 (s)	
$\equiv\text{Si}-\text{Cl}$	550–470 (s) 250–150	

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm^{-1}	Remarks
Silicon compounds (<i>continued</i>)		
>SiCl_2	595–535 (s) 540–460 (m)	
—SiCl_3	625–570 (s) 535–450 (m)	
Boron compounds		
Boranes >BH or —BH_2	2 640–2 450 (m-s) 2 640–2 570 (m-s) 2 535–2 485 (m-s) 2 380–2 315 (s) 2 285–2 265 (s) 2 140–2 080 (w-m) 2 580–2 450 (m)	Free H in BH Free H in BH_2 plus second band In complexes; second band for BH_2 Bridged H Borazoles and borazines
BH_4^-	2 310–2 195 (s)	Two bands
B—N	1 550–1 330 750–635	Borazines and borazoles
B—O	1 390–1 310 (s) 1 280–1 200	BO stretching Metal orthoborates
B—Cl B—Br	1 090–890 (s)	Plus other bands at lower frequencies for BX_2 and BX_3
B—F	1 500–840 (var)	Isotope splitting present
XBF_2	1 500–1 410 (s) 1 300–1 200 (s)	
X_2BF	1 360–1 300 (s)	
BF_3 complexes	1 260–1 125 (s) 1 030–800 (s)	Band splitting may be added to isotopic splittings.
BF_4^-	ca 1 030 (vs)	

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm^{-1}	Remarks
Halogen compounds		
C—F		
Aliphatic, mono-F	1 110–1 000 (vs) 780–680 (s)	Two bands Number of bands
Aliphatic, di-F	1 250–1 050 (vs)	
Aliphatic, poly-F	1 360–1 090 (vs)	
Aromatic	1 270–1 100 (m) 680–520 (m-s) 420–375 (var) 340–240 (s)	
—CF ₃		
Aliphatic	1 350–1 120 (vs) 780–680 (s) 680–590 (s) 600–540 (s) 555–505 (s)	
Aromatic	1 330–1 310 (m-s) 600–580 (s)	
C—Cl		
Primary alkanes	730–720 (s) 685–680 (s) 660–650 (s)	
Secondary alkanes	ca 760 (m) 675–655 (m-s) 615–605 (s)	
Tertiary alkanes	635–610 (m-s) 580–560 (m-s)	
Poly-Cl	800–700 (vs)	
Aryl:		
1,2-	1 060–1 035 (m)	
1,3-	1 080–1 075 (m)	
1,4-	1 100–1 090 (m)	
Chloroformates	ca 690 (s) 485–470 (s)	
Axial Cl	730–580 (s)	
Equatorial Cl	780–740 (s)	
C—Br		
Primary alkanes	645–635 (s) 565–555 (s) 440–430 (var)	
Secondary alkanes	620–605 (s) 590–575 (m-w) 540–530 (s)	

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm^{-1}	Remarks
Halogen compounds (<i>continued</i>)		
C—Br (<i>continued</i>)		
Tertiary alkanes	600–595 (m-s) 525–505 (s)	
Axial	690–550 (s)	
Equatorial	750–685 (s)	
Aryl:		
1,2-	1 045–1 025 (m)	
1,3-; 1,4-	1 075–1 065 (m)	
Other bands	400–260 (s) 325–175 (m-s) 290–225 (m-s)	
C—I		
Primary alkanes	600–585 (s) 515–500 (s)	
Secondary alkanes	ca 575 (s) 550–520 (s) 490–480 (s)	
Tertiary alkanes	580–560 (s) 510–485 (m) 485–465 (s)	
Aromatic	1 060–1 055 (m-s) 310–160 (s)	
Axial	265–185	
Equatorial	ca 640 (s) ca 655 (s)	
Inorganic ions		
Ammonium	3 300–3 030	Several bands, all strong
Cyanate	2 220–2 130 (s)	
Cyanide	2 200–2 000	
Carbonate	1 450–1 410	
Hydrogen sulfate	1 190–1 160 (s) 1 180–1 000 (s) 880–840 (m)	
Nitrate	1 410–1 350 (vs) 860–800 (m)	
Nitrite	1 275–1 230 (s) 835–800 (m)	Shoulder

TABLE 6.17 Absorption Frequencies of Miscellaneous Bands (*continued*)

Group	Band, cm^{-1}	Remarks
Inorganic ions (<i>continued</i>)		
Phosphate	1 100–1 000	
Sulfate	1 130–1 080 (s)	
Thiocyanate	ca 2 050 (s)	

TABLE 6.18 Absorption Frequencies in the Near Infrared*Values in parentheses are molar absorptivity*

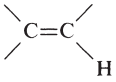
Class	Band, cm^{-1}	Remarks
Acetylenes	9 800–9 430 6 580–6 400 (1.0)	Overtone of $\equiv\text{CH}$ stretching
Alcohols (nonhydrogen-bonded)	7 140–7 010 (2.0)	Overtone of OH stretching
Aldehydes Aliphatic Aromatic Formate	4 640–4 520 (0.5) ca 8 000 ca 4 525 ca 4 445 4 775–4 630 (1.0)	Combination of $\text{C}=\text{O}$ and CH stretchings
Alkanes $-\text{CH}_3$ $-\text{CH}_2-$ $\equiv\text{CH}$ Cyclopropane	9 000–8 350 (0.02) 5 850–5 660 (0.1) 4 510–4 280 (0.3) 9 170–8 475 (0.02) 5 830–6 640 (0.1) 4 420–4 070 (0.25) 8 550–8 130 7 000–6 800 5 650–5 560 6 160–6 060 4 500–4 400	All bands very weak
Alkenes  $>\text{C}=\text{CH}_2$ and $-\text{CH}=\text{CH}_2$	6 850–6 370 (1.0) 7 580–7 300 (0.02) 6 140–5 980 (0.2) 4 760–4 700 (1.2)	

TABLE 6.18 Absorption Frequencies in the Near Infrared (*continued*)

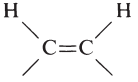
Class	Band, cm^{-1}	Remarks
Alkenes (continued)  $-\text{O}-\text{CH}=\text{CH}_2$ $-\text{CO}-\text{CH}=\text{CH}_2$	4760–4660 (0.15) 6250–6040 (0.3) 7580–7410 (0.02) 6190–5990 (0.3) 4820–4750 (0.2–0.5)	<i>Trans</i> (<i>E</i>) isomers have no unique bands.
Amides Primary Secondary	7400–6540 (0.7) 5160–5060 (3.0) 5040–4990 (0.5) 4960–4880 (0.5) 7330–7140 (0.5) 5050–4960 (0.4)	Two bands; overtone of NH stretch Second overtone of C=O stretch; second overtone of NH deformation; combination of C=O and NH Overtone of NH stretch Combination of NH stretch and NH bending
Amines, aliphatic Primary Secondary	9710–9350 6670–6450 (0.5) 5075–4900 (0.7) 9800–9350 6580–6410 (0.5)	Second overtone of NH stretch Two bands; overtone of NH stretch Two bands; combination of NH stretch and NH bending Second overtone of NH stretch Overtone of NH stretch
Amines, aromatic Primary Secondary	9950–9520 (0.4) 7040–6850 (0.2) 6760–6580 (1.4) 5140–5040 (1.5) 10000–9710 6800–6580 (0.5)	
Aryl-H	7660–7330 (0.1) 6170–5880 (0.1)	Overtone of CH stretch
Carbonyl	5200–5100	
Carboxylic acids	7000–6800	
Epoxide (terminal)	6135–5960 (0.2) 4665–4520 (1.2)	Cyclopropane bands in same region

TABLE 6.18 Absorption Frequencies in the Near Infrared (*continued*)

Class	Band, cm^{-1}	Remarks
Glycols	7 140–7 040	
Hydroperoxides		
Aliphatic	6 940–6 750 (2.0) 4 960–4 880 (0.8)	Two bands
Aromatic	7 040–6 760 (1.0) 4 950–4 850 (1.3)	
Imides	9 900–9 620 6 540–6 370	
Nitriles	5 350–5 200 (0.1)	
Oximes	7 140–7 050	
Phosphines	5 350–5 260 (0.2)	
Phenols		
Nonbonded	7 140–6 800 (3.0) 5 000–4 950	
Intramolecularly bonded	7 000–6 700	
Thiols	5 100–4 950 (0.05)	

TABLE 6.19 Infrared Transmitting Materials

Material	Wavelength range, μm	Wavenumber range, cm^{-1}	Refractive index at $2\ \mu\text{m}$
NaCl, rock salt	0.25–17	40 000–590	1.52
KBr, potassium bromide	0.25–25	40 000–400	1.53
KCl, potassium chloride	0.30–20	33 000–500	1.5
AgCl, silver chloride*	0.40–23	25 000–435	2.0
AgBr, silver bromide*	0.50–35	20 000–286	2.2
CaF ₂ , calcium fluoride (Irtran-3)	0.15–9	66 700–1 110	1.40
BaF ₂ , barium fluoride	0.20–11.5	50 000–870	1.46
MgO, magnesium oxide (Irtran-5)	0.39–9.4	25 600–1 060	1.71
CsBr, cesium bromide	1–37	10 000–270	1.67
CsI, cesium iodide	1–50	10 000–200	1.74
TlBr–TlI, thallium bromide–iodide (KRS-5)*	0.50–35	20 000–286	2.37
ZnS, zinc sulfide (Irtran-2)	0.57–14.7	17 500–680	2.26

* Useful for internal reflection work.

TABLE 6.19 Infrared Transmitting Materials (*continued*)

Material	Wavelength range, μm	Wavenumber range, cm ⁻¹	Refractive index at 2 μm
ZnSe, zinc selenide* (vacuum deposited) (Irtran-4)	1–18	10 000–556	2.45
CdTe, cadmium telluride (Irtran-6)	2–28	5 000–360	2.67
Al ₂ O ₃ , sapphire*	0.20–6.5	50 000–1 538	1.76
SiO ₂ , fused quartz	0.16–3.7	62 500–2 700	
Ge, germanium*	0.50–16.7	20 000–600	4.0
Si, silicon*	0.20–6.2	50 000–1 613	3.5
Polyethylene	16–300	625–33	1.54

* Useful for internal reflection work.

TABLE 6.20 Infrared Transmission Characteristics of Selected Solvents

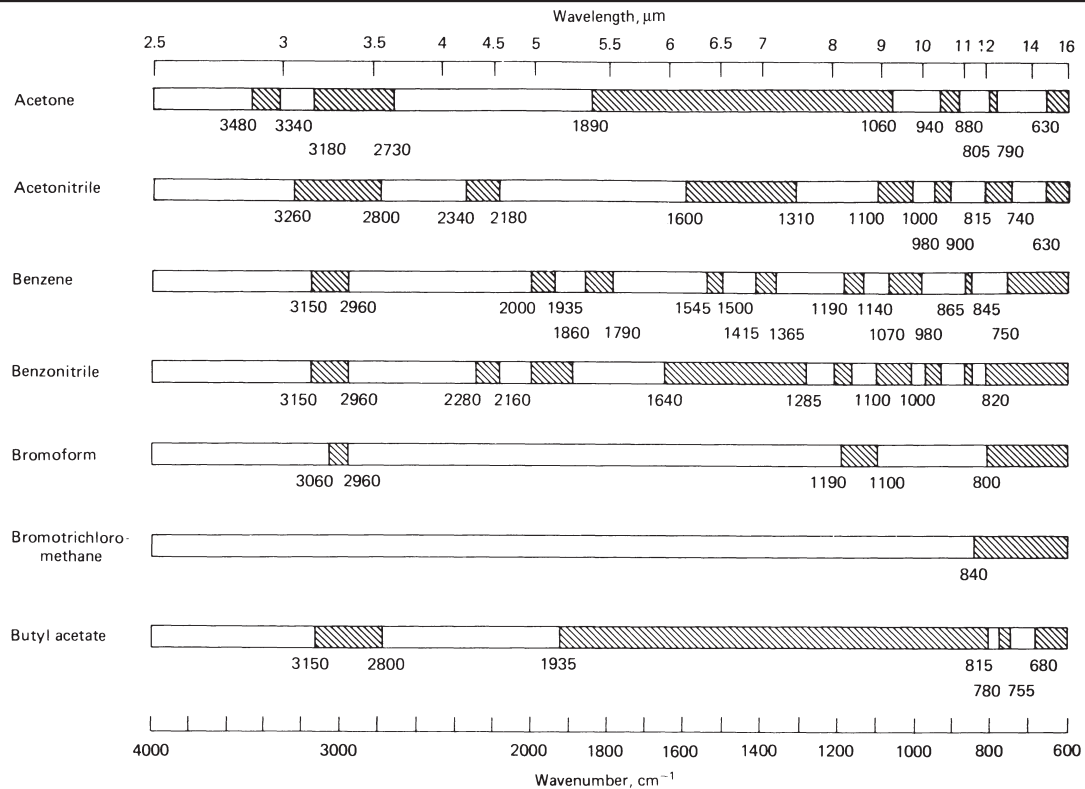
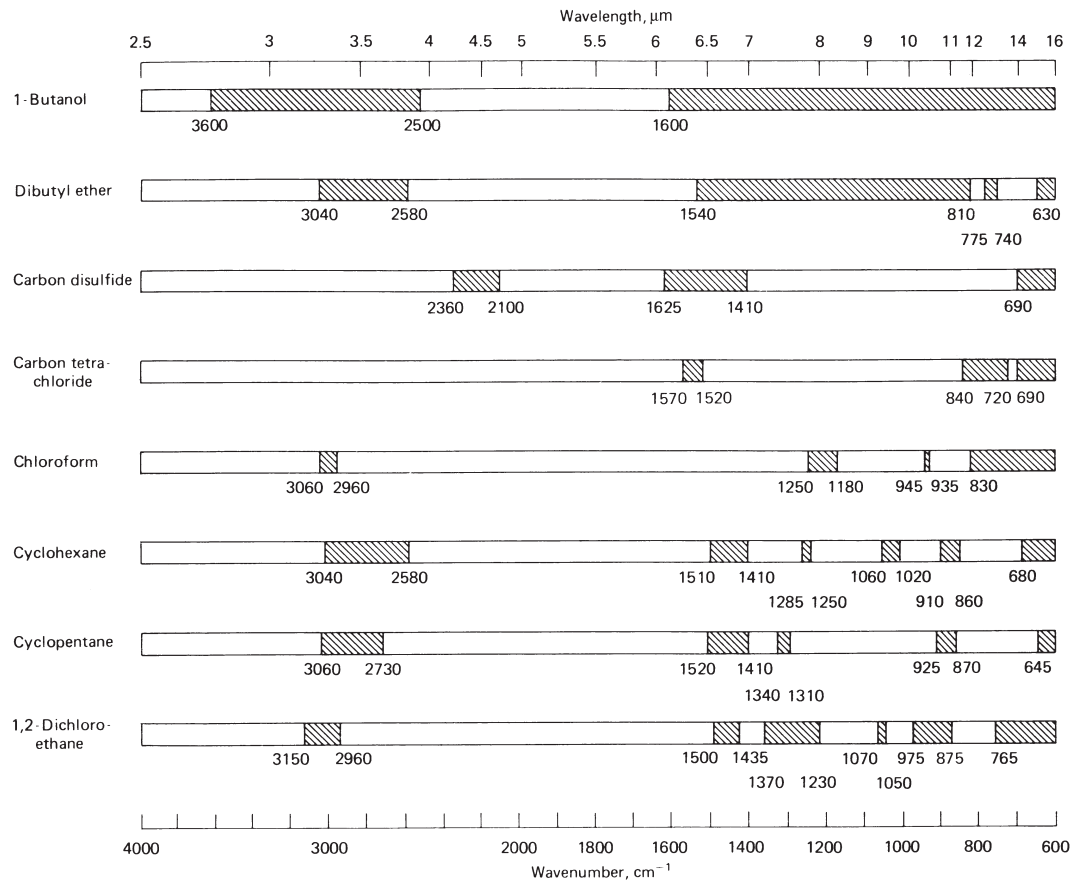
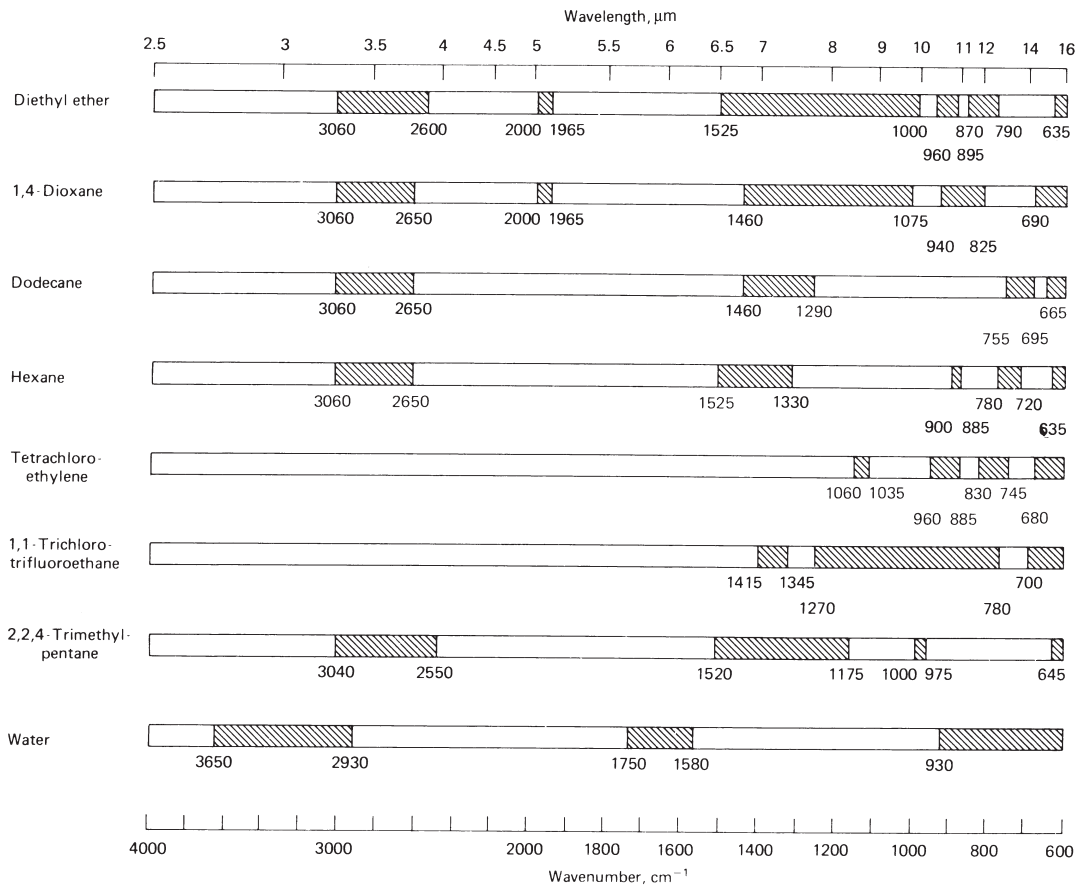


TABLE 6.20 Infrared Transmission Characteristics of Selected Solvents (*continued*)



RAMAN SPECTROSCOPY

Infrared and Raman spectroscopy are related by the fact that both permit the detection of bond vibrations. Like IR spectroscopy, the spectral bands are reported in cm^{-1} . An important difference is that the wavelength and intensity of inelastically scattered light is measured in the Raman spectroscopic method. The “Raman effect” causes the scattered radiation to shift according to the energies of molecular vibrations. Although Raman spectroscopy involves a physical principle different from that in IR spectroscopy, the two techniques are complementary.

Infrared spectroscopy relies on a changing dipole during a bond vibration for absorption of energy to occur. In Raman, it is a change in polarizability in the bond that permits absorption. The simple molecule carbon dioxide, $\text{O}=\text{C}=\text{O}$, is an instructive example. Both $\text{C}=\text{O}$ bonds have dipoles but they oppose each other and the net dipole is 0 Debye (0D). The symmetrical stretch in which both $\text{C}=\text{O}$ bonds simultaneously extend and contract does not change the dipole but is detectable by Raman because the polarizability of the system alters.

Raman scattering is not a very efficient process and an energy source of considerable power is required. This is typically an argon (Ar) laser. A variety of chemical bonds and systems can be detected by modern Raman spectrometers and typical data are summarized in Tables 6.21–6.30.

TABLE 6.21 Raman Frequencies of Single Bonds to Hydrogen and Carbon

Abbreviations Used in the Table

m, moderately strong	vw, very weak
m-s, moderate to strong	w, weak
m-vs, moderate to very strong	w-m, weak to moderately strong
s, strong	w-m, weak to moderately strong
vs, very strong	w-vs, weak to very strong

Group	Band, cm^{-1}	Remarks
Saturated C—H and C—C		
—CH ₃	2969–2967 (s) 2884–2883 (s) ca 1205 (s) 1150–1135 1060–1056 975–835 (s) 280–220	In aryl compounds In unbranched alkyls In unbranched alkyls Terminal rocking of methyl group CH ₂ —CH ₃ torsion
—CH ₂ —	2949–2912 (s) 2861–2849 (s) 1473–1443 (m-vs) 1305–1295 (s) 1140–1070 (m) 888–837 (w) 425–150 500–490	Intensity proportional to number of CH ₂ groups Often two bands; see above Substituent on aromatic ring

TABLE 6.21 Raman Frequencies of Single Bonds to Hydrogen and Carbon (*continued*)

Group	Band, cm^{-1}	Remarks
Saturated C—H and C—C (<i>continued</i>)		
—CH(CH ₃) ₂	1 350–1 330 (m) 835–750 (s)	If attached to C=C bond, 870–800 cm^{-1} . If attached to aryl ring, 740 cm^{-1}
—C(CH ₃) ₃	1 265–1 240 (m) 1 220–1 200 (m) 760–685 (vs)	Not seen in <i>tert</i> -butyl bromide Not seen in <i>tert</i> -butyl bromide If attached to C=C or aromatic ring, 760–720 cm^{-1}
Internal tertiary carbon atom	855–805 (w) 455–410	
Internal quaternary carbon atom	710–680 (vs) 490–470	
Two adjacent tertiary carbon atoms	730–920 770–725	Often a band at 530–524 cm^{-1} indicates presence of adjacent tertiary and quaternary carbon atoms.
Dialkyl substitution at α -carbon atom	800–700 (m-s) 680–650 (vs) 605–550	
Cyclopropane	3 101–3 090 3 038–3 019 1 210–1 180 (s)	Shifts to 1 200 cm^{-1} for monoalkyl or 1,2-dialkyl substitution and to 1 320 cm^{-1} for <i>gem</i> -1,1- dialkyl substitution
Cyclobutane	1 001–960 (vs)	Shifts to 933 cm^{-1} for monoalkyl, to 887 cm^{-1} for <i>cis</i> -1,3-dialkyl, and to 891 cm^{-1} plus 855 cm^{-1} (doublet) for <i>trans</i> -1,3-dialkyl substitution
Cyclopentane	900–800 (s)	
Cyclohexane	825–815 (vs) 810–795 (vs)	Boat configuration Chair configuration

TABLE 6.21 Raman Frequencies of Single Bonds to Hydrogen and Carbon (*continued*)


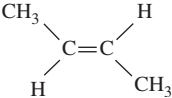
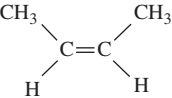
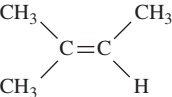
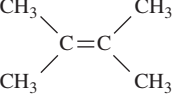
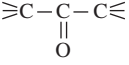

Group	Band, cm^{-1}	Remarks
Saturated C—H and C—C (<i>continued</i>)		
Cycloheptane	ca 733	
Cyclooctane	ca 703	
	1 392–1 377 450–400 (vw) 270–250 (m)	
	1 380–1 379 492–455 (vw) 220–200 (m)	
	1 372–1 368 970–952 (m) 592–545 (vw) 420–400 (m) 310–290 (m)	
	1 385–1 375 522–488 (w)	
	1 392–1 386 690–678 (m-s) 510–485 (m) 424–388 (w)	
	1 170–1 100 (w-m) 600–580 (m-s)	
	1 120–1 090 (m-vs) 600–510 (w-m)	Tertiary or quaternary carbon adjacent to carbonyl group lowers the frequency 300 cm^{-1}
—CH ₂ —CO—	1 420–1 410 (s)	
—CHO	2 850–2 810 (m) 2 720–2 695 (vs)	Often appears as a shoulder

TABLE 6.21 Raman Frequencies of Single Bonds to Hydrogen and Carbon (*continued*)


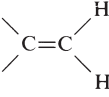
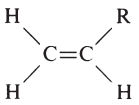
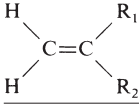
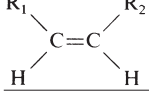
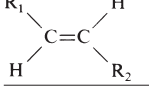
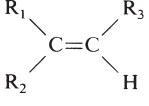
Group	Band, cm^{-1}	Remarks
Unsaturated C—H		
$\text{—C}\equiv\text{C—H}$	3 340–3 270 (w-m)	Alkyl substituents at higher frequencies; unsaturated or aryl substituents at lower frequencies
	3 040–2 995 (m)	
	3 095–3 050 (m) 2 990–2 983 (s)	Asymmetric $=\text{CH}_2$ stretch Symmetric $=\text{CH}_2$ stretch
	1 419–1 415 (m) 1 309–1 2 888 (m)	Plus $=\text{CH}$ and $=\text{CH}$ stretching bands
	1 413–1 399 (m) 909–885 (m) 711–684 (w)	Plus $=\text{CH}_2$ stretching bands
	1 270–1 251 (m)	Plus $=\text{CH}$ stretching band
	1 314–1 290 (m)	Plus $=\text{CH}$ stretching band
	1 360–1 322 (w) 830–800 (vw)	Plus $=\text{CH}$ stretching band
Hydroxy O—H		
Free —OH Intermolecularly bonded Aromatic —OH	3 650–3 250 (w) 3 400–3 300 (w) ca 3 160 (s)	
—OH	1 460–1 320 (w) 1 276–1 205 (w-m) 1 260 (w-m)	Common to all OH substituents Primary Secondary

TABLE 6.21 Raman Frequencies of Single Bonds to Hydrogen and Carbon (*continued*)

Group	Band, cm^{-1}	Remarks
Hydroxy O—H (<i>continued</i>)		
C—C—OH primary	1 070–1 050 (m-s) 1 030–960 (m-s) 480–430 (w-m)	CCO stretching CCO deformation
C—C—OH Secondary	1 135–1 120 (m-s) 825–815 (vs) 500–490 (w-m)	
Tertiary	1 210–1 200 (m-s) 755–730 (vs) 360–350 (w-m)	
—CO—O—H	1 305–1 270	CO stretching
N—H and C—N bonds		
Amine >N—H Associated Nonbonded Salts	3 400–3 250 (s) 3 550–3 250 (s) 2 986–2 974	Primary amines show two bands. Often obscured by intense CH stretching bands
—NH ₂	1 650–1 590 (w-vs)	Bending
Amides Primary	3 540–3 500 (w) 3 400–3 380 (w) 1 310–1 250 (s)	Both bands lowered ca 150 cm^{-1} in solid state and H bonding Interaction of NH bending and CN stretching; lowered 50 cm^{-1} in nonbonded state
Secondary	1 150–1 095 (m) 3 491–3 404 (m-s) 1 190–1 130 (m) 931–865 (m-s) 430–395 (w-m)	Rocking of NH ₂ Two bands; lowered in frequency on H bonding and in solid state
—CO—N	607–555 (m)	O=CN bending
C—N—C C	1 070–1 045 (m)	Stretching
>C—N< Primary carbon Secondary α carbon	1 090–1 060 (m) 1 140–1 035 (m)	CN stretching Two bands but often obscured. Strong band at 800 cm^{-1}
Tertiary α carbon	1 240–1 020 (m)	Two bands. Strong band also at 745 cm^{-1}

TABLE 6.22 Raman Frequencies of Triple Bonds*Abbreviations Used in the Table*

m, moderately strong

s-vs, strong to very strong

m-s, moderate to strong

vs, very strong

s, strong

Group	Band, cm^{-1}	Remarks
$\text{R}-\text{C}\equiv\text{CH}$	2 160–2 100 (vs) 650–600 (m) 356–335 (s)	Monoalkyl substituted; $\text{C}\equiv\text{C}$ stretch $\text{C}\equiv\text{CH}$ deformation $\text{C}\equiv\text{C}-\text{C}$ bending of monoalkyls
$\text{R}_1-\text{C}\equiv\text{C}-\text{R}_2$	2 300–2 190 (vs)	$\text{C}\equiv\text{C}$ stretching of disubstituted alkyls; sometimes two bands
$-\text{C}\equiv\text{C}-\text{C}\equiv\text{C}-$	2 264–2 251 (vs)	
$-\text{C}\equiv\text{N}$	2 260–2 240 (vs) 2 234–2 200 (vs) 840–800 (s-vs) 385–350 (m-s) 200–160 (vs)	Unsaturated nonaryl substituents lower the frequency and enhance the intensity. Lowered ca 30 cm^{-1} with aryl and conjugated aliphatics CCCN symmetrical stretching Aliphatic nitriles
$\text{H}-\text{C}\equiv\text{N}$	2 094 (vs)	
Azides $-\text{N}=\text{N}^+=\text{N}$	2 170–2 080 (s) 1 258–1 206 (s)	Asymmetric NNN stretching Symmetric NNN stretching; HN_3 at $1\,300\text{ cm}^{-1}$
Diazonium salts $\text{R}-\text{N}^+=\text{N}$	2 300–2 240 (s)	
Isonitriles $-\text{N}^+\equiv\text{C}^-$	2 146–2 134 2 124–2 109	Stretching of aliphatics Stretching of aromatics
Thiocyanates $-\text{S}-\text{C}\equiv\text{N}$	2 260–2 240 (vs) 650–600 (s)	Stretching of $\text{C}\equiv\text{N}$ Stretching of SC bond

TABLE 6.23 Raman Frequencies of Cumulated Double Bonds*Abbreviations Used in the Table*

s, strong

vw, very weak

vs, very strong

w, weak

Group	Band, cm^{-1}	Remarks
Allenenes $\text{C}=\text{C}=\text{C}$	2000–1960 (s) 1080–1060 (vs) 356	Pseudo-asymmetric stretching Symmetric stretching $\text{C}=\text{C}=\text{C}$ bending
Carbodiimides (cyanamides) $-\text{N}=\text{C}=\text{N}-$	2140–2125 (s) 2150–2100 (vs) 1460 1150–1140 (vs)	Asymmetric stretching of aliphatics Asymmetric stretching of aromatics; two bands Symmetrical stretching of aliphatics Symmetric stretching of aryls
Cumulenes (trienes) $\text{C}=\text{C}=\text{C}=\text{C}$	2080–2030 (vs) 878	
Isocyanates $-\text{N}=\text{C}=\text{O}$	2300–2250 (vw) 1450–1400 (s)	Asymmetric stretching Symmetric stretching
Isothiocyanates $-\text{N}=\text{C}=\text{S}$	2220–2100 690–650	Two bands Alkyl derivatives
Ketenes $\text{C}=\text{C}=\text{O}$	2060–2040 (vs) 1130 (s) 1374 (s) 1120 (s)	Pseudo-asymmetric stretching Pseudo-symmetric stretching Alkyl derivatives Aryl derivatives
Sulfinylamines $\text{R}-\text{N}=\text{S}=\text{O}$	1306–1214 (w) 1155–989 (s)	Asymmetric stretching Symmetric stretching

TABLE 6.24 Raman Frequencies of Carbonyl Bonds*Abbreviations Used in the Table*

m, moderately strong
m-s, moderate to strong
s, strong

s-vs, strong to very strong
vs, very strong
w, weak

Group	Band, cm^{-1}	Remarks
Acid anhydrides —CO—O—CO— Saturated Conjugated, noncyclic	1 850–1 780 (m) 1 771–1 770 (m) 1 775 1 720	
Acid fluorides —CO—F Alkyl Aryl	1 840–1 835 1 812–1 800	
Acid chlorides —CO—Cl Alkyl Aryl	1 810–1 770 (s) 1 774 1 731	
Acid bromides —CO—Br Alkyl Aryl	1 812–1 788 1 775–1 754	
Acid iodides —CO—I Alkyl Aryl	ca 1 806 ca 1 752	
Lactones	1 850–1 730 (s)	
Esters Saturated Aryl and α,β -unsaturated Diesters Oxalates Phthalates $\text{C}\equiv\text{C}-\text{CO}-\text{O}-$ Carbamates	1 741–1 725 1 727–1 714 1 763–1 761 1 738–1 728 1 716–1 708 1 694–1 688	Alkyl branching on carbon adjacent to $\text{C}=\text{O}$ lowers frequency by $5\text{--}15\text{ cm}^{-1}$.
Aldehydes	1 740–1 720 (s-vs)	
Ketones Saturated Aryl	1 725–1 700 (vs) 1 700–1 650 (m)	

TABLE 6.24 Raman Frequencies of Carbonyl Bonds (*continued*)

Group	Band, cm^{-1}	Remarks
Ketones (<i>continued</i>)		
Alicyclic		
$n = 4$	1 782 (m)	
$n = 5$	1 744 (m)	
$n \geq 6$	1 725–1 699 (m)	
Carboxylic acids		
Mono-	1 686–1 625 (s)	These α -substituents increase the frequency: F, Cl, Br, OH. Solid state; often two bands In solution; very broad band
Poly-	1 782–1 645	
Amino acids	1 750–1 710 1 743–1 729	
Carboxylate ions		
Amino acid anion	1 690–1 550 (w) 1 440–1 340 (vs) 1 743–1 729 1 600–1 570 (w)	Often masked by water deformation band near $1\,630\text{cm}^{-1}$
Amides (see also Table 6.21)		
Primary		
Associated	1 686–1 576 (m-s) 1 650–1 620 (m)	
Nonbonded	1 715–1 675 (m) 1 620–1 585 (m)	
Secondary		
Associated	1 680–1 630 (w) 1 570–1 510 (w) 1 490–1 440	Both <i>cis</i> (<i>Z</i>) and <i>trans</i> (<i>E</i>) forms <i>Trans</i> (<i>E</i>) form <i>Cis</i> (<i>Z</i>) form Both <i>cis</i> (<i>Z</i>) and <i>trans</i> (<i>E</i>) forms <i>Trans</i> (<i>E</i>) form (no <i>cis</i> band)
Nonbonded	1 700–1 650 1 550–1 500	
Tertiary	1 670–1 630 (m)	
Lactams	1 750–1 700 (m)	

TABLE 6.25 Raman Frequencies of Other Double Bonds*Abbreviations Used in the Table*

m, moderately strong

vs, very strong

m-s, moderate to strong

w, weak

s, strong

s-vs, strong to very strong

w-m, weak to moderately strong

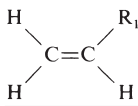
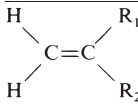
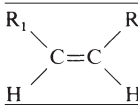
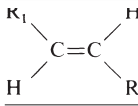
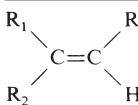
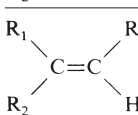
Group	Band, cm ⁻¹		Remarks	
Alkenes >C=C<				
>C=C<	1 680–1 576 (m-s)		General range	
	1 648–1 638 (vs)		C=C stretching	
	ca 1 650 (vs) 270–252 (w)		C=C stretching C=C—C skeletal deformation	
	ca 1 660 (vs) 970–952 (w)		C=C stretching Asymmetric CC stretching	
	1 676–1 665 (s)		C—C stretching	
	1 678–1 664 (vs) 522–488 (w)		C=C stretching C=C—C skeletal deformation	
	1 680–1 665 (s) 690–678 (m-s) 510–485 (m) 424–388 (w)		C=C stretching Symmetrical CC stretching Skeletal deformation Skeletal deformation	
Haloalkene	X = fluorine	X = chlorine	X = bromine	X-iodine
>C=C< stretch of haloalkanes				
H ₂ C=CHX	1 654	1 603–1 601	1 596–1 593	1 581
HXC=CHX				
<i>cis</i> (Z)	1 712	1 590–1 587	1 587–1 583	1 543
<i>trans</i> (E)	1 694	1 578–1 576	1 582–1 581	1 537
H ₂ C=CX ₂	1 728	1 616–1 611	1 593	
X ₂ C=CHX	1 792	1 589–1 582	1 552	
X ₂ C=CX ₂	1 872	1 577–1 571	1 547	1 465 (solid)

TABLE 6.25 Raman Frequencies of Other Double Bonds (*continued*)

Group	Band, cm^{-1}	Remarks
>C=N—bonds		
Aldimines (azomethines) $\begin{array}{c} \text{H} \\ \diagdown \\ \text{C}=\text{N}-\text{R}_2 \\ \diagup \\ \text{R}_1 \end{array}$	1 673–1 639 1 405–1 400 (s)	Dialkyl substituents at higher frequency; diaryl substituents at lower end of range
Aldoximes and Ketoximes >C=N—OH	1 680–1 617 (vs) 1 335–1 330 (w)	
Azines >C=N—N=C<	1 625–1 608 (s)	
Hydrazones $\begin{array}{c} \text{H} & & \text{H} \\ \diagdown & & \diagup \\ \text{C}=\text{N}-\text{N} & & \\ \diagup & & \diagdown \\ \text{R}_1 & & \text{R}_2 \end{array}$	1 660–1 610 (s-vs)	
Imido ethers $\begin{array}{c} \text{O} \\ \diagdown \\ \text{C}=\text{NH} \\ \diagup \end{array}$	1 658–1 648	NH stretching at $3\,360\text{--}3\,327\text{ cm}^{-1}$
Semicarbazones and thiosemicarbazones $\begin{array}{c} & & \text{H} \\ & & \diagup \\ \diagdown & \text{C}=\text{N}-\text{N} & \\ \diagup & & \diagdown \\ & & \text{C} \quad \text{NH}_2 \\ & & \parallel \\ & & \text{O (or S)} \end{array}$	1 665–1 642 (vs) 1 620–1 610 (vs)	Aliphatic. Thiosemicarbazones fall in lower end of range. Aromatic derivatives
Azo compounds —N=N—		
—N=N—	1 580–1 570 (vs) 1 442–1 380 (vs) 1 060–1 030 (vs)	Nonconjugated Conjugated to aromatic ring CN stretching in aryl compounds
Nitro compounds N=O		
Alkyl nitrites	1 660–1 620 (s)	N=O stretching
Alkyl nitrates	1 635–1 622 (w-m) 1 285–1 260 (vs) 610–562 (m)	Asymmetric NO_2 stretching Symmetric NO_2 stretching NO_2 deformation

TABLE 6.25 Raman Frequencies of Other Double Bonds (*continued*)

Group	Band, cm^{-1}	Remarks
Nitro compounds $\text{N}=\text{O}$ (<i>continued</i>)		
Nitroalkanes		
Primary	1 560–1 548 (m-s) 1 395–1 370 (s)	Sensitive to substituents attached to CNO_2 group
	915–898 (m-s) 894–873 (m-s) 618–609 (w) 640–615 (w) 494–472 (w-m)	
Secondary	1 553–1 547 (m) 1 375–1 360 (s) 908–868 (m) 863–847 (s) 625–613 (m)	Shoulder Broad; useful to distinguish from secondary nitroalkanes
Tertiary	560–516 (s) 1 543–1 533 (m) 1 355–1 345 (s)	Sharp band
Nitrogen oxides N^+O^-	1 612–1 602 (s) 1 252 (m) 1 049–1 017 (s) 835 (s) 541 (w) 469 (w)	

TABLE 6.26 Raman Frequencies of Aromatic Compounds*Abbreviations Used in the Table*

m, moderately strong	var, of variable strength
m-s, moderate to strong	vs, very strong
m-vs, moderate to very strong	w, weak
s, strong	w-m, weak to moderately strong
s-vs, strong to very strong	

Group	Band, cm^{-1}	Remarks
Common features		
Aromatic compounds	3 070–3 020 (s) 1 630–1 570 (m-s)	CH stretching C—C stretching
Substitution patterns of the benzene ring		
Monosubstituted	1 180–1 170 (w-m) 1 035–1 015 (s) 1 010–990 (vs) 630–605 (w)	Characteristic feature; found also with 1,3- and 1,3,5-substitutions
1,2-Disubstituted	1 230–1 215 (m) 1 060–1 020 (s) 740–715 (m)	Characteristic feature Lowered 60 cm^{-1} for halogen substituents
1,3-Disubstituted	1 010–990 (vs) 750–640 (s)	Characteristic feature
1,4-Disubstituted	1 230–1 200 (s-vs) 1 180–1 150 (m) 830–750 (vs) 650–630 (m-w)	Lower frequency with Cl substituents
Isolated hydrogen	1 379 (s-vs) 1 290–1 200 (s) 745–670 (m-vs) 580–480 (s)	Characteristic feature
1,2,3-Trisubstituted	1 100–1 050 (m) 670–500 (vs) 490–430 (w)	The lighter the mass of the substituent, the higher the frequency
1,2,4-Trisubstituted	750–650 (vs) 580–540 (var) 500–450 (var)	Lighter mass at higher frequencies

TABLE 6.26 Raman Frequencies of Aromatic Compounds (*continued*)

Group	Band, cm^{-1}	Remarks
Substitution patterns of the benzene ring (<i>continued</i>)		
1,3,5-Trisubstituted	1 010–990 (vs)	
Completely substituted	1 296 (s) 550 (vs) 450 (m) 361 (m)	
Other aromatic compounds		
Naphthalenes	1 390–1 370 1 026–1 012 767–762 535–512 519–512	Ring breathing α or β substituents β substituents α substituents β substituents
Disubstituted naphthalenes	773–737 (s) 726–705 (s) 690–634 (s) 608 575–569 544–537	1,2-; 1,3-; 2,3-; 2,6-; 2,7- 1,3-; 1,4-(two bands); 1,6-; 1,7- (two bands) 1,2-; 1,4-(two bands); 1,5-; 1,8- (two bands) 1,3- 1,2-; 1,3-; 1,6- 1,2-; 1,7-; 1,8-
Anthracenes	1 415–1 385	Ring breathing

TABLE 6.27 Raman Frequencies of Sulfur Compounds*Abbreviations Used in the Table*

m, moderately strong

m-s, moderate to strong

s, strong

s-vs, strong to very strong

vs, very strong

w-m, weak to moderately strong

Group	Band, cm^{-1}	Remarks
—S—H	2 590–2 560 (s)	SH stretching for both aliphatic and aromatic
>C=S	1 065–1 050 (m) 735–690 (vs)	Solid state
>S=O In $(\text{RO}_2)_2\text{SO}$ In $(\text{R}_2\text{N})_2\text{SO}$	1 209–1 198 1 108	One or two bands

TABLE 6.27 Raman Frequencies of Sulfur Compounds (*continued*)

Group	Band, cm ⁻¹	Remarks
>S=O (<i>continued</i>) In R ₂ SO SOF ₂ SOCl ₂ SOBr ₂	1 070–1 010 (w-m) 1 308 1 233 1 121	Broad
—SO ₂ —	1 330–1 260 (m-s) 1 155–1 110 (s) 610–540 (m) 512–485 (m)	Asymmetric SO ₂ stretching Symmetric SO ₂ stretching Scissoring mode of aryls Scissoring mode of alkyls
—SO ₂ —N<	ca 1 322 (m) 1 163–1 138 (s) 524–510 (s)	Asymmetric SO ₂ stretching Symmetric SO ₂ stretching Scissoring mode
—SO ₂ —O	1 363–1 338 (w-m) 1 192–1 165 (vs) 589–517 (w-m)	SO ₂ stretching. Aryl substituents occur at higher range. Scissoring (two bands). Aryl substituents occur at higher range of frequencies.
—SO ₂ —S—	1 334–1 305 (m-s) 1 128–1 126 (s) 559–553 (m-s)	
X—SO ₂ —X	1 412–1 361 (w-m) (F) (Cl) 1 263–1 168 (s) (F) (Cl) 596–531 (s)	
—O—SO ₂ —O—	1 388–1 372 (s) 1 196–1 188 (vs)	
—O—C—S— $\quad \parallel$ $\quad \text{S}$	670–620 (vs) 480–450 (vs)	C=S stretching CS stretching
>C—SH	920 (m) 850–820 (m)	C—SH deformation of aryls
>C—S—	752 (vs), 731 (vs) 742–722 (m-s) 698 (w), 678 (s) 693–639 (s) 651–610 (s-vs) 589–585 (vs)	With vinyl group attached With CH ₃ attached With allyl group attached Ethyl or longer alkyl chain Isopropyl group attached <i>tert</i> -Butyl group attached

TABLE 6.27 Raman Frequencies of Sulfur Compounds (*continued*)

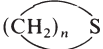
Group	Band, cm^{-1}	Remarks
$\equiv\text{C}-\text{S}-$ (<i>continued</i>)  $n = 2$ $n = 4$ $n = 5$	 1 112 688 659	
$\equiv\text{C}-(\text{S}-\text{S})_n-\text{C}\equiv$ Didi- <i>n</i> -alkyl disulfides Di- <i>tert</i> -butyl disulfide Trisulfides	715–620 (vs) 525–510 (vs) 576 (s) 543 (m) 510–480 (s)	Two bands; CS stretching Two bands; SS stretching CS stretching SS stretching SS stretching

TABLE 6.28 Raman Frequencies of Ethers*Abbreviations Used in the Table*

m, moderately strong

var, of variable strength

s, strong

vs, very strong

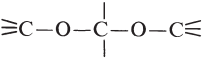
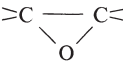
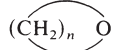
Group	Band, cm^{-1}	Remarks
$\equiv\text{C}-\text{O}-\text{C}\equiv$ Aliphatic	1 200–1 070 (m) 930–830 (s) 800–700 (s)	Asymmetrical COC stretching. Symmetrical substitution gives higher frequencies Symmetrical COC stretching Branching at α carbon gives higher frequencies.
Aromatic	550–400 1 310–1 210 (m) 1 050–1 010 (m)	
	1 145–1 129 (m) 900–800 (vs) 537–370 (s) 396–295	
	1 280–1 240 (s)	Ring breathing
$-\text{O}-\text{O}-$	800–770 (var)	
 $n = 3$ $n = 4$ $n = 5$	1 040–1 010 (s) 920–900 (s) 820–800 (s)	

TABLE 6.29 Raman Frequencies of Halogen Compounds*Abbreviations Used in the Table*

m-s, moderate to strong
s, strong

var, of variable strength
vs, very strong

Group	Band, cm^{-1}	Remarks
C—F	1400–870	Correlations of limited applicability because of vibrational coupling with stretching
C—Cl Primary Secondary Tertiary	350–290 (s) 660–650 (vs) 760–605 (s) 620–540 (var)	CCl bending; general May be one to four bands May be one to three bands
=C—Cl	844–564 438–396 381–170	
=CCl ₂	601–441 300–235	
C—Br	690–490 (s) 305–258 (m-s)	Often several bands; primary at higher range of frequencies. Tertiary has very strong band at ca 520 cm^{-1} .
=C—Br	745–565 356–318 240–115	
=CBr ₂	467–265 185–145	
C—I	663–595 309 154–85	
=C—I	ca 180	Solid state
=CI ₂	ca 265 ca 105	Solid state Solid state

TABLE 6.30 Raman Frequencies of Miscellaneous Compounds*Abbreviations Used in the Table*

m, moderately strong

vs, very strong

s, strong

vvs, very very strong

Group	Band, cm^{-1}	Remarks
C—As	570–550 (vs) 240–220 (vs)	CAs stretching CAsC deformation
C—Pb	480–420 (s)	CPb stretching
C—Hg	570–510 (vvs)	CHg stretching
C—Si	1300–1200 (s)	CSi stretching
C—Sn	600–450 (s)	CSn stretching
P—H	2350–2240 (m)	PH stretching
Heterocyclic rings		
Trimethylene oxide	1029	2-Substituted
Trimethylene imine	1026	
Tetrahydrofuran	914	
Pyrrolidine	899	
1,3-Dioxolane	939	
1,4-Dioxane	834	
Piperidine	815	
Tetrahydropyran	818	
Morpholine	832	
Piperazine	836	
Furan	1515–1460 1140	
Pyrazole	1040–990	
Pyrrole	1420–1360 (vs) 1144	
Thiophene	1410 (s) 1365 (s) 1085 (vs) 1035 (s) 832 (vs) 610 (s)	
Pyridine	1030 (vs) 990 (vs)	

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Nuclear Magnetic Resonance (NMR) Spectroscopy is by far the most widely used analytical technique in the modern organic chemistry lab. Numerous monographs have been written on this subject. It would be impossible to cover all of the significant points here. The reader who is interested in knowing what the proton (^1H) or carbon (^{13}C) spectrum of a particular compound is directed to the Aldrich Library of NMR Spectra or the Sadtler Library.

A number of resources are also available online. These include software for the prediction and analysis of spectral data and databases. Resources include:

Proton NMR basics:

<http://jchemed.chem.wisc.edu/JCESoft/Programs/PNMRB/>

NMR database:

www.acornnmr.com/database.htm

NMR prediction:

www.acdlabs.com/products/spec_lab/predict_nmr/

NMR library:

www.acdlabs.com/products/spec_lab/exp_spectra/spec_libraries/aldrich.html

NMR Periodic Table for half-integer quadrupole spins:

www.pascal-man.com/periodic-table/periodictable.html

Nuclear Magnetic Resonance

Table 6.31 presents the nuclear properties of the elements. Hydrogen (^1H) is an almost ideal nucleus for NMR spectroscopy. First, its natural abundance is high so most of the nuclei present in the sample will be detected in the NMR experiment. Second, its sensitivity is high meaning that its signal is readily detected. The nuclei that have been most generally used in organic chemistry are ^1H and ^{13}C although the natural abundance of the latter is low. Advances in instruments have made the acquisition of ^{13}C -NMR spectra routine. Several other nuclei have high natural abundance and occur frequently in organic compounds. These include ^7Li , ^{11}B , ^{14}N , ^{19}F , ^{23}Na , and ^{35}Cl , which are shown in bold type in Table 6.31. Modern NMR spectrometers permit the acquisition of NMR spectra from many nuclei depending on the probe. The most favorable nuclei are those that have spin $1/2$, high natural abundance, high sensitivity, and no quadrupole moment. Of course, the importance of the problem under study will ultimately dictate whether the investigator will invest the time and effort to obtain the spectrum when the experiment is difficult.

Table 6.31 Nuclear properties of the elements

In the following table the magnetic moment μ is in multiples of the nuclear magneton μ_N ($eh/4\pi Mc$) with diamagnetic correction, the spin I is in multiples of $h/2\pi$, and the electric quadrupole moment Q is in multiples of 10^{-28} square meters. Nuclei with spin $\frac{1}{2}$ have no quadrupole moment. The sign of μ and Q is uncertain for those nuclides for which no sign is given. Sensitivity is for equal number of nuclei at constant field. NMR frequency at any magnetic field is the entry for column 5 multiplied by the value of the magnetic field in kilogauss. For example, in a magnetic field of 14.0924 kG, protons (^1H) will precess at a frequency of $4.25760 \times 14.0924 \text{ kG} = 60.000 \text{ MHz}$. In a magnetic field of 23.4924 kG, protons will precess at $4.25760 \times 23.4924 \text{ kG} = 100.00 \text{ MHz}$.

TABLE 6.31 Nuclear Properties of the Elements

Nuclide	Natural abundance, %	Spin <i>I</i>	Sensitivity at constant field relative to ¹ H	NMR frequency for a 1000 G field, MHz	Magnetic moment μ/μ_N , J·T ⁻¹	Electric quadrupole moment <i>Q</i> , 10 ⁻²⁸ m ²
¹ n	—	—1/2	0.322	2.916 70	—1.913 12	—
¹ H	99.985	1/2	1.000	4.257 60	+2.792 78	—
² H	0.015	1	0.009 64	0.653 57	+0.857 42	+0.002 8
³ H	—	1/2	1.21	4.541 31	+2.978 9	—
³ He	0.000 13	—1/2	0.443	3.243 38	—2.127 6	—
⁶ Li	7.42	1	0.008 51	0.626 55	+0.822 03	—0.000 8
⁷ Li	92.58	3/2	0.294	1.654 65	+3.256 36	—0.04
⁹ Be	100	—3/2	0.013 9	0.598 27	—1.177 45	0.05
¹⁰ B	19.7	3	0.019 9	0.457 4	+1.800 6	+0.111
¹¹ B	80.3	3/2	0.165	1.365 95	+2.688 5	+0.041
¹³ C	1.108	1/2	0.015 9	1.070 54	+0.702 4	—
¹⁴ N	99.635	1	0.001 01	0.307 6	+0.403 75	+0.01
¹⁵ N	0.365	—1/2	0.001 04	0.431 5	—0.283 1	—
¹⁷ O	0.037	—5/2	0.029 1	0.577 39	—1.893 7	—0.004
¹⁹ F	100	1/2	0.834	4.005 43	+2.628 8	—
²¹ Ne	0.257	—3/2	0.027 2	0.336 11	—0.661 76	+0.09
²² Na	—	3	0.018 1	0.443 4	1.746	—
²³ Na	100	3/2	100	1.126 21	+2.217 40	+0.10
²⁴ Na	—	4	0.001 15	0.322	1.690	—
²⁵ Mg	10.11	—5/2	0.026 8	0.260 6	—0.855 4	+0.22
²⁷ Al	100	5/2	0.207	1.109 40	+3.641 3	+0.15
²⁹ Si	4.71	—1/2	0.078 5	0.845 8	—0.555 26	—
³¹ P	100	1/2	0.066 4	1.723 8	+1.131 7	—
³³ S	0.76	3/2	0.002 26	0.326 6	+0.643 5	—0.055
³⁵ S	—	3/2	0.008 50	0.508	—	+0.038
³⁵ Cl	75.53	3/2	0.004 71	0.417 1	+0.821 81	—0.080
³⁶ Cl	—	2	0.012 1	0.489 3	+1.285 3	—0.10
³⁷ Cl	24.47	3/2	0.002 72	0.347 2	+0.684 07	—0.006 2
³⁹ K	93.22	3/2	0.000 508	0.198 64	+0.391 43	+0.049
⁴⁰ K	0.011 8	4	0.005 21	0.247 0	—1.298 1	—0.061
⁴¹ K	6.77	3/2	0.000 083 9	0.109 03	+0.214 9	+0.060
⁴³ Ca	0.145	7/2	0.063 9	0.286 54	—1.317 2	—
⁴⁵ Sc	100	7/2	0.301	1.034 34	+4.755 9	—0.22
⁴⁷ Ti	7.32	—5/2	0.002 10	0.239 97	—0.788 46	+0.29
⁴⁹ Ti	5.46	—7/2	0.003 76	0.240 04	—1.104 14	+0.24
⁵⁰ V	0.25	6	0.055 3	0.424 3	+3.347 0	0.06
⁵¹ V	99.75	7/2	0.383	1.119 22	+5.148 5	—0.05
⁵³ Cr	9.55	3/2	0.000 10	0.240 63	—0.473 5	+0.03
⁵⁵ Mn	100	5/2	0.178	1.055 42	+3.449	+0.4
⁵⁷ Fe	2.17	1/2	0.000 033 3	0.138	+0.090 42	—
⁵⁹ Co	100	7/2	0.281	1.007 2	+4.616	+0.38
⁶¹ Ni	1.25	3/2	0.003 50	0.380 48	—0.749 8	+0.16
⁶³ Cu	69.1	3/2	0.093 8	1.128 5	+2.222 8	—0.211
⁶⁵ Cu	30.9	3/2	0.116	1.209 0	+2.381 2	—0.195
⁶⁷ Zn	4.11	5/2	0.002 86	0.266 3	+0.875 24	+0.16
⁶⁹ Ga	60.2	3/2	0.069 3	1.021 88	+2.014 5	+0.19

TABLE 6.31 Nuclear Properties of the Elements 9 (continued)

Nuclide	Natural abundance, %	Spin <i>I</i>	Sensitivity at constant field relative to ¹ H	NMR frequency for a 1000G field, MHz	Magnetic moment μ/μ_N , J·T ⁻¹	Electric quadrupole moment <i>Q</i> , 10 ⁻²⁸ m ²
⁷¹ Ga	39.8	3/2	0.142	1.29840	+2.5597	+0.12
⁷⁵ As	100	3/2	0.0251	0.7292	+1.439	+0.29
⁷⁷ Se	7.58	1/2	0.00697	0.8118	+0.534	—
⁷⁹ Br	50.52	3/2	0.0786	1.0669	+2.1055	+0.37
⁸¹ Br	49.48	3/2	0.0984	1.1498	+2.2696	+0.31
⁸⁷ Rb	27.85	3/2	0.177	1.2923	+2.7500	+0.13
⁹³ Nb	100	9/2	0.482	1.04048	+6.167	-0.22
¹¹³ In	4.23	-1/2	0.345	0.9312	-0.6225	—
¹¹⁹ Sn	8.58	-1/2	0.0518	1.5868	-1.0461	—
¹²¹ Sb	57.25	5/2	0.160	1.0192	+3.3592	-0.28
¹²³ Sb	42.75	7/2	0.0457	0.5519	+2.5466	-0.36
¹²⁵ Te	6.99	-1/2	0.0316	1.3453	-0.8872	—
¹²⁷ I	100	5/2	0.0935	0.8517	+2.8091	-0.79
¹²⁹ Xe	26.44	-1/2	0.0212	1.17779	-0.7768	—
¹⁹⁵ Pt	33.8	1/2	0.00994	0.91523	+0.6022	—
¹⁹⁹ Hg	16.84	1/2	0.00572	0.7612	+0.50415	—
²⁰³ Tl	29.50	1/2	0.187	2.4332	+1.6115	—
²⁰⁷ Pb	21.7	1/2	0.00913	0.8898	10.5783	—

Chemical Shifts

In essence, the chemical shift of a nucleus such as proton (¹H) is its resonance frequency. It is usually expressed in parts per million (ppm) relative to a standard. The most common standard is tetramethylsilane [(CH₃)₄Si, TMS] which defines 0 on the delta (δ) scale and 10 on the older, less used τ scale. A small amount of TMS is typically added to the NMR solution to be examined. The presence of an internal standard minimizes experimental variations. This is particularly important because the chemical shift is typically a change of only a few hertz per megahertz, hence the part per million (ppm) scale. The separation of peaks will be greater in hertz at higher field but spectra obtained at different field strengths are comparable on the ppm scale. Common reference standards are listed in Table 6.32.

TABLE 6.32 Proton Chemical Shifts of Reference Compounds Relative to Tetramethylsilane

Compound	Chemical shift δ, ppm*	Solvent(s)
Tetramethylsilane, (CH ₃) ₄ Si	0.0	CDCl ₃ , CCl ₄
3-(Trimethylsilyl)-1-propanesulfonic acid, sodium salt (DSS), (CH ₃) ₃ SiCH ₂ CH ₂ COONa	0.0	D ₂ O
Sodium acetate	1.90	D ₂ O
1,2-Dibromoethane	3.63	CDCl ₃

TABLE 6.32 Proton Chemical Shifts of Reference Compounds
Relative to Tetramethylsilane (*continued*)

Compound	Chemical shift δ , ppm*	Solvent(s)
1,1,2,2-Tetrachloroethane, $\text{Cl}_2\text{HCCHCl}_2$	5.95	CDCl_3 , CCl_4
1,4-Benzoquinone	6.78	CDCl_3 , CCl_4
1,4-Dichlorobenzene	7.23	CCl_4
Chloroform, CHCl_3	7.27	CDCl_3 , CCl_4
Benzene	7.37	CDCl_3 , CCl_4
1,3,5-Trinitrobenzene	9.21	$\text{DMSO}-d_6^\dagger$ CDCl_3

*Shift relative to TMS, first entry in table; \dagger Dimethylsulfoxide- d_6

A typical solution prepared for NMR analysis rarely contains more than a few percent of solute. Thus, protons on the solvent could significantly distort the spectrum. When ^1H -NMR are desired, solvents having no protons (CS_2 or CCl_4) or deuterated solvents are used. Table 6.33 gives the common NMR solvents used. Although modern manufacturing methods typically produce NMR solvents having high isotopic purity, incomplete deuteration of a protonic solvent will result in a residual signal.

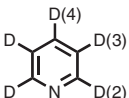
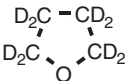
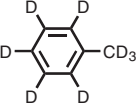
TABLE 6.33 Common NMR Solvents

Solvent	Detail	Group*	δ (ppm)
Acetic acid- d_4	$\text{D}_3\text{C}-\text{COOD}$	CD_2H OH	2.05 11.5 \dagger
Acetone- d_6	CD_3COCD_3	CD_2H	2.057
Acetonitrile- d_3	$\text{CD}_3\text{C}\equiv\text{N}$	CD_2H	1.95
Benzene- d_6	C_6D_6	$\text{C}-\text{H}$	6.78
<i>tert</i> -Butanol- d_1	$(\text{CH}_3)_3\text{COD}$	CD_2H	1.28
Chloroform- d_1	Cl_3CD	Cl_3CH	7.25
Cyclohexane- d_{12}	C_6D_{12}	CHD	1.40
Deuterium oxide	D_2O	HOD	4.7 \dagger
Dimethylformamide- d_7	$(\text{CD}_3)_2\text{N}-\text{CD}=\text{O}$	CD_2H $-\text{CH}=\text{O}$	2.75; 2.95 8.05
Dimethylsulfoxide- d_6 ($\text{DMSO}-d_6$)	CD_3SOCD_3	CD_2H	2.51
1,4-Dioxane- d_8	$\text{D}_2\text{C}-\overset{\text{O}}{\underset{ }{\text{C}}}-\text{CD}_2$	Absorbed H_2O	3.3 \dagger
	$\text{D}_2\text{C}-\overset{\text{O}}{\underset{ }{\text{C}}}-\text{CD}_2$	Methylene	3.55
Hexamethylphosphoramide- d_{18} , HMPA- d_{18} , HMPT- d_{18}	$(\text{D}_3\text{C})_2\text{N}-\overset{\text{O}}{\underset{\text{N}(\text{CD}_3)_2}{\underset{ }{\text{P}}}}-\text{N}(\text{CD}_3)_2$	Methyl	2.60
Methanol- d_4	CD_3OD	CD_2H	3.35
		OH	4.8 \dagger

*Impurity peak resulting from incomplete deuteration or exchange.

 \dagger These values may vary greatly depending on the solute and its concentration.

TABLE 6.33 Common NMR Solvents (continued)

Solvent	Detail	Group*	δ(ppm)
Dichloromethane- <i>d</i> ₂	Cl ₂ CD ₂	Cl ₂ CDH	5.35
Pyridine- <i>d</i> ₅		C-2—H	8.5
		C-3—H	7.0
		C-4—H	7.35
Tetrahydrofuran- <i>d</i> ₆		CD-2—H	3.58
		CD-3—H	1.73
Toluene- <i>d</i> ₈		CD ₂ H	2.3
		Ring CD	7.1
Trifluoroacetic acid- <i>d</i> ₁	F ₃ C—COOD	Hydroxyl	11.3†

*Impurity peak resulting from incomplete deuteration or exchange. †These values may vary greatly depending on the solute and its concentration.

TABLE 6.34 Proton Chemical Shifts

Values are given on the δ scale; τ = 10.00 − δ.

Abbreviations Used in the Table

R, alkyl group Ar, aryl group

Substituent group	Methyl protons	Methylene protons	Methine proton
HC—C—CH ₂	0.95	1.20	1.55
HC—C—NR ₂	1.05	1.45	1.70
HC—C—C=C	1.00	1.35	1.70
HC—C—C=O	1.05	1.55	1.95
HC—C—NRAr	1.10	1.50	1.80
HC—C—H(C=O)R	1.10	1.50	1.90
HC—C—(C=O)NR ₂	1.10	1.50	1.80
HC—C—(C=O)Ar	1.15	1.55	1.90
HC—C—(C=O)OR	1.15	1.70	1.90
HC—C—Ar	1.15	1.55	1.80
HC—C—OH	1.20	1.50	1.75
HC—C—OR	1.20	1.50	1.75
HC—C—C≡CR	1.20	1.50	1.80
HC—C—C≡N	1.25	1.65	2.00
HC—C—SR	1.25	1.60	1.90
HC—C—OAr	1.30	1.55	2.00
HC—C—O(C=O)R	1.30	1.60	1.80
HC—C—SH	1.30	1.60	1.65
HC—C—(S=O)R			
and HC—C—SO ₂ R	1.35	1.70	
HC—C—NR ₃ ⁺	1.40	1.75	2.05

TABLE 6.34 Proton Chemical Shifts (*continued*)

Substituent group	Methyl protons	Methylene protons	Methine proton
HC—C—O—N=O	1.40		
HC—C—O(C=O)CF ₃	1.40	1.65	
HC—C—Cl	1.55	1.80	1.95
HC—C—F	1.55	1.85	2.15
HC—C—NO ₂	1.60	2.05	2.50
HC—C—O(C=O)Ar	1.65	1.75	1.85
HC—C—I	1.75	1.80	2.10
HC—C—Br	1.80	1.85	1.90
HC—CH ₂	0.90	1.30	1.50
HC—C=C	1.60	2.05	
HC—C≡C	1.70	2.20	2.80
HC—(C=O)OR	2.00	2.25	2.50
HC—(C=O)NR ₂	2.00	2.25	2.40
HC—SR	2.05	2.55	3.00
HC—O—O	2.10	2.30	2.55
HC—(C=O)R	2.10	2.35	2.65
HC—C≡N	2.15	2.45	2.90
HC—I	2.15	3.15	4.25
HC—CHO	2.20	2.40	
HC—Ar	2.25	2.45	2.85
HC—NR ₂	2.25	2.40	2.80
HC—SSR	2.35	2.70	
HC—(C=O)Ar	2.40	2.70	3.40
HC—SAr	2.40		
HC—NR ₂ Ar	2.60	3.10	3.60
HC—SO ₂ R and HC—(SO)R	2.60	3.05	
HC—Br	2.70	3.40	4.10
HC—NR ₃ ⁺	2.95	3.10	3.60
HC—NH(C=O)R	2.95	3.35	3.85
HC—SO ₃ R	2.95		
HC—Cl	3.05	3.45	4.05
HC—OH and HC—OR	3.20	3.40	3.60
HC—PAr ₃	3.20	3.40	
HC—NH ₂	3.50	3.75	4.05
HC—O(C=O)R	3.65	4.10	4.95
HC—OAr	3.80	4.00	4.60
HC—O(C=O)Ar	3.80	4.20	5.05
HC—O(C=O)CF	3.95	4.30	
HC—F	4.25	4.50	4.80
HC—NO ₂	4.30	4.35	4.60
Cyclopropane		0.20	0.40
Cyclobutane		2.45	
Cyclopentane		1.65	
Cyclohexane		1.50	1.80
Cycloheptane		1.25	

TABLE 6.34 Proton Chemical Shifts (*continued*)

Substituent group	Proton shift	Substituent group	Proton shift
$\text{HC}\equiv\text{CH}$	2.35	$\text{HO}-\text{C}=\text{O}$	10–12
$\text{HC}\equiv\text{CAr}$	2.90	$\text{HO}-\text{SO}_2$	11–12
$\text{HC}\equiv\text{C}-\text{C}=\text{C}$	2.75	$\text{HO}-\text{Ar}$	4.5–6.5
HAr	7.20	$\text{HO}-\text{R}$	0.5–4.5
$\text{HCO}-\text{O}$	8.1	$\text{HS}-\text{Ar}$	2.8–3.6
$\text{HCO}-\text{R}$	9.4–10.0	$\text{HS}-\text{R}$	1–2
$\text{HCO}-\text{Ar}$	9.7–10.5	$\text{HN}-\text{Ar}$	3–6
$\text{HO}-\text{N}=\text{C}$ (oxime)	9–12	$\text{HN}-\text{R}$	0.5–5

Saturated heterocyclic ring systems

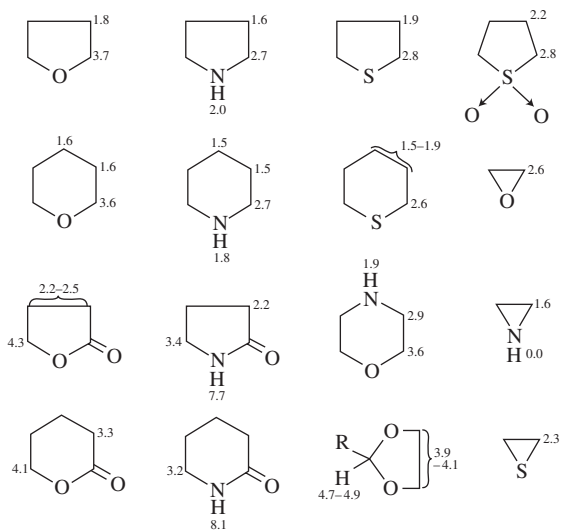


TABLE 6.34 Proton Chemical Shifts (*continued*)

Substituent group	Methyl protons	Methylene protons	Methine proton
Unsaturated cyclic systems			

TABLE 6.35 Estimation of Chemical Shift for Protons of $\text{—CH}_2\text{—}$ and >CH— Groups

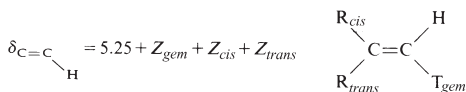
$$\delta_{\text{CH}_2} = 0.23 + C_1 + C_2 \quad \delta_{\text{CH}} = 0.23 + C_1 + C_2 + C_3$$

X*	C	X*	C	X*	C
—CH_3	0.5	—SR	1.6	—OR	2.4
—CF_3	1.1	$\text{—C}\equiv\text{C—Ar}$	1.7	—Cl	2.5
>C=C<	1.3	—CN	1.7	—OH	2.6
$\text{—C}\equiv\text{C—R}$	1.4	—CO—R	1.7	—N=C=S	2.9
—COOR	1.5	—I	1.8	—OCOR	3.1
—NR_2	1.6	—Ph	1.8	—OPh	3.2
—CONR_2	1.6	—Br	2.3		

*R, alkyl group; Ar, aryl group; Ph, phenyl group.

TABLE 6.36 Estimation of Chemical Shift of Proton Attached to a Double Bond

Positive Z values indicate a downfield shift, and an arrow indicates the point of attachment of the substituent group to the double bond.



R	Z_{gem} , ppm	Z_{cis} , ppm	Z_{trans} , ppm
→H	0	0	0
→alkyl	0.45	-0.22	-0.28
→alkyl—ring (5- or 6-member)	0.69	-0.25	-0.28
→CH ₂ O—	0.64	-0.01	-0.02
→CH ₂ S—	0.71	-0.13	-0.22
→CH ₂ X (X: F, Cl, Br)	0.70	0.11	-0.04
→CH ₂ N<	0.58	-0.10	-0.08
↘C=C (isolated)	1.00	-0.09	-0.23
↘C=C (conjugated)	1.24	0.02	-0.05
→C≡N	0.27	0.75	0.55
→C≡C—	0.47	0.38	0.12
↘C=O (isolated)	1.10	1.12	0.87
↘C=O (conjugated)	1.06	0.91	0.74
→COOH (isolated)	0.97	1.41	0.71
→COOH (conjugated)	0.80	0.98	0.32
→COOR (isolated)	0.80	1.18	0.55
→COOR (conjugated)	0.78	1.01	0.46
	1.02	0.95	1.17
	1.37	0.98	0.46
	1.11	1.46	1.01
→OR (R: aliphatic)	1.22	-1.07	-1.21
→OR (R: conjugated)	1.21	-0.60	-1.00
→OCOR	2.11	-0.35	-0.64
→CH ₂ —; →CH ₂ —C≡N	0.69	-0.08	-0.06
→CH ₂ —aromatic ring	1.05	-0.29	-0.32
→F	1.54	-0.40	-1.02
→Cl	1.08	0.18	0.13
→Br	1.07	0.45	0.55
→I	1.14	0.81	0.88
→N—R (R: aliphatic)	0.80	-1.26	-1.21

TABLE 6.36 Estimation of Chemical Shift of Proton Attached to a Double Bond (*continued*)

R	Z_{gem} , ppm	Z_{cis} , ppm	Z_{trans} , ppm
$\begin{array}{c} \\ \rightarrow \text{N}-\text{R} \text{ (R: conjugated)} \\ \end{array}$	1.17	-0.53	-0.99
$\begin{array}{c} \\ \rightarrow \text{N}-\text{C}=\text{O} \\ \end{array}$	2.08	-0.57	-0.72
$\rightarrow \text{aromatic}$	1.38	0.36	-0.07
$\rightarrow \text{CF}_3$	0.66	0.61	0.32
$\rightarrow \text{aromatic (o-substituted)}$	1.65	0.19	0.09
$\rightarrow \text{SR}$	1.11	-0.29	-0.13
$\rightarrow \text{SO}_2$	1.55	1.16	0.93

TABLE 6.37 Chemical Shifts in Monosubstituted Benzene

$$\delta = 7.27 + \Delta_i$$

Substituent	Δ_{ortho}	Δ_{meta}	Δ_{para}
NO ₂	0.94	0.18	0.39
CHO	0.58	0.20	0.26
COOH	0.80	0.16	0.25
COOCH ₃	0.71	0.08	0.20
COCl	0.82	0.21	0.35
CCl ₃	0.8	0.2	0.2
COCH ₃	0.62	0.10	0.25
CN	0.26	0.18	0.30
CONH ₂	0.65	0.20	0.22
$\overset{+}{\text{N}}\text{H}_3$	0.4	0.2	0.2
CH ₂ X*	0.0-0.1	0.0-0.1	0.0-0.1
CH ₃	-0.16	-0.09	-0.17
CH ₂ CH ₃	-0.15	-0.06	-0.18
CH(CH ₃) ₂	-0.14	-0.09	-0.18
C(CH ₃) ₂	-0.09	0.05	-0.23
F	-0.30	-0.02	-0.23
Cl	0.01	-0.06	-0.08
Br	0.19	-0.12	-0.05
I	0.39	-0.25	-0.02
NH ₂	-0.76	-0.25	-0.63
OCH ₃	-0.46	-0.10	-0.41
OH	-0.49	-0.13	-0.2
OCOR	-0.2	0.1	-0.2
NHCH ₃	-0.8	-0.3	-0.6
N(CH ₃) ₂	-0.60	-0.10	-0.62

*X = Cl, alkyl, OH, or NH₂.

TABLE 6.38 Proton Spin Coupling Constants

Structure	<i>J</i> , Hz	Structure	<i>J</i> , Hz
	12–15		<i>cis</i> (Z) 2 <i>trans</i> (E) 6 gem 4
$\text{CH}-\text{CH}$ (free rotation)	6–8		2–3 1.8 3–4 3.5 2–4 0–1 2–5 1–2
$>\text{CH}-\text{OH}$ (no exchange)	5		2–3 5–6 3–4 3.5–5.0 2–4 1.5 2–5 3.4
$>\text{CH}-\text{NH}$	4–8		<i>o</i> 6–12 <i>m</i> 4–8 <i>p</i> 1.5–2.5
$\text{CH}-\text{SH}$	6–8		<i>o</i> 2.5 <i>m</i> 1.5 <i>p</i> 0
	1–3		<i>a-a</i> 8–10 <i>a-e</i> 2–3 <i>e-e</i> 2–3
$-\text{N}=\text{C}-\text{H}$	8–16	Cyclopentane <i>cis</i> (Z)	4–6
	0–3	<i>trans</i> (E)	4–6
	6–14	Cyclobutane <i>cis</i> (Z)	8
	11–18	<i>trans</i> (E)	8
	0.5–3	Cyclopropane <i>cis</i> (Z)	9–11
	0.5–3	<i>trans</i> (E)	6–8
	4–10	gem	4–6
$>\text{C}=\text{CH}-\text{CH}=\text{C}<$	10–13		<i>o</i> 6–10 <i>m</i> 1–3 <i>p</i> 0–1
$=\text{CH}-\text{C}=\text{O}$	6		1–2 8–9 2–3 6
$-\text{CH}_2-\text{C}\equiv\text{C}-\text{CH}$	0–3		2–3 5–6 3–4 7–9 2–4 1–2 3–5 1–2 2–5 0–1 2–6 0–1
$>\text{CH}-\text{C}\equiv\text{CH}$	0–3		
	0–2		
	2–4		
	5–7		
	6–9		
	10–13		
	4–5		
	3		
	5–6		
	0		
	7		
	6		

TABLE 6.38 Proton Spin Coupling Constants (*continued*)

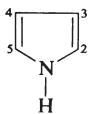
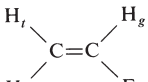

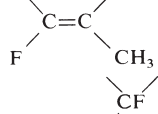
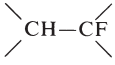

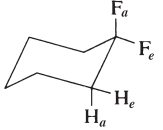
Structure	<i>J</i> , Hz	Structure	<i>J</i> , Hz
 1-2 1-3 2-3 3-4 2-4 2-5	2-3 2-3 2-3 3-4 1-2 1-3	 <i>gem</i> <i>cis (Z)</i> <i>trans (E)</i>	72-90 -3 to 20 12-40
 45-52		 2-4	
 <i>gauche</i> <i>trans (Z)</i>	0-12 10-45	 0-6	
		 <i>a-a</i> <i>a-e</i> <i>e-e</i>	21 34 12
			< 5-8

TABLE 6.39 Carbon-13 Chemical Shifts

Values given in ppm on the δ scale, relative to tetramethylsilane

Substituent group	Primary carbon	Secondary carbon	Tertiary carbon	Quaternary carbon
<i>Alkanes</i>				
C—C	5–30	25–45	23–58	28–50
C—O	45–60	42–71	62–78	73–86
C—N	13–45	44–58	50–70	60–75
C—S	10–30	22–42	55–67	53–62
C—halide (I to Cl)	3–25	3–40	34–58	35–75
Substituent group	δ , ppm	Substituent group	δ , ppm	
Cyclopropane	–5–5	Alcohols R—OH	45–87	
Cycloalkane C ₄ –C ₁₀	5–25	Ethers R—O—R	57–87	
Mercaptanes	5–70	Nitro R—NO ₂	60–78	
Amines		Alkynes		
R ₂ N—C	20–70	HC≡CR	63–73	
Aryl—N	128–138	RC≡CR	72–95	
Sulfoxides, sulfones	35–55	Acetals, ketals	88–112	
Thiocyanates R—SCN	96–118	Esters		
Alkenes		Saturated	158–165	
H ₂ C=	100–122	α,β -Unsaturated	165–176	
R ₂ C=	110–150	Isocyanides R—NC	162–175	

TABLE 6.39 Carbon-13 Chemical Shifts (*continued*)

Substituent group	δ , ppm	Substituent group	δ , ppm
Heteroaromatics		Carboxylic acids	
C \equiv N	100–152	Nonconjugated	162–165
C $_{\alpha}$	142–160	Conjugated	165–184
Cyanates R—OCN	105–120	Salts (anion)	175–195
Isocyanates R—NCO	115–135	Ketones	
Isothiocyanates R—NCS	115–142	α -Halo	160–200
Nitriles, cyanides	117–124	Nonconjugated	192–202
Aromatics		α,β -Unsaturated	202–220
Aryl-C	125–145	Imides	165–180
Aryl-P	119–128	Acyl chlorides R—CO—Cl	165–183
Aryl-N	128–138	Thioureas	165–185
Aryl-O	133–152	Aldehydes	
Azomethines	145–162	α -Halo	170–190
Carbonates	159–162	Nonconjugated	182–192
Ureas	150–170	Conjugated	192–208
Anhydrides	150–175	Thioketones R—CS—R	190–202
Amides	154–178	Carbonyl M(CO) $_n$	190–218
Oximes	155–165	Allenes =C=	197–205

Saturated heterocyclic ring systems

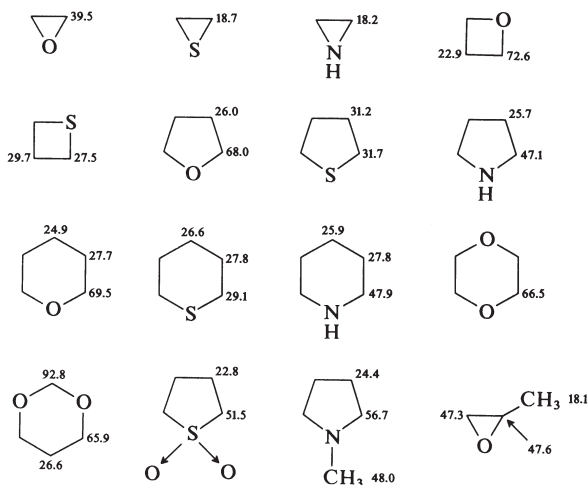
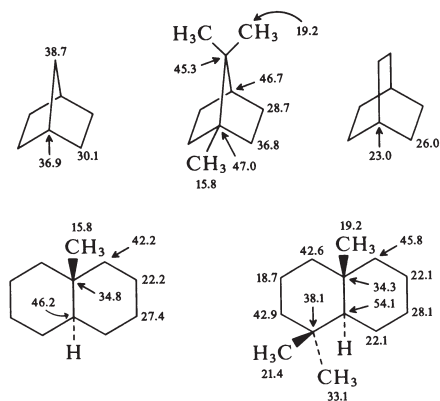


TABLE 6.39 Carbon-13 Chemical Shifts (*continued*)

Unsaturated cyclic systems

TABLE 6.39 Carbon-13 Chemical Shifts (*continued*)

Saturated alicyclic ring systems

**TABLE 6.40** Estimation of Chemical Shifts of Alkane Carbons*Relative to tetramethylsilane*

Positive terms indicate a downfield shift.

$$\delta_C = -2.6 + 9.1n_\alpha + 9.4n_\beta - 2.5n_\gamma + 0.3n_\delta + 0.1n_\epsilon \text{ (plus any correction factors)}$$

where n_α is the number of carbons bonded directly to the i th carbon atom and n_β , n_γ , n_δ , and n_ϵ are the number of carbon atoms two, three, four, and five bonds removed. The constant is the chemical shift for methane.

Chain branching*	Correction factor	Chain branching*	Correction factor
1°(3°)	-1.1	4°(1°)	-1.5
1°(4°)	-3.4	2°(4°)	-7.2
2°(3°)	-2.5	3°(3°)	-9.5
3°(2°)	-3.7	4°(2°)	-8.4

*1° signifies a CH_3- group; 2°, a $-\text{CH}_2-$ group; 3°, a $>\text{CH}-$ group; and 4°, a $>\text{C}<$ group. 1°(3°) signifies a methyl group bound to a $>\text{CH}-$ group, and so on.

Examples: For 3-methylpentane, $\text{CH}_3-\text{CH}_2-\text{CH}(\text{CH}_3)-\text{CH}_2-\text{CH}_3$,

$$\delta_{C=2} = -2.6 + 9.1(2) + 9.4(2) - 2.5 - 1(1)[2^\circ(3^\circ)] = 29.4$$

$$\delta_{C=3} = -2.6 + 9.1(3) + 9.4(2) + (2)[3^\circ(2^\circ)] = 36.2$$

TABLE 6.41 Effect of Substituent Groups on Alkyl Chemical Shifts

These increments are added to the shift value of the appropriate carbon atom as calculated from Table 6.40.



Substituent group Y*	α carbon		β carbon		γ carbon
	Straight	Branched	Straight	Branched	
—CO—OH	20.9	16	2.5	2	−2.2
—COO [−] (anion)	24.4	20	4.1	3	−1.6
—CO—OR	20.5	17	2.5	2	−2
—CO—Cl	33	28		2	
—CO—NH ₂	22	2.5			−0.5
—CHO	31		0		−2
—CO—R	30	24	1	1	−2
—OH	48.3	40.8	10.2	7.7	−5.8
—OR	58	51	8	5	−4
—O—CO—NH ₂	51		8		
—O—CO—R	51	45	6	5	−3
—C—CO—Ar	53				
—F	68	63	9	6	−4
—Cl	31.2	32	10.5	10	−4.6
—Br	20.0	25	10.6	10	−3.1
—I	−8	4	11.3	12	−1.0
—NH ₂	29.3	24	11.3	10	−4.6
—NH ₃ ⁺	26	24	8	6	−5
—NHR	36.9	31	8.3	6	−3.5
—NR ₂	42		6		−3
—NR ₃ ⁺	31		5		−7
—NO ₂	63	57	4	4	
—CN	4	1	3	3	−3
—SH	11	11	12	11	−6
—SR	20		7		−3
—CH=CH ₂	20		6		−0.5
—C ₆ H ₅	23	17	9	7	−2
—C≡CH	4.5		5.5		−3.5

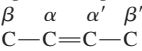
*R, alkyl group; Ar, aryl group.

TABLE 6.42 Estimation of Chemical Shift of Carbon Attached to a Double Bond

The olefinic carbon chemical shift is calculated from the equation

$$\delta_c = 123.3 + 10.6n_\alpha + 7.2n_\beta - 7.9n_{\alpha'} - 1.8n_{\beta'} \text{ (plus any steric correction terms)}$$

where n is the number of carbon atoms at the particular position, namely,



Substituents on both sides of the double bond are considered separately. Additional vinyl carbons are treated as if they were alkyl carbons. The method is applicable to alicyclic alkenes; in small rings carbons are counted twice, that is, from both sides of the double bond where applicable. The constant in the equation is the chemical shift for ethylene. The effect of other substituent groups is tabulated below.

Substituent group	β	α	α'	β'
—OR	2	29	−39	−1
—OH	6			−1
—O—CO—CH ₃	−3	18	−27	4
—CO—CH ₃		15	6	
—CHO		13.6	13.2	
—CO—OH		5.2	9.1	
—CO—OR		6	7	
—CN		−15.4	14.3	
—F		24.9	−34.3	
—Cl	−1	3.3	−5.4	2
—Br	0	−7.2	−0.7	2
—I		−37.4	7.7	
—C ₆ H ₅		12	−11	

Substituent pair		Steric correction term
α, α'	<i>trans</i> (E)	0
α, α'	<i>cis</i> (Z)	−1.1
α, α	<i>gem</i>	−4.8
α', α'		+2.5
β, β		+2.3

TABLE 6.43 Carbon-13 Chemical Shifts in Substituted Benzenes

$$\delta_{\text{C}} = 128.5 + \Delta$$

Substituent group	$\Delta_{\text{C}-1}$	Δ_{ortho}	Δ_{meta}	Δ_{para}
—CH ₃	9.3	0.8	−0.1	−2.9
—CH ₂ CH ₃	15.6	−0.4	0	−2.6
—CH(CH ₃) ₂	20.2	−2.5	0.1	−2.4
—C(CH ₃) ₃	22.4	−3.1	−0.1	−2.9
—CH ₂ O—CO—CH ₃	7.7	0	0	0
—C ₆ H ₅	13.1	−1.1	0.4	−1.2
—CH=CH ₂	9.5	−2.0	0.2	−0.5
—C≡CH	−6.1	3.8	0.4	−0.2
—CH ₂ OH	12.3	−1.4	−1.4	−1.4
—CO—OH	2.1	1.5	0	5.1
—COO [−] (anion)	8	1	0	3
—CO—OCH ₃	2.1	1.1	0.1	4.5
—CO—CH ₃	9.1	0.1	0	4.2
—CHO	8.6	1.3	0.6	5.5
—CO—Cl	4.6	2.4	1	6.2
—CO—CF ₃	−5.6	1.8	0.7	6.7
—CO—C ₆ H ₅	9.4	1.7	−0.2	3.6
—CN	−15.4	3.6	0.6	3.9
—OH	26.9	−12.7	1.4	−7.3
—OCH ₃	31.4	−14.0	1.0	−7.7
—OC ₆ H ₅	29.2	−9.4	1.6	−5.1
—O—CO—CH ₃	23.0	−6.4	1.3	−2.3
—NH ₂	18.0	−13.3	0.9	−9.8
—N(CH ₃) ₂	22.4	−15.7	0.8	−11.5
—N(C ₆ H ₅) ₂	19	−4	1	−6
—NHC ₆ H ₅	14.6	−10.7	0.7	−7.7
—NH—CO—CH ₃	11.1	−9.9	0.2	−5.6
—NO ₂	20.0	−4.8	0.9	5.8
—F	34.8	−12.9	1.4	−4.5
—Cl	6.2	0.4	1.3	−1.9
—Br	−5.5	3.4	1.7	−1.6
—I	−32.2	9.9	2.6	−1.4
—CF ₃	−9.0	−2.2	0.3	3.2
—NCO	5.7	−3.6	1.2	−2.8
—SH	2.3	1.1	1.1	−3.1
—SCH ₃	10.2	−1.8	0.4	−3.6
—SO ₂ —NH ₂	15.3	−2.9	0.4	3.3
—Si(CH ₃) ₃	13.4	4.4	−1.1	−1.1

TABLE 6.44 Carbon-13 Chemical Shifts in Substituted Pyridines*

$$\delta_c(k) = C_k + \Delta_i$$

Substituent group	$C_2 = C_6 = 149.6$ Δ_{C-2} or Δ_{C-6}	Δ_{23}	Δ_{24}	Δ_{25}	Δ_{26}
—CH ₃	9.1	-1.0	-0.1	-3.4	-0.1
—CH ₂ CH ₃	14.0	-2.1	0.1	-3.1	0.2
—CO—CH ₃	4.3	-2.8	0.7	3.0	-0.2
—CHO	3.5	-2.6	1.3	4.1	0.7
—OH	14.9	-17.2	0.4	-3.1	-6.8
—OCH ₃	15.3	-13.1	2.1	-7.5	-2.2
—NH ₂	11.3	-14.7	2.3	10.6	-0.9
—NO ₂	8.0	-5.1	5.5	6.6	0.4
—CN	-15.8	5.0	-1.7	3.6	1.9
—F	14.4	-14.7	5.1	-2.7	-1.7
—Cl	2.3	0.7	3.3	-1.2	0.6
—Br	-6.7	4.8	3.3	-0.5	1.4

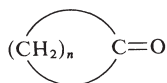
Substituent group	Δ_{32}	$C_3 = C_5 = 124.2$ Δ_{C-3} or Δ_{C-5}	Δ_{34}	Δ_{35}	
—CH ₃	1.3	9.0	0.2	-0.8	-2.3
—CH ₂ CH ₃	0.3	15.0	-1.5	-0.3	-1.8
—CO—CH ₃	0.5	-0.3	-3.7	-2.7	4.2
—CHO	2.4	7.9	0	0.6	5.4
—OH	-10.7	31.4	-12.2	1.3	-8.6
—NH ₂	-11.9	21.5	-14.2	0.9	-10.8
—CN	3.6	-13.7	4.4	0.6	4.2
—Cl	-0.3	8.2	-0.2	0.7	-1.4
—Br	2.1	-2.6	2.9	1.2	-0.9
—I	7.1	-28.4	9.1	2.4	0.3

Substituent group	$\Delta_{42} = \Delta_{46}$	$\Delta_{43} = \Delta_{45}$	$C_4 = 136.2$ Δ_{C-4}
—CH ₃	0.5	0.8	10.8
—CH ₂ CH ₃	0	-0.3	15.9
—CH=CH ₂	0.3	-2.9	8.6
—CO—CH ₃	1.6	-2.6	6.8
—CHO	1.7	-0.6	5.5
—NH ₂	0.9	-13.8	19.6
—CN	2.1	2.2	-15.7
—Br	3.0	3.4	-3.0

*May be used for disubstituted, polyheterocyclic, and polynuclear systems if deviations due to steric and mesomeric effects are allowed for.

TABLE 6.45 Carbon-13 Chemical Shifts of Carbonyl Group

X	Y	δ_{C}	X	Y	δ_{C}
H—	—CH ₃	199.7	CH ₃ —	—CH=CH ₂	196.9
H—	—CCl ₃	175.3	CH ₃ —	—C ₆ H ₅	197.6
H—	—NH ₂	165.5	CH ₃ —	—CH ₂ —CO—CH ₃	201.9
				(keto)	
H—	—N(CH ₃) ₂	162.4			191.4
				(enol)	
H—	2-Furyl	153.3	CH ₃ —	—CH ₂ CHO	167.7
H—	2-Pyrrolyl	134.0	CH ₃ —	—C ₆ H ₅ —CH ₃	196 (<i>m, p</i>)
H—	2-Thienyl	143.3			199 (<i>o</i>)
(CH ₃) ₂ CH—	—OH	184.8	CH ₃ —	—2,6-(CH ₃) ₂ C ₆ H ₃	206
C ₆ H ₅ —	—OH	172.6	CH ₃ —	—OH	178
CF ₃ —	—OH	163.0	CH ₃ —	—O [−] (anion)	181.5
CCl ₃ —	—OH	168.0	CH ₃ —	—OCH ₃	170.7
CH ₃ CH(NH ₂)—	—OH	176.5	CH ₃ —	—O—CH=CH ₂	167.7
CF ₃ —	—OCH ₂ CH ₃	158.1	CH ₃ —	—O—CH(CH ₃) ₂	170.3
H ₂ N—	—OCH ₂ CH ₃	157.8	CH ₃ —	—O—CO—CH ₃	167.3
2-Furyl	—OCH ₃	159.1	CH ₃ —	—NH ₂	172.7
(CH ₃) ₂ N—	—C ₆ H ₅	170.8	CH ₃ —	—NHCH ₃	172
CH ₂ =CHCH ₂ O—			CH ₃ —	—N(CH ₃) ₂	169.5
CO—	—OCH ₂ CH=CH ₂	157.6	CH ₃ —	—Cl	169.6
CH ₃ CH ₂ —	—CH ₂ CH ₃	211.4	CH ₃ —	—Br	165.6
CH ₃ —CH ₂ —	—O—CO—CH ₂ CH ₃	170.3	CH ₃ —	—I	158.9
CH ₃ —	—CH ₃	205.8			
CH ₃ —	—CH ₂ CH ₃	207			



n	δ_{C}
3	207.9
4	218.2
5	211.3
6	211.4
7	216.0

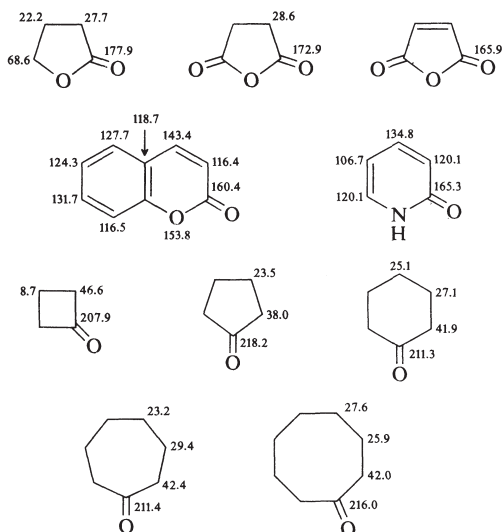


TABLE 6.46 One-Bond Carbon–Hydrogen Spin Coupling Constants

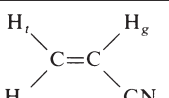
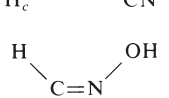
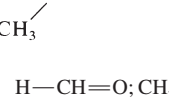
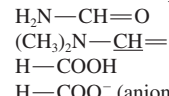
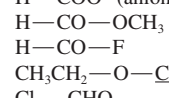
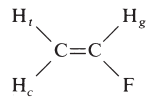
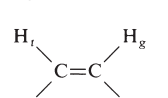
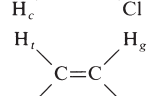


Structure	J_{CH} , Hz	Structure	J_{CH} , Hz
H—CH ₃	125.0	 <i>gem</i>	177
H—CH ₂ CH ₃	124.9	 <i>cis (Z)</i>	163
CH ₃ —CH ₂ —CH ₃	119.2	 <i>trans (E)</i>	165
H—C(CH ₃) ₂	114.2	 <i>cis (Z)</i>	163
H—CH ₂ CH ₂ OH	126.9	 <i>trans (E)</i>	177
H—CH ₂ CH=CH ₂	122.4		
H—CH ₂ C ₆ H ₅	129.4	H—CH=O; CH ₃ —CH=O	172
H—CH ₂ C≡CH	132.0	H ₂ N—CH=O	188.3
H—CH ₂ CN	136.1	(CH ₃) ₂ N—CH=O	191
H—CH(CN) ₂	145.2	H—COOH	222
H—CH ₂ —halogen	149–152	H—COO [−] (anion)	195
H—CHF ₂	184.5	H—CO—OCH ₃	226
H—CHCl ₂	178.0	H—CO—F	267
H—CH ₂ NH ₂	133.0	CH ₃ CH ₂ —O—CHO	225.6
H—CH ₂ NH ₃ ⁺	145.0	Cl ₃ —CHO	207
H—CH ₂ OH (or H—CH ₂ OR)	140–141	H—C≡CH	249
H—CH(OR) ₂	161–162	H—C≡CCH ₃	248
H—C(OR) ₃	186	H—C≡CC ₆ H ₅	251
H—C(OH)R ₂	143	H—C≡CCH ₂ OH	241
H—CH ₂ NO ₂	146.0	H—CN	269
H—CH(NO ₂) ₂	169.4	Cyclopropane	161
H—CH ₂ COOH	130.0	Cyclobutane	136
H—CH(COOH) ₂	132.0	Cyclopentane	131
H—CH=CH ₂	156.2	Cyclohexane	123
H—C(CH ₃)=C(CH ₃) ₂	148.4	Tetrahydrofuran	2,5 149
H—CH=C(<i>tert</i> -C ₄ H ₉) ₂	152		3,4 133
H—C(<i>tert</i> -C ₄ H ₉)=C(<i>tert</i> -C ₄ H ₉) ₂	143	1,4-Dioxane	145
Methylenecycloalkane		Benzene	159
C ₄ —C ₇	153–155	Fluorobenzene	2,6 155
H—CH=C=CH ₂	168		3,5 163
H—C(C ₆ H ₅)=CH(C ₆ H ₅)			4 161
<i>cis (Z)</i>	155	Bromobenzene	2,6 171
<i>trans (E)</i>	151		3,5 164
Cyclopropene	220		4 161
 <i>gem</i>	200	Benzonitrile	2,6 173
 <i>cis (Z)</i>	159		3,6 166
 <i>trans (E)</i>	162		4 163
 <i>gem</i>	195	Nitrobenzene	2,6 171
<i>cis (Z)</i>	163		3,5 167
<i>trans (E)</i>	161		4 163
<i>gem</i>	162	Mesitylene	2,6 154
<i>cis (Z)</i>	157		3,5 170
<i>trans (E)</i>	162		4 163
			152

TABLE 6.46 One-Bond Carbon–Hydrogen Spin Coupling Constants (*continued*)













Structure	J_{CH} , Hz	Structure	J_{CH} , Hz
2,4,6-Trimethylpyridine	158		
 2,5	183	 2	208
 3,4	170	 4	199
 2,5	201		205
 3,4	175		216
 2,5	185		
 3,4	167		
 3,5	190		
 4	178		

TABLE 6.47 Two-Bond Carbon–Hydrogen Spin Coupling Constants



Structure	$^2J_{\text{CH}}$, Hz	Structure	$^2J_{\text{CH}}$, Hz
$\text{CH}_3\text{—CH}_2\text{—H}$	−4.5	$(\text{CH}_2)_n\text{—C=CH}_2$ $n=4$	4.2
$\text{CCl}_3\text{—CH}_2\text{—H}$	5.9	$(\text{CH}_2)_n\text{—C=CH}_2$ $n=5$	5.2
$\text{ClCH}_2\text{—CH}_2\text{Cl}$	−3.4	H—C=C—H $n=6$	5.5
$\text{Cl}_2\text{CH—CHCl}_2$	1.2	 <i>cis</i> (Z)	16.0
$\text{CH}_3\text{—CHO}$	26.7	 <i>trans</i> (E)	0.8
$\text{CH}_2=\text{CH}_2$	−2.4	$\text{HC}\equiv\text{CH}$	49.3
$(\text{CH}_3)_2\text{C=O}$	5.5	$\text{C}_6\text{H}_5\text{O—C}\equiv\text{CH}$	61.0
$\text{CH}_2=\text{CH—CH=O}$	26.9	$\text{HC}\equiv\text{C—CHO}$	33.2
$(\text{C}_2\text{H}_5)_2\text{CH—CHO}$	26.9	$\text{ClCH}_2\text{—CHO}$	32.5
$\text{H}_2\text{NCH=CH—CHO}$	6.0	$\text{Cl}_2\text{CH—CHO}$	35.3
$\text{H}_2\text{NCH—CH—CHO}$	20.0	$\text{Cl}_3\text{C—CHO}$	46.3
C_6H_6	1.0	$\text{C}_6\text{H}_5\text{—C}\equiv\text{C}\equiv\text{CH}_3$	10.8

TABLE 6.48 Carbon–Carbon Spin Coupling Constants

Structure*	J_{CC} , Hz	Structure*	J_{CC} , Hz
$\text{H}_3\text{C—CH}_3$	35	$\text{H}_3\text{C—CH}_2\text{NH}_2$	37
$\text{H}_3\text{C—CHR}_2$	37	C—C=O	38–40
$\text{H}_3\text{C—CH}_2\text{Ar}$	34	C—C—C=O	36
$\text{H}_3\text{C—CH}_2\text{CN}$	33	C—C—Ar	43
$\text{H}_3\text{C—CH}_2\text{—CH}_2\text{OH}$		C—CO—O^- (anion)	52
C-1, C-2	38	C—CO—N	52
C-2, C-3	34	C—CO—OH	57

TABLE 6.48 Carbon–Carbon Spin Coupling Constants (continued)

Structure*	J_{CC} , Hz	Structure*	J_{CC} , Hz
C—CO—OR	59	C ₆ H ₅ NH ₂	
C—CN	52–57	1–2	61
C—C≡C ² J_{CC} = 11.8	67	2–3	58
H ₂ C=CH ₂	68	3–4	57
>C=C—CO—OH	70–71	³ J_{2-5}	7.9
>C=C—CN	71	C ₆ H ₅ CH ₃	44
>C=C—Ar	67–70	Pyridine	
C ₆ H ₆	57	2–3	54
C ₆ H ₅ NO ₂		3–4	56
1–2	55	³ J_{2-5}	14
2–3, 3–4	56	Furan	69
³ J_{2-5}	7.6	Pyrrole	69
C ₆ H ₅ I		Thiophene	64
1–2	60	H ₂ C=C=C(CH ₃) ₂	100
2–3	53	—C≡C—	170–176
3–4	58		
³ J_{2-5}	8.6	Structure	² J_{CC} , Hz
C ₆ H ₅ —OCH ₃			
2–3	58	<u>CH</u> ₃ —CO— <u>CH</u> ₃	16
3–4	56	<u>CH</u> ₃ —C≡ <u>CH</u>	11.8
		<u>CH</u> ₃ CH ₂ — <u>CN</u>	33

* R, alkyl group; Ar, aryl group.

TABLE 6.49 Carbon–Fluorine Spin Coupling Constants


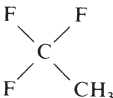

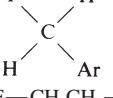


Structure*	J_{CF} , Hz	Structure*	J_{CF} , Hz
	–158		–271
	–235		–165
	–274	F—CH ₂ CH ₂ — or F—CR ₃	–167
	–259	<i>p</i> -F—C ₆ H ₄ —OR	–237
		<i>p</i> -F—C ₆ H ₄ —R	–241
		<i>p</i> -F—C ₆ H ₄ —CF ₃	–252
		<i>p</i> -F—C ₆ H ₄ —CO—CH ₃	–253
		<i>p</i> -F—C ₆ H ₄ —NO ₂	–257
		F—C ₆ H ₅	
		² J_{CF} = 21.0	–244
		³ J_{CF} = 7.7	
		⁴ J_{CF} = 3.4	

TABLE 6.49 Carbon-Fluorine Spin Coupling Constants (*continued*)

Structure*	J_{CF} , Hz	Structure*	J_{CF} , Hz
$\begin{array}{c} \text{F} \\ \diagdown \\ \text{C}=\text{CH}_2 \\ \diagup \\ \text{F} \end{array}$	-287	$\begin{array}{c} \text{F} \quad \text{H} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{F} \quad \text{CH}_2\text{OH} \end{array}$	-241
$\begin{array}{c} \text{F} \\ \diagdown \\ \text{C}=\text{O} \\ \diagup \\ \text{F} \end{array}$	-308	$\begin{array}{c} \text{F} \quad \text{F} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{F} \quad \text{CH}_2\text{OH} \end{array}$	-278
$\begin{array}{c} \text{F} \\ \diagdown \\ \text{C}=\text{O} \\ \diagup \\ \text{R} \end{array}$	-353	$\begin{array}{c} \text{F} \quad \text{F} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{F} \quad \text{OCF}_3 \end{array}$	-265
$\begin{array}{c} \text{F} \\ \diagdown \\ \text{C}=\text{O} \\ \diagup \\ \text{H} \end{array}$	-369	$\begin{array}{c} \text{F} \quad \text{F} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{F} \quad \text{CO}-\text{CH}_3 \end{array}$	-289

* Ar, aryl group; R, alkyl group.

TABLE 6.50 Carbon-13 Chemical Shifts of Deuterated Solvents*Relative to tetramethylsilane*

Solvent	Group	δ , ppm
Acetic- d_3 acid- d_1	Methyl	20.0
	Carbonyl	205.8
Acetone- d_6	Methyl	28.1
	Carbonyl	178.4
Acetonitrile- d_3	Methyl	1.3
	Carbonyl	117.7
Benzene- d_6		128.5
Carbon disulfide		193
Carbon tetrachloride		97
Chloroform- d_1		77
Cyclohexane- d_{12}		25.2
Dimethyl sulfoxide- d_6		39.5
1,4-Dioxane- d_6		67
Formic acid- d_1	Carbonyl	165.5
Methanol- d_4		47-49
Methylene chloride- d_2		53.8
Nitromethane- d_3		57.3
Pyridine- d_5	C_3, C_5	123.5
	C_4	135.5
	C_2, C_6	149.9

TABLE 6.51 Carbon-13 Spin Coupling Constants with Various Nuclei

Nuclei	Structure	¹ J, Hz	² J, Hz	³ J, Hz	⁴ J, Hz
² H	CDCl ₃	32			
	CD ₃ —CO—CD ₃	20			
	(CD ₃) ₂ SO	22			
	C ₆ D ₆	26			
⁷ Li	CH ₃ Li	15			
¹¹ B	(C ₆ H ₅) ₄ B [−]	49		3	
¹⁴ N	(CH ₃) ₄ N ⁺	10			
	CH ₃ NC	8			
²⁹ Si	(CH ₃) ₄ Si	52			
³¹ P	(CH ₃) ₃ P	14			
	(C ₄ H ₉) ₃ P	11	12	5	
	(C ₆ H ₅) ₃ P	12	20	7	0
	(CH ₃) ₄ P ⁺	56			
	(C ₄ H ₉) ₄ P ⁺	48	4	15	
	(C ₆ H ₅) ₄ P ⁺	88	11	13	3
	R(RO) ₂ P = O	142	5–7		
	(C ₄ H ₉ O) ₃ P = O		6	7	
	(CH ₃) ₂ Se	62			
	(CH ₃) ₃ Se ⁺	50			
¹¹³ Cd	(CH ₃) ₂ Cd	513, 537			
¹¹⁹ Sn	(CH ₃) ₄ Sn	340			
	(CH ₃) ₂ SnC ₆ H ₅	474	37	47	11
¹²⁵ Te	(CH ₃) ₂ Te	162			
¹⁹⁹ Hg	(CH ₃) ₂ Hg	687			
	(C ₆ H ₅) ₂ Hg	1186	88	102	18
²⁰⁷ Pb	(CH ₃) ₂ Pb	250			
	(C ₆ H ₅) ₄ Pb	481	68	81	20

TABLE 6.52 Boron-11 Chemical Shifts

Values given in ppm on the δ scale, relative to B(OCH₃)₃

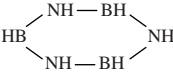
Structure	δ, ppm	Structure	δ, ppm
R ₃ B	−67 to −68	C ₆ H ₅ BCl ₂	−36
Ar ₃ B	−43	C ₆ H ₅ B(OH) ₂	−14
BF ₃	24	C ₆ H ₅ B(OR) ₂	−10
BCl ₃	−12	M(BH ₄)	55–61
BBr ₃	−6	B(BF ₄)	19–20
BI ₃	41		
B(OH) ₃	36		−12
B(OR) ₃	0–1		
B(NR ₂) ₃	−13		

TABLE 6.52 Boron-11 Chemical Shifts (*continued*)

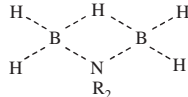
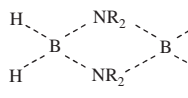
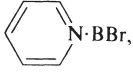
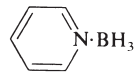
Structure	δ , ppm	Structure	δ , ppm	
	37	$R_2O(\text{or ROH}) \cdot BCl_3$ $R_2O(\text{or ROH}) \cdot BBr_3$ $R_2O(\text{or ROH}) \cdot BI_3$	-7 to -8 23-24 74-82	
	15		24	
$(CH_3)_2N-B(CH_3)_2$	62	Boranes	1	
Addition complexes		B_2H_6		
$R_2O \cdot BH_3$	18-19	B_4H_{10}		
$R_3N \cdot BH_3$	25	(BH_2)	25	
$R_2NH \cdot BH_3$	33	(BH)	60	
	31		Base	Apex
$R_2O(\text{or ROH}) \cdot BF_3$	17-19	B_5H_9	31	70
		B_3H_{11}	-16	50
		$B_{10}H_{14}$	7	54

TABLE 6.53 Nitrogen-15 (or Nitrogen-14) Chemical Shifts*Values given in ppm on the δ scale, relative to NH_3 liquid*

Substituent group	δ , ppm	Substituent group	δ , ppm
Aliphatic amines		Ureas	
Primary	1-59	Aliphatic	63-84
Secondary	7-81	Aryl	105-108
Tertiary	14-44	Sulfonamides	79-164
Cyclo, primary	29-44	Amides	
Aryl amines	40-100	HCO-NHR	
Aryl hydrazines	40-100	R = primary	100-115
Piperidines,		R = secondary	104-148
decahydroquinolines	30-82	R = tertiary	96-133
Amine cations		HCO-NH-Aryl	138-141
Primary	19-59	RCO-NHR or	103-130
Secondary	40-74	RCO-NR ₂	
Tertiary	30-67	RCO-NH-Aryl	131-136
Quaternary	43-70	Aryl-CO-H-Aryl	ca 126
Enamines, tertiary type		Guanidines	
Alkyl	29-82	Amino	30-60
Cycloalkyl	55-104	Imino	166-207
Aminophosphines	59-100	Thioureas	85-111
Amine N-oxides	95-122	Thioamides	135-154

TABLE 6.53 Nitrogen-15 (or Nitrogen-14) Chemical Shifts (*continued*)

Substituent group	δ , ppm	Substituent group	δ , ppm
Cyanamides		Diazo	
R_2N-	-12 to -38	Internal	226-303
$-CN$	175-200	Terminal	315-440
Carbodiimides	95-120	Nitrilium ions	123-150
Isocyanates		Azinium ions	185-220
Alkyl, primary	14-32	Azine <i>N</i> -oxides	230-300
Alkyl, secondary and tertiary	54-57	Nitrones	270-285
Aryl	ca 46	Imides	170-178
Isothiocyanates	90-107	Imimes	310-359
Azides	52-80	Oximes	340-380
	108-122	Nitramines	
	240-260	Amine	252-280
Lactams	113-122	$-NO_2$	328-355
Hydrazones		Nitrates	310-353
Amino	141-167	<i>gem</i> -Polynitroalkanes	310-353
Imino	319-327	Nitro	
Cyanates	155-182	Aryl	350-382
Nitrile <i>N</i> -oxides, fulminates	195-225	Alkyl	372-410
Isonitriles		Hetero, unsaturated	354-367
Alkyl, primary	162-178	Azoxy	330-356
Alkyl, secondary	191-199	Azo	504-570
Aryl	ca 180	Nitrosamines	222-250
Nitriles			525-550
Alkyl	235-241	Nitrites	555-582
Aryl	258-268	Thionitrites	720-790
Thiocyanates	265-280	Nitroso	
Diazonium		Aliphatic amines, NO	535-560
Internal	222-230	Aryl	804-913
Terminal	315-322		

TABLE 6.53 Nitrogen-15 (or Nitrogen-14) Chemical Shifts (*continued*)

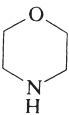
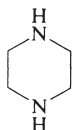

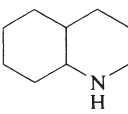









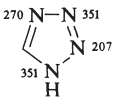




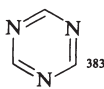
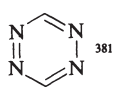
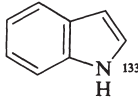
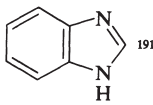
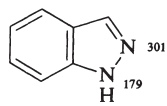
Substituent group	δ , ppm	Substituent group	δ , ppm
Saturated cyclic systems			
$(\text{CH}_2)_n\text{N}-\text{H}$ $n=2$ $n=3$ $n=4$ $n=5$ 	 -8.5 25.3 36.7 37.7 32.1	   <i>cis</i> (<i>Z</i>) <i>trans</i> (<i>E</i>)	 35.5 7.5 (in C_6H_6) 18.0 (in H_2O) 42.4 52.9
Unsaturated cyclic systems			
			
			
			
			
			

TABLE 6.53 Nitrogen-15 (or Nitrogen-14) Chemical Shifts (*continued*)

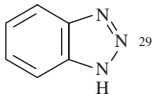
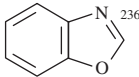
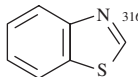
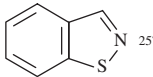
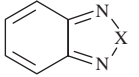
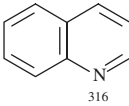
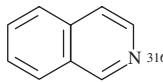
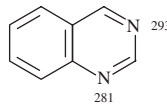
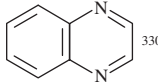
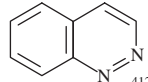
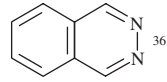
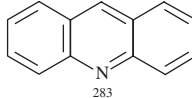
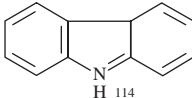
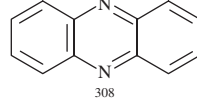
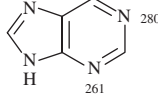
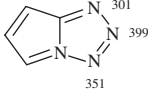
Unsaturated cyclic systems (<i>continued</i>)										
										
		<table> <tr> <th>X</th> <th>δ, ppm</th> </tr> <tr> <td>O</td> <td>517</td> </tr> <tr> <td>S</td> <td>331</td> </tr> <tr> <td>Se</td> <td>373</td> </tr> </table>	X	δ , ppm	O	517	S	331	Se	373
X	δ , ppm									
O	517									
S	331									
Se	373									
										
										
										
										

TABLE 6.54 Nitrogen-15 Chemical Shifts in Monosubstituted Pyridine

$$\delta = 317.3 + \Delta_i$$

Substituent	Δ_{C-2}	Δ_{C-3}	Δ_{C-4}
—CH ₃	−0.4	0.3	−8.0
—CH ₂ CH ₃	−1.8		−6.6
—CH(CH ₃) ₂	−5.1		−5.9
—C(CH ₃) ₃	−2.5		−5.8
—CN	−0.9	−0.8	10.6
—CHO	10	11	29
—CO—CH ₃	−9	15	11
—CO—OCH ₂ CH ₃	11.8		−5
—OCH ₃	−49	0	−23
—OH	−126	−2	−118
—NO ₂	−23	1	22
—NH ₂	−45	10	−46
—F	−42	−18	
—Cl	−4	4	−6
—Br	2	8	7

TABLE 6.55 Nitrogen-15 Chemical Shifts for Standards*Values given in ppm, relative to NH₃ liquid at 23 °C*

Substance	δ , ppm	Conditions
Nitromethane (neat)	380.2	For organic solvents and acidic aqueous solutions
Potassium (or sodium) nitrate (saturated aqueous solution)	376.5	For neutral and basic aqueous solutions
C(NO ₂) ₄	331	For nitro compounds
(CH ₃) ₂ —CHO (neat)	103.8	For organic solvents and aqueous solutions
(C ₂ H ₅) ₄ N ⁺ Cl [−]	64.4	Saturated aqueous solution
(CH ₃) ₄ N ⁺ Cl [−]	43.5	Saturated aqueous solution
NH ₄ Cl	27.3	Saturated aqueous solution
NH ₄ NO ₃	20.7	Saturated aqueous solution
NH ₃	0.0	Liquid, 25 °C
	−15.9	Vapor, 5 atm

TABLE 6.56 Nitrogen-15 to Hydrogen-1 Spin Coupling Constants

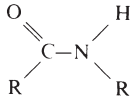
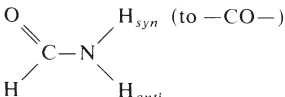

Structure	<i>J</i> , Hz	Structure	<i>J</i> , Hz
R—NH ₂ and R ₂ NH	61–67		88–92
Aryl—NH ₂	78	Pyrrole	97
<i>p</i> -CH ₃ O—aryl—NH ₂	79	HC≡NH ⁺	133–136
<i>p</i> -O ₂ N—aryl—NH ₂	90–93	>P—NH ₂	82–90
Amine salts (alkyl and aryl)	73–76	(R ₃ Si) ₂ NH	67
Aryl—NHOH	79	CF ₃ —S—NH ₂	81
Aryl—NHCH ₃	87	(CF ₃ —S) ₂ NH	99
Aryl—NHCH ₂ F	90	Pyridinium ion	90
Aryl—NHNH ₂	90	Quinolinium ion	96
<i>p</i> -O ₂ N—aryl—NHNH ₂	99		
Aryl—SO ₂ —NH ₂	81		
Aryl—SO ₂ —NHR	86		
 (to —CO—)	88		
	92–93		

TABLE 6.57 Nitrogen-15 to Carbon-13 Spin Coupling Constants

Structure	<i>J</i> , Hz	Structure	<i>J</i> , Hz
Alkyl amines	4–4.5	Alkyl—NO ₂	11
Cyclic alkyl amines	2–2.5	R—CN	18
Alkyl amines protonated	4–5	CH ₃ —N ⁺ ≡C [−]	
Aryl amines	10–14	H ₃ C—N	10
Aryl amines protonated	9	—N≡C	9
CH ₃ CO—NH ₂	14–15	Diaryl azoxy	
H ₂ N—CO—NH ₂	20	<i>anti</i>	18
Aryl—NO ₂	15	<i>syn</i>	13

TABLE 6.58 Nitrogen-15 to Fluorine-19 Spin Coupling Constants



Structure	<i>J</i> , Hz	Structure	<i>J</i> , Hz
NF ₃	155	Pyridine	
F ₄ N ₂	164	2-F	52
FNO ₂	158	3-F	4
F ₃ NO	190	2,6-di-F	37
F ₃ C—O—NF ₂	164–176	Pyridinium ion	
FCO—NF ₂	221	2-F	23
(NF ₄) ⁺ SbF ₆ [−]	323	3-F	3
(NF ₄) ⁺ AsF ₆ [−]	328	Quinoline, 8-F	3
(N ₂ F) ⁺ AsF ₆ [−]	459	Aniline	
F ₃ C—NO ₂	215	2-F	0
		3-F	0
		4-F	1.5
 (² <i>J</i> = 10)	190	Anilinium ion	
 (² <i>J</i> = 52)		2-F	1.4
		3-F	0.2
		4-F	0
		203	

TABLE 6.59 Fluorine-19 Chemical Shifts

Values given in ppm on the δ scale, relative to CCl₃F

Substituent group	δ, ppm	Substituent group	δ, ppm
—SO ₂ —F	−67 to −42 (aryl) (alkyl)	R—CF ₂ Cl	61–71
—CO—F	−29 to −20	>C—CF ₃ and aryl—CF ₃	56–73
>N—CO—F	−5	—CS—CF ₃	70
Aryl—CF ₂ Cl	49	>CF—CF ₃	71–73
—CF ₂ I	56	—S—CF ₃	41
—CF ₂ Br	63	—S—CF ₂ —S—	39
		>P—CF ₃	46–66

TABLE 6.59 Fluorine-19 Chemical Shifts (*continued*)

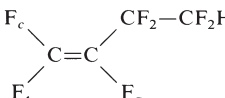
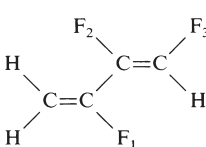




Substituent group	δ , ppm	Substituent group	δ , ppm
$>\text{N}-\text{CF}_3$	40–58	Perfluorocycloalkane	131–138
$>\text{N}-\text{CF}_2-\text{C}$	85–127	$>\text{CF}-\text{CF}_3$	163–198
$-\text{O}-\text{CF}_2-\text{R}$	70–91	$>\text{CF}(\text{CF}_3)_2$	180–191
$-\text{O}-\text{CF}_2-\text{CF}_3$	70–91	$-\text{CFH}-$	198–231
$-\text{CH}_2-\text{CF}_3$	76–77	$-\text{CFH}_2$	235–244
$\text{HO}-\text{CO}-\text{CF}_3$	77	$\text{F}_2\text{C}=\text{CF}_2$	133
$-\text{CHF}-\text{CF}_3$	81		
$-\text{CF}_2-\text{CF}_3$	78–88		
$-\text{CS}-\text{F}$	81	<i>cis</i> (Z)	108
$\text{CF}_3-\text{C}-\text{N}<$	84–96	<i>trans</i> (E)	92
$-\text{CO}-\text{CF}_2-\text{CF}_3$	83	<i>gem</i>	192
$-\text{CF}_2-$	86–126		
$-\text{CF}_2\text{Br}$	91		
$-\text{C}-\text{CF}_2-\text{S}-$	91–98	F-1	126
$-\text{CF}=\text{}$	180–192	F-2	155
$-\text{CF}_2-\text{CF}_3$	111	F-3	162
$-\text{CO}-\text{CF}_2-$	116–131	$\text{ClFC}=\text{CH}-\text{CF}_3$	61
$-\text{C}(\text{halide})-\text{CF}_2-$	119–128	Cycloalkenes	
$-\text{CF}_2-\text{CF}_3$	121–125	$=\text{CF}-\text{CF}_2-$	
$-\text{CF}_2-\text{CF}_2-$	121–129	$\text{C}(\text{CF}_3 \text{ or } \text{H})-$	101–113
$-\text{CF}_2-\text{CH}_2-$	122–133	$-\text{CF}_2-\text{CF}_2-$	
$-\text{CF}_2-\text{CHF}_2$	128–132	$\text{C}(\text{CF}_3 \text{ or } \text{CH}_3)=$	110–114
$-\text{CF}_2\text{H}$	136–143	$-\text{CF}_2-\text{CF}_2-\text{CH}=\text{}$	113–116
	151–156	$-\text{CF}_2-\text{CF}_2-\text{CF}=\text{}$	119–122
	147	Aryl—F	113
	96–133	$\text{C}_{10}\text{H}_7-\text{F}$	
	159	F-1	127
Cyclohexane-F	210	F-2	114
(axial)		$\text{C}_6\text{H}_5-\text{C}_6\text{H}_4-\text{F}$	
to		F-2	117
240		F-3	113
(equatorial)		F-4	109
		C_6F_6	163

TABLE 6.60 Fluorine-19 Chemical Shifts for Standards

Substance	Formula	δ , ppm
Trichlorofluoromethane	CFCl_3	0.0
α,α,α -Trifluorotoluene	$\text{C}_6\text{H}_5\text{CF}_3$	63.8
Trifluoroacetic acid	CF_3COOH	76.5
Carbon tetrafluoride	CF_4	76.7
Fluorobenzene	$\text{C}_6\text{H}_5\text{F}$	113.1
Perfluorocyclobutane	C_4F_8	138.0

TABLE 6.61 Fluorine-19 to Fluorine-19 Spin Coupling Constants

Structure	J_{FF} , Hz
$\text{F}_2\text{C}_{\text{gem}}\text{cycloalkane}$	212–260
Unsaturated compounds >C=C<	
gem	30–90
trans	115–130
cis	9–58
Aromatic compounds, monocyclic	
ortho	18–22
meta	0–7
para	12–15
Alkanes	
$\text{CFCl}_2\text{—CF}_2\text{—CFCl}_2$	6
$\text{CFCl}_2\text{—CF}_2\text{—CCl}_3$	5
$\text{CF}_2\text{Cl—CF}_2\text{—CF}_2\text{Cl}$	1
$\text{CF}_3\text{—CF}_2\text{—CF}_2\text{Cl}$ (or —CF_3)	< 1
$\text{CF}_3\text{—CF}_2\text{—CF}_2\text{Cl}$	2
$\text{CF}_3\text{—CF}_2\text{—CF}_2\text{Cl}$	9
$\text{CF}_3\text{—CF}_2\text{—CF}_3$	7

TABLE 6.62 Silicon-29 Chemical Shifts

Values given in ppm on the δ scale relative to tetramethylsilane

Substituent group X in $(\text{CH}_3)_{4-n}\text{SiX}_n$	n			
	1	2	3	4
—F	35	9	−52	−109
—Cl	30	32	13	−19
—Br	26	20	−18	−94
—I	9	−34	−18	−346
—H	−19	−42	−65	−93
$\text{—C}_2\text{H}_5$	2	5	7	8

TABLE 6.62 Silicon-29 Chemical Shifts (*continued*)

Substituent group X in (CH ₃) _{4-n} SiX _n	<i>n</i>			
	1	2	3	4
—C ₆ H ₅	—5	—9	—12	
—CH=CH ₂	—7	—14	—21	—23
—Oalkyl	14–17	—3 to —6	—41 to —45	—79 to —83
—Oaryl	17	—6	—54	—101
—O—CO—alkyl	22	4	—43	—75
—N(CH ₃) ₂	6	—2	—18	—28

Structure	δ, ppm	Structure	δ, ppm
Hydrides			
H ₃ Si—	—39 to —60	$\begin{array}{c} \text{O—} \\ \\ \text{CH}_3\text{—Si—O—} \end{array}$ (branching)	—65 to —66
—H ₂ Si—	—5 to —37	$\begin{array}{c} \text{O—} \\ \\ \text{—O—Si—O—} \end{array}$ (cross-linked)	—105 to —110
HSi≡	—2 to —39		
Silicates			
Orthosilicate anions	—69 to —72		
Silicon in end position	—77 to —81		
Silicon in middle	—85 to —89		
Branching silicons	—93 to —97		
Cross-linked silicons	—107 to —120		
Methyl siloxanes			
(CH ₃) ₂ Si—O— (end position)	6–8	Polysilanes	
$\begin{array}{c} \text{O—} \\ \\ (\text{CH}_3)_2\text{Si} \end{array}$ (middle)	—18 to —23	F ₃ Si—SiF ₃	—74
$\begin{array}{c} \text{O—} \\ \\ \text{CH}_3\text{Si(H)} \end{array}$ (middle)	—35 to —36	Cl ₃ Si—SiCl ₃	—8
		(CH ₃ O) ₃ Si—Si(OCH ₃) ₃	—53
		(CH ₃) ₃ Si—Si(CH ₃) ₃	—20
		(CH ₃) ₂ Si[Si(CH ₃) ₃] ₂	—48
		HSi[Si(CH ₃) ₃] ₃	—117
		Si[Si(CH ₃) ₃] ₄	—135

TABLE 6.63 Phosphorus-31 Chemical Shifts*Values given in ppm on the δ scale, relative to 85% H₃PO₄*

Structure	Identical atoms attached directly to phosphorus	Non-identically substituted phosphorus		
		R = CH ₃	R = C ₂ H ₅	R = C ₆ H ₅
P ₄	461			
PR ₃		62	20	6
PHR ₂		99	56	41
PH ₂ R		164	128	122
PH ₃	241			
PF ₃	—97			
PRF ₂			—168	—207

TABLE 6.63 Phosphorus-31 Chemical Shifts (*continued*)

Structure	Identical atoms attached directly to phosphorus	Non-identically substituted phosphorus		
		R = CH ₃	R = C ₂ H ₅	R = C ₆ H ₅
PCl ₃	−220			
PRCl ₂		−192	−196	−162
PR ₂ Cl		−94	−119	−81
PBr ₃	−227			
PRBr ₂		−184	−194	−152
PR ₂ Br		−91	−116	−71
PI ₃	−178			
P(CN) ₃	136			
P(SiR ₃) ₃		251		
P(OR) ₃		−141	−139	−127
P(OR) ₂ Cl		−169	−165	−157
P(OR)Cl ₂		−114	−177	−173
P(SR) ₃		−125	−115	−132
P(SR) ₂ Cl		−188	−186	−183
P(SR)Cl ₂		−206	−211	−204
P(SR) ₂ Br				−184
P(SR)Br ₂		−204		
P(NR ₂) ₃		−123	−118	
P(NR ₂)Cl ₂		−166	−162	−151
PR(NR ₂) ₂		−86	−100	−100
PR ₂ (NR ₂)		−39	−62	
F ₂ P—PF ₂	−226			
Cl ₂ P—PCl ₂	−155			
I ₂ P—PI ₂	−170			
PH ₂ [−] K ⁺	255			
P(CF ₃) ₃	3			
P ₄ O ₆	−113			
Structure	Identical atoms attached directly to phosphorus	Non-identically substituted phosphorus		
		X = F	X = Cl	X = Br
P(NCO) ₃	−97			
P(NCO) ₂ X		−128	−128	−127
P(NCO)X ₂		−131	−166	
P(NCS) ₃	−86			
P(NCS) ₂ X			−114	−112
P(NCS)X ₂			−155	−153
Structure	Identical atoms attached directly to phosphorus	Non-identically substituted phosphorus		
		R = CH ₃	R = C ₂ H ₅	R = C ₆ H ₅
O=PR ₃		−36	−48	−25
O=PHR ₂		−63		−23
O=PF ₃	36			

TABLE 6.63 Phosphorus-31 Chemical Shifts (*continued*)

Structure	Identical atoms attached directly to phosphorus	Non-identically substituted phosphorus		
		R = CH ₃	R = C ₂ H ₅	R = C ₆ H ₅
O=PRF ₂	-2	-27	-29	-11
O=PCl ₃				
O=PRCl ₂		-45	-53	-34
O=PR ₂ Cl		-65	-77	-43
O=P(OR) ₃		-1	1	18
O=P(OR) ₂ Cl		-6	-3	6
O=P(OR)Cl ₂		-6	-6	-2
O=PH(OR) ₂		-19	-15	
O=PR ₂ (OC ₂ H ₅)		-50	-52	-31
O=PR(OC ₂ H ₅) ₂		-30	-33	-17
O=P(NR ₂) ₃		-23	-24	-2
O=PR ₂ (NR ₂)		-44		-26
O=P(OR) ₂ NH ₂		-15	-12	-3
O=P(OR) ₂ (NCS)			19	29
O=P(SR) ₃		-66	-61	-55
O=PBr ₃	103			
O=P(NCO) ₃	41			
O=P(NCS) ₃	62			
O=P(NH ₂) ₃	-22			

Structure	Identical atoms attached directly to phosphorus	Structure	Identical atoms attached directly to phosphorus
PF ₅	35	$\begin{array}{c} \text{O} \\ \\ -\text{O}-\text{P}-\text{O}- \\ \\ \text{OR} \end{array}$ (middle group)	ca 18
PF ₆ ⁻ H ⁺	144		
PBr ₅	101	$\begin{array}{c} \text{O} \\ \\ -\text{O}-\text{P}-\text{O}- \\ \\ \text{O} \\ \\ \text{P (etc.)} \end{array}$ (branch group)	ca 30
P(OC ₂ H ₅) ₅	71		
PO ₄ ³⁻	-6		
O=P[OSi(CH ₃) ₃] ₃	33		
H ₄ P ₂ O ₇	11		
Phosphonates	-24 to -2		
Phosphonium cations			
Alkyl	-43 to -32		
Aryl	-35 to -18		
(O ₃ P—PO ₃) ⁴⁻	-9		
Polyphosphates			
O=P—O— (OR) ₂ (end group)	ca 6		

TABLE 6.63 Phosphorus-31 Chemical Shifts (continued)

Structure	Identical atoms attached directly to phosphorus	Non-identically substituted phosphorus		
		R = CH ₃	R = C ₂ H ₅	R = C ₆ H ₅
S=PR ₃	-29	-59	-55	-43
S=PCl ₃				
S=PRCl ₂		-80	-94	-75
S=PR ₂ Cl		-87	-109	-80
S=PBr ₃	112			
S=PRBr ₂		-21	-42	-20
S=PR ₂ Br		-64	-98	
S=P(OR) ₃		-73	-68	-53
S=P(OR)Cl ₂		-59	-56	-54
S=P(OR) ₂ Cl		-73	-68	-59
S=PH(OR) ₂		-74	-69	-59
S=P(SR) ₃		-98	-92	-92
S=P(NH ₂) ₃	-60			
S=P(NR ₂) ₃		-82	-78	
Se=P(OR) ₃		-78	-71	-58
Se=P(SR) ₃		-82	-76	
P(OR) ₅			71	86
PRF ₄		30	30	42
PR ₂ F ₃		-9	-6	

TABLE 6.64 Phosphorus-31 Spin Coupling Constants

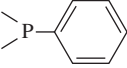
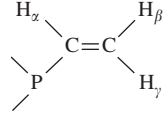


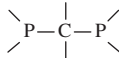

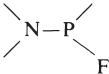
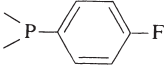
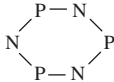
Substituent group	J _{PH} , Hz	Substituent group	J _{PH} , Hz
>PH	180–225	>P–N–CH	8–25
–PH ₂ [–]	134	>P–C–CH	0–4
RPH ₂	160–210		
>P–CH ₃	1–6	<i>ortho</i>	7–10
>P–CH ₂ –	14	<i>meta</i>	2–4
			
α	12–22	O=PHR ₂	210–500
β	30–40	O–PH(S)R	490–540
γ	14–20	O ₂ PHR	500–575
(Halogen) ₂ P=CH	16–20	O ₂ PH(N)	560–630
>P–NH	10–28	O ₂ PH(S or Se)	630–655
>P–O–CH ₃	11–15	O ₃ PH	630–760
>P–O–CH ₂ –R	6–10	S(or Se)= 	490–650
>P–O–CHR ₂	3–7	S(or Se)=PHR ₂	420–454
>P–SCH	5–20		

TABLE 6.64 Phosphorus-31 Spin Coupling Constants

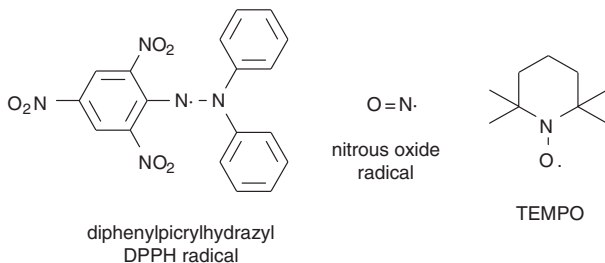
Substituent group	J_{PH} , Hz	Substituent group	J_{PH} , Hz
$\text{O}=\text{P}-\text{CH}_3$	7–15	 axial F equatorial	600–860
$\text{O}=\text{P}-\text{CH}=\text{C}$	15–30	$\text{O}=\text{P}-\text{CF}$	800–1 000
$\text{O}=\text{P}-\text{CH}-\text{Aryl}$ (or $\text{C}=\text{O}$)	15–30	$\text{O}=\text{P}-\text{F}$	110–113
$(\text{Halogen})_2\text{P}-\text{N}-\text{CH}$	9–18	$\text{P}-\text{O}-\text{P}-\text{F}$	980–1 190
$\text{S}=\text{P}-\text{CH}$	11–15	Substituent group	J_{PB} , Hz
$\equiv\text{P}-\text{CH}_3^+$	12–17	$\text{H}_3\text{B}-\text{P}-\text{N}$	80
$\equiv\text{P}-\text{H}^+$	490–600		
Substituent group	J_{PP} , Hz	Substituent group	J_{PP} , Hz
$>\text{P}-\text{F}$	1 320–1 420 (1F) (3F)	$>\text{P}-\text{P}<$	220–400
RPF_2	1 140–1 290	$\text{O}=\text{P}-\text{P}=\text{O}$	330–500
R_2PF	1 020–1 110	$\text{S}=\text{P}-\text{P}=\text{S}$	15–500
$\text{RP}(\text{N})\text{F}$	920–985 (alkyl) (aryl)		ca 70
	1 225–1 305	$>\text{P}-\text{O}-\text{P}<$	20–40
$(\text{OCN})\text{PF}$	1 310	$>\text{P}-\text{S}-\text{P}<$	86–90
	1 100–1 200	$\text{O}=\text{P}-\text{O}-\text{P}=\text{O}$	15–25
$>\text{P}-\text{CF}$	60–90	$\text{O}=\text{P}-\text{N}(\text{H})=\text{P}=\text{O}$	8–30
	0–60 1–7 0–3		5–66
<i>ortho</i>		$\text{P}=\text{N}-\text{P}=\text{N}-$	5–65
<i>meta</i>			
<i>para</i>			

ELECTRON SPIN RESONANCE

Electron paramagnetic resonance (EPR) is also referred to as electron spin resonance (ESR). In many respects, it is similar to NMR and the corresponding principles, discussed in the previous section, apply. The critical difference is that an unpaired electron spin is detected in this method instead of a nuclear spin. The method applies only to paramagnetic systems. The electron spin is more readily detected than is a nuclear spin and magnets on EPR instruments are correspondingly smaller and less expensive.

Certain transition metals such as cobalt (Co), copper (Cu), iron (Fe), manganese (Mn), nickel (Ni), and vanadium (V) have unpaired spins and are readily detectable by EPR. Likewise, organic radicals can be detected and studied. Numerous organic radicals have been studied by this method. When an unpaired electron spin is present, it will be observed at a characteristic resonance position. The resonance line is split by nuclei such as protons resulting in spin–spin coupling as observed in NMR. The coupling constant is referred to as “*g*” in EPR rather than “*J*” as in NMR. It is referred to as the hyperfine splitting or hyperfine coupling constant.

Certain radicals are especially stable and are of biological consequence or have been used as antioxidants. TEMPO radicals (TEMPO = 2,2,6,6-tetramethylpiperidin-1-oxyl) have been particularly well studied because they are readily prepared and extremely stable.



A noticeable difference between NMR and EPR is that NMR is typically presented in absorption mode whereas EPR normally is presented in derivative mode. The EPR spectrum may be analyzed mathematically to determine the coupling pattern and thus the structural relationships. A database of software useful in EPR research is available at <http://epr.niehs.nih.gov/software.html>.

Involves protons unless otherwise indicated.

H^\bullet 508 Li^\bullet 81 Na^\bullet 632 K^\bullet 165 Cs^\bullet 3280 $\text{H}\dot{\text{C}}-\text{H}$ 15 $\text{H}_2\dot{\text{C}}-\text{H}$ (^1H) 22.8
 (^{13}C) 41

$\text{CH}_3-\dot{\text{C}}-\text{H}$ 26.8 22.3 $\text{CH}_3-\text{CH}_2-\dot{\text{C}}-\text{H}$ 30.3 22.1 $(\text{CH}_3)_2-\dot{\text{C}}-\text{H}$ 24.7 21.2
 $(\text{CH}_3)_3-\dot{\text{C}}$ 22.7 $\text{H}^\bullet \quad \text{C}=\text{C}^\bullet \quad \text{H}$ 68 16 34 $\text{CH}_2=\text{CH}-\text{CH}_2-\dot{\text{C}}\text{H}-\text{H}$ 0.6 28.5 22.2

\triangle^\bullet α 6.5 \square^\bullet α 21.3
 β 23.4 γ 1.1

$\text{C}_5\text{H}_5^\bullet$ 6.0 $\text{C}_7\text{H}_7^\bullet$ 3.9

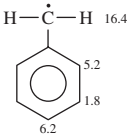
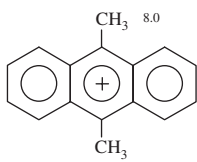
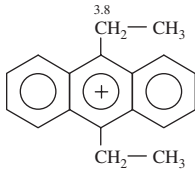
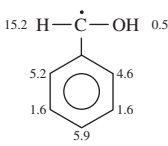
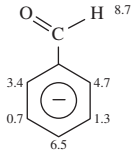
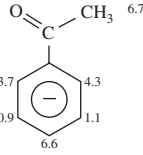
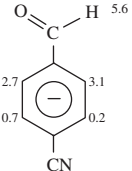
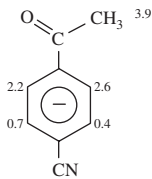
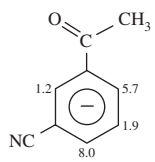
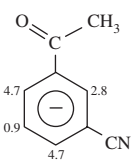
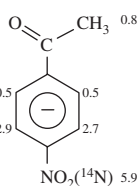
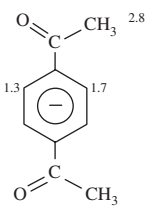
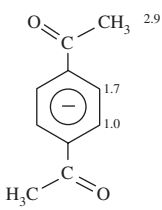
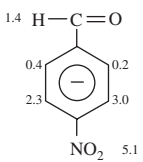
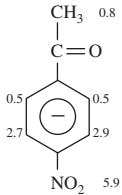
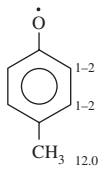
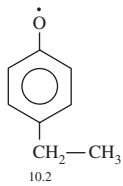
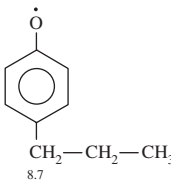
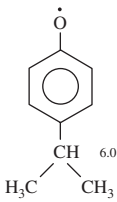
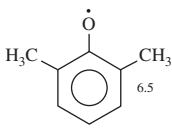
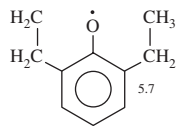
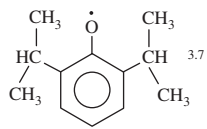
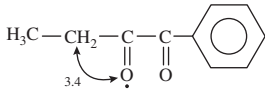
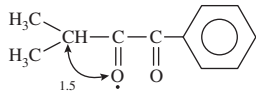
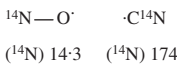
$\text{C}_8\text{H}_8^\bullet$ 3.2 $\text{H}-\text{C}\equiv\text{C}^\bullet$ 16.1 $\text{H}_2\text{C}=\text{C}^\bullet=\text{CH}_2$ 14.8 4.1 13.9

$\text{C}_6\text{H}_6^\oplus$ 2.9 $\text{C}_{10}\text{H}_8^\oplus$ 1.8 4.9 $\text{C}_{14}\text{H}_{10}^\oplus$ 6.5 3.1 1.4

$\text{C}_6\text{H}_6^\ominus$ (^1H) 3.8 $\text{C}_{10}\text{H}_8^\ominus$ 5.0 1.9 $\text{C}_{14}\text{H}_{10}^\ominus$ 2.7 5.3 1.5
 (^{13}C) 2.8

$\text{C}_6\text{H}_5\text{CH}_3^\ominus$ 0.8 5.1 0.6 $\text{C}_{10}\text{H}_7\text{CH}_3^\ominus$ 3.9 $\text{C}_{14}\text{H}_{11}\text{CH}_2\text{CH}_3^\ominus$ 2.3 2.9 0.6 3.7 4.4 4.4

TABLE 6.65 Spin-Spin Coupling (Hyperfine Splitting Constants) (*continued*)

Chemical structures and their corresponding σ and π bond dissociation energies (in kcal/mol) are shown below:

Monosubstituted Benzenes:

- $\text{C}_6\text{H}_5\text{NO}_2$: σ = 10.0, π = 3.4
- $\text{C}_6\text{H}_4(\text{NO}_2)_2$ (1,2): σ = 32, π = 0.4, 1.6, 0.1, 1.6
- $\text{C}_6\text{H}_4(\text{NO}_2)_2$ (1,3): σ = 4.7, π = 4.2, 1.0, 4.2, 3.1, 4.7
- $\text{C}_6\text{H}_2(\text{NO}_2)_4$: σ = 1.7, π = 1.1, 1.1, 1.7

Disubstituted Benzenes:

- $\text{C}_6\text{H}_3(\text{NO}_2)(\text{tert-butyl})$: σ = 14.9, π = 2.5, 1.1, 1.1, 2.5
- $\text{C}_6\text{H}_2(\text{NO}_2)(\text{tert-butyl})_2$: σ = 17.8, π = 0.9, 0.9, 0.9, 0.9
- $\text{C}_6\text{H}_3(\text{NO}_2)(\text{CH}_3)_2$: σ = 17.8, π = 0.9, 0.9, 1.4, 0.9

Amines:

- $\text{C}_6\text{H}_5\text{NH}_2$: σ = 12.2, π = 3.4, 1.1, 1.1, 1.1
- $\text{C}_6\text{H}_4(\text{NO}_2)\text{N}(\text{CH}_3)_2$: σ = 1.7, π = 3.3, 1.1, 1.1, 0.7
- $\text{C}_6\text{H}_5\text{N}$ (pyridine): ^1H = 2.6, ^{14}H = 7.1
- $\text{C}_6\text{H}_5\text{N}^+$ (pyridinium): ^1H = 3.3, ^{14}H = 7.6

Radical Anions:

- $[\text{C}_6\text{H}_5\text{C}(\text{H})_2]^-$: σ = 4.4, π = 1.9, 3.0, 0.3, 0.8, 3.9
- $[\text{C}_6\text{H}_5\text{N}(\text{N})]^-$: σ = 4.8, π = 2.8, 2.0, 0.8, 0.8, 2.8

Carbonyl Compounds:

- $\text{H}-\text{C}(=\text{O})-\text{H}$: σ = 137
- $\text{H}-\text{C}(=\text{O})-\text{OH}$: σ = 1-2.5
- $\text{HO}-\text{C}(\text{OH})-\text{CH}_3$: σ = 17.1
- $\text{HO}-\text{C}(\text{OH})-\text{CH}_2\text{OH}$: σ = 10.1

Carboxylic Acids:

- $\text{HO}-\text{C}(\text{OH})_2-\text{H}$: σ = 3.9

Nitro Compounds:

- CH_3-NO_2 : σ = 11.4, π = 25.8
- $\text{CH}_3-\text{CH}_2-\text{NO}_2$: σ = 8.3, π = 9.8, 25.5
- $\text{CH}_3-\text{C}(\text{NO}_2)_2-\text{CH}_3$: σ = 4.6, π = 1.8, 25.2

Imine:

- $\text{R}-\text{C}(\text{H})=\text{N}-\text{O}$: σ = 26.2 (anti), 29.2 (syn), π = 6.2 (syn), 31.6

Quinone:

- $\text{O}=\text{C}_6\text{H}_4=\text{O}$: σ = 1.2, π = 3.7, 33.0

Cyclohexanone:

- $\text{C}_6\text{H}_{10}\text{O}$: σ = 10.6

Cyclohexanone Derivatives:


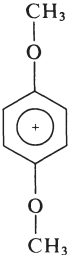
- $\text{C}_6\text{H}_9\text{O}$: σ = 13.5, π = 7.5

axial equatorial

(all positions)

(all positions)

TABLE 6.65 Spin–Spin Coupling (Hyperfine Splitting Constants) (continued)

		3.5 <i>trans</i> (<i>E</i>) 3.0 1.5	3.3 <i>cis</i> (<i>Z</i>) 2.7 1.8
(all positions)		Ring H	

IONIZATION POTENTIALS

The ionization potential is the energy required to remove an electron from an element or compound. Table 6.66A presents the ionization potentials for molecular species. The values are given in electron volts (eV). The values in parentheses are uncertainties in the final figure(s). Smaller numbers indicate lower energies or greater ease of electron removal. Table 6.66B is arranged alphabetically by element. Within an element, the compounds are arranged by increasing molecular weight.

TABLE 6.66A Ionization Potentials of Molecular Species

1 eV = 23.061 kcal·mol^{−1}
Values in parentheses are uncertainties in the final figure(s).

Species	Ionization potential, eV	Species	Ionization potential, eV
Diborane(6)	12.0	2-Methyl-1-propene	9.23(2)
Pentaborane(9)	10.5	Cyclobutane	10.58
Hexaborane(10)	9.3(1)	Butane	10.63(3)
Trimethylborane	8.8(2)	Isobutane	10.57
Triethylborane	9.0(2)	Cyclopentadiene	8.97
Methane	12.6	1,2-Pentadiene	9.42
CD ₄	12.888	1,3-Pentadiene	8.68
Acetylene	11.4	1,4-Pentadiene	9.58
C ₂ D ₂	11.416(6)	2,3-Pentadiene	8.68
Ethylene	10.5	2-Methyl-1,4-butadiene	8.845(5)
Ethane	11.5	Cyclopentene	9.01(1)
Propyne	10.36	1-Pentene	9.50(2)
Allene	10.16(2)	<i>cis</i> -2-Pentene	9.11
Cyclopropene	9.95	<i>trans</i> -2-Pentene	9.06
Cyclopropane	10.09(2)	2-Methyl-1-butene	9.12(2)
Propane	11.1	3-Methyl-1-butane	9.51(3)
1,2-Butadiene	9.57(2)	3-Methyl-2-butene	8.69(2)
1,3-Butadiene	9.07	Cyclopentane	10.53(5)
1-Butyne	10.18(1)	Pentane	10.35
2-Butyne	9.9(1)	Isopentane	10.32
1-Butene	9.6	Neopentane	10.35

TABLE 6.66A Ionization Potentials of Molecular Species (*continued*)

Species	Ionization potential, eV	Species	Ionization potential, eV
<i>cis</i> -2-Butene	9.13	Benzene	9.24
<i>trans</i> -2-Butene	9.13	Hexa-1,3-diene-5-yne	9.50
1,3-Hexadiyne	9.25	2,2,4-Trimethylpentane	9.86
1,4-Hexadiyne	9.75	2,2,3,3-Tetramethylbutane	9.79
1,5-Hexadiyne	10.35	Indene	8.81
2,4-Hexadiyne	9.75	β -Methylstyrene	8.35(1)
1-Methylcyclopentadiene	8.43(5)	Propylbenzene	8.72(1)
2-Methylcyclopentadiene	8.46(5)	Isopropylbenzene	8.69(1)
Cyclohexene	8.72	1,2,3-Trimethylbenzene	8.48
1-Hexene	9.45(2)	1,2,4-Trimethylbenzene	8.27
2,3-Dimethyl-2-butene	8.30	1,3,5-Trimethylbenzene	8.4
Cyclohexane	9.8	Naphthalene	8.12
Hexane	10.18	Azulene	7.42
2-Methylpentane	10.12	Butylbenzene	8.69(1)
3-Ethylbutane	10.08	<i>sec</i> -Butylbenzene	8.68(1)
2,2-Dimethylbutane	10.06	<i>tert</i> -Butylbenzene	8.68(1)
2,3-Dimethylbutane	10.02	1,2,3,5-Tetramethylbenzene	8.47(5)
Toluene	8.82(1)	1,2,4,5-Tetramethylbenzene	8.03
Cycloheptatriene	8.5	<i>cis</i> -Decalin	9.61(2)
Bicyclo[2.2.1]heptane	8.67	<i>trans</i> -Decalin	9.61(2)
Bicyclo[3.2.0]heptane	9.37	1-Methylnaphthalene	7.96(1)
1,2-Dimethylcyclopentadiene	8.1(1)	2-Methylnaphthalene	7.955(10)
5,5-Dimethylcyclopentadiene	8.22(5)	Pentamethylbenzene	7.92(2)
1,3-Cycloheptadiene	8.55	Hexamethylcyclopentadiene	7.74(5)
Norbornene	8.95(15)	Biphenyl	8.27(1)
4-Methylcyclohexene	8.91(1)	Hexamethylbenzene	7.85(2)
Methylcyclohexane	9.85(3)	Fluorene	8.63
Heptane	9.90(5)	Diphenylacetylene	8.85(5)
Phenylacetylene	8.815(5)	Anthracene	7.55
Styrene	8.47(2)	Phenanthrene	8.1
Cyclooctatetraene	8.0	1,2-Benzanthracene	8.01
Cubane	8.74(15)	1-Phenyldecane	9.05(10)
Ethylbenzene	8.76(1)	3-Phenyldecane	8.95(10)
<i>o</i> -Xylene	8.56	7-Phenyltridecane	8.91(10)
<i>m</i> -Xylene	8.58	1-Phenylicosane	9.34(10)
<i>p</i> -Xylene	8.44	2-Phenylicosane	9.22(10)
7-Methylcycloheptatriene	8.39(10)	3-Phenylicosane	8.95(10)
1-Methylspiroheptadiene	8.02(10)	4-Phenylicosane	9.01(10)
6-Methylspiroheptadiene	8.4(1)	5-Phenylicosane	9.04(10)
1,2,3-Trimethylcyclopentadiene	7.96(5)	7-Phenylicosane	8.97(10)
1,5,5-Trimethylcyclopentadiene	8.0(1)	9-Phenylicosane	9.06(10)
4-Vinylcyclohexene	8.93(2)	N ₂	15.576
<i>cis</i> -1,2-Dimethylcyclohexane	10.08(2)	NH ₃	10.2
<i>trans</i> -1,2-Dimethylcyclohexane	10.08(3)	N ₂ H ₂	9.85(10)
		N ₂ H ₄	8.74(6)
		HCN	13.8
		C ₂ N ₂	13.6

TABLE 6.66A Ionization Potentials of Molecular Species (*continued*)

Species	Ionization potential, eV	Species	Ionization potential, eV
Methylamine	8.97	<i>N,N</i> -Dimethyl- <i>p</i> -toluidine	7.33
Acetonitrile	12.2	Tripropylamine	7.23
Ethyleneimine	9.94(15)	<i>N</i> -Butylaniline	7.53
Ethylamine	8.86(2)	<i>N,N</i> -Diethylaniline	6.99
Dimethylamine	8.24(2)	<i>N,N</i> -Dimethyl-4-ethylaniline	7.38
Acrylonitrile	10.91(1)	<i>N,N</i> -2,4-Tetramethylaniline	7.17
Propionitrile	11.84(2)	<i>N,N</i> -2,6-Tetramethylaniline	7.22
Propylamine	8.78(2)	<i>N,N</i> -3,5-Tetramethylaniline	7.25
Isopropylamine	8.72(3)	<i>N,N</i> -Diethyl-4-toluidine	6.93
Trimethylamine	7.82(2)	<i>N,N</i> -Dimethyl-4-isopropylaniline	7.41
3-Butenonitrile	10.39(1)	Diphenylamine	7.25(3)
Pyrrole	8.20(1)	<i>N,N</i> -Dipropylaniline	6.96
Butyronitrile	11.67(5)	<i>N,N</i> -Dimethyl-4- <i>tert</i> -butylaniline	7.43
Pyrrolidine	8.41	<i>N,N</i> -Dibutylaniline	6.95
Butylamine	8.71(3)	Triphenylamine	6.86(3)
<i>sec</i> -Butylamine	8.70	Diazirine	10.18(5)
Isobutylamine	8.70	Diazomethane	8.999(1)
<i>tert</i> -Butylamine	8.64	Methylhydrazine	8.00(6)
Diethylamine	8.01(1)	1,1-Dimethylhydrazine	7.67(5)
Pyridine	9.3	1,2-Dimethylhydrazine	7.75(10)
Aniline	7.7	<i>o</i> -Diazine	9.9
2-Methylpyridine	9.02(3)	<i>m</i> -Diazine	9.9
3-Methylpyridine	9.04(3)	<i>p</i> -Diazine	9.8
4-Methylpyridine	9.04(3)	1,1-Diethylhydrazine	7.59(5)
Cyclohexylamine	8.86	1-Butyl-1-methylhydrazine	7.62(5)
Dipropylamine	7.84(2)	<i>p</i> -Bis(dimethylamino)benzene	6.9
Diisopropylamine	7.73(3)	Methyl azide	9.5(1)
Triethylamine	7.50(2)	O ₂	12.063(1)
Benzonitrile	9.705(10)	O ₃	12.3(1)
<i>N</i> -Methylaniline	7.32	Water (and D ₂ O)	12.6
<i>m</i> -Toluidine	7.50(2)	H ₂ O ₂	11.0
2,3-Dimethylpyridine	8.85(2)	CO	14.013(4)
2,4-Dimethylpyridine	8.85(3)	CO ₂	13.769(30)
2,6-Dimethylpyridine	8.85(2)	NO	9.25
Phenylacetoneitrile	9.4(5)	N ₂ O	12.894
3-Methylbenzonitrile	9.66(5)	NO ₂	9.79
4-Methylbenzonitrile	9.76	Formaldehyde	10.88
<i>N</i> -Ethylcyclohexylamine	7.56	Methanol	10.84
<i>N,N</i> -Dimethylcyclohexylamine	7.12	Acetaldehyde	10.2
Dibutylamine	7.69(3)	Ethylene oxide	10.6
<i>N</i> -Propylaniline	7.54	Ethanol	10.49
<i>N</i> -Ethyl- <i>N</i> -methylaniline	7.37	Dimethyl ether	9.98
<i>N,N</i> -Dimethyl- <i>o</i> -toluidine	7.37	Propenal	10.10(1)
<i>N,N</i> -Dimethyl- <i>m</i> -toluidine	7.35	Diphenyl ether	8.82(5)
Propionaldehyde	9.98		

TABLE 6.66A Ionization Potentials of Molecular Species (*continued*)

Species	Ionization potential, eV	Species	Ionization potential, eV
Acetone	9.69	Benzophenone	9.4
Allyl alcohol	9.67(5)	4-Methylbenzophenone	9.13(5)
Methyl vinyl ether	8.93(2)	Formic acid	11.05(1)
Propylene oxide	10.22(2)	Acetic acid	10.69(3)
Trimethylene oxide	9.667(5)	Methyl formate	10.815(5)
1-Propanol	10.1	Propionic acid	10.24(1)
2-Propanol	10.15	Ethyl formate	10.61(1)
Furan	8.89	Methyl acetate	10.27(2)
2-Butenal	9.73(1)	Dimethoxymethane	10.00(5)
Butyraldehyde	9.86(2)	Vinyl acetate	9.19(5)
2-Methylpropionaldehyde	9.74(3)	2,3-Butanedione	9.24(3)
2-Butanone	9.5	Butanoic acid	10.16(5)
Tetrahydrofuran	9.42	Isobutyric acid	10.02(5)
1-Butanol	10.04	Propyl formate	10.54(1)
Diethyl ether	9.6	Ethyl acetate	10.11(2)
Cyclopentanone	9.26(1)	Methyl propionate	10.15(3)
Dihydropyran	8.34(1)	1,4-Dioxane	9.13(3)
Pentanal	9.82(5)	1,1-Dimethoxyethane	9.65(3)
3-Methylbutyraldehyde	9.71(5)	2-Furaldehyde	9.21(1)
2-Pentanone	9.37(2)	2,4-Pentanedione	8.87(3)
3-Methyl-2-butanone	9.30(2)	Butyl formate	10.50(2)
3-Pentanone	9.32(1)	Isobutyl formate	10.46(2)
Cyclopentanone	9.25(1)	Propyl acetate	10.04(3)
Phenol	8.51	Isopropyl acetate	9.99(1)
4-Methyl-3-penten-2-one	9.08(3)	Ethyl propionate	10.00(2)
Cyclohexanone	9.14(1)	Methyl butyrate	10.07(3)
2-Hexanone	9.35	Methyl isobutyrate	9.98(2)
4-Methyl-2-pentanone	9.30	Diethoxymethane	9.70(5)
3,3-Dimethyl-2-butanone	9.17(3)	1,4-Quinone	9.67(2)
Dipropyl ether	9.27(5)	Butyl acetate	9.56(3)
Diisopropyl ether	9.20(5)	Isobutyl acetate	9.97
Benzaldehyde	9.52	<i>sec</i> -Butyl acetate	9.91(3)
Tropone	9.68(2)	Benzoic acid	9.73(9)
Benzyl alcohol	9.14(5)	<i>p</i> -Hydroxybenzaldehyde	9.32(2)
Methoxybenzene	8.21(2)	α -Hydroxyacetophenone	9.33(5)
<i>m</i> -Cresol	8.52(5)	Methyl benzoate	9.35(6)
2-Heptanone	9.33(3)	<i>p</i> -Methoxybenzaldehyde	8.60(3)
Acetophenone	9.27(3)	<i>m</i> -Hydroxyacetophenone	8.67(5)
4-Methylbenzaldehyde	9.33(5)	<i>p</i> -Hydroxyacetophenone	8.70(3)
Benzyl methyl ether	8.85(3)	α -Methoxyacetophenone	8.60(5)
Ethyl phenyl ether	8.13(2)	<i>m</i> -Methoxyacetophenone	8.53(5)
3-Methylanisole	8.31(5)	<i>p</i> -Methoxyacetophenone	8.62(5)
Propiophenone	9.27(5)	Methyl <i>p</i> -methylbenzoate	8.94(4)
3-Methylacetophenone	9.15(5)	<i>p</i> -Hydroxybenzophenone	8.59(5)
Phenyl benzoate	8.98(5)	N ₂ F ₄	12.04(10)
Benzil	8.78(5)	OF ₂	13.6
Methyl methoxyacetate	9.56(5)	XeF ₂	11.5(2)
Methyl <i>p</i> -methoxybenzoate	8.43(4)	Fluoromethane	12.85(1)

TABLE 6.66A Ionization Potentials of Molecular Species (*continued*)

Species	Ionization potential, eV	Species	Ionization potential, eV
Diphenyl carbonate	9.01(5)	Fluoroethylene	10.37
Acetamide	9.77(2)	Fluorobenzene	9.2
<i>N,N</i> -Dimethylformamide	9.12(2)	1,2-Difluorobenzene	9.31
<i>N</i> -Methylacetamide	8.90(2)	1,4-Difluorobenzene	9.15
<i>NN</i> -Dimethylacetamide	8.81(3)	Trifluoroethylene	10.14
<i>N,N</i> -Diethylformamide	8.89(2)	3,3,3-Trifluoro-1-propene	10.9
2-Pyridinecarboxaldehyde	9.75(5)	<i>o</i> -Fluorophenol	8.66(1)
4-Pyridinecarboxaldehyde	10.12(5)	PH ₃	9.98
<i>N,N</i> -Diethylacetamide	8.60(2)	PF ₃	9.71
Phenyl isocyanate	8.77(2)	Methylphosphine	9.72(15)
Benzamide	9.4(2)	Ethylphosphine	9.47(50)
<i>p</i> -Aminobenzaldehyde	8.25(2)	Trimethylphosphine	8.6(2)
<i>p</i> -Methoxyaniline	7.82	Triphenylphosphine	7.36(5)
Acetanilide	8.39(10)	S ₆	9.7
<i>m</i> -Aminoacetophenone	8.09(5)	S ₇	9.2(3)
<i>p</i> -Aminoacetophenone	8.17(2)	Hydrogen sulfide	10.4
α -Cyanoacetophenone	9.56(5)	Carbon disulfide	10.080
Nitromethane	11.1	Sulfur dioxide	12.34(2)
Nitroethane	10.88(5)	Methanethiol	9.440(5)
1-Nitropropane	10.81(3)	Ethylene sulfide	8.87(15)
2-Nitropropane	10.71(5)	Ethanethiol	9.285(5)
Nitrobenzene	9.92	Dimethyl sulfide	8.685(5)
<i>m</i> -Nitrotoluene	9.65(5)	Propylene sulfide	8.6(2)
<i>p</i> -Nitrotoluene	9.87	1-Propanethiol	9.195
<i>o</i> -Nitroaniline	8.66	Ethyl methyl sulfide	8.55(1)
<i>m</i> -Nitroaniline	8.7	Thiophene	8.860(5)
<i>p</i> -Nitroaniline	8.85	Methyl 1-propenyl sulfide	8.7(2)
Ethyl nitrate	11.22	1-Butanethiol	9.14(2)
Propyl nitrate	11.07(2)	Diethyl sulfide	8.430(5)
<i>p</i> -Nitrophenol	9.52	Methyl propyl sulfide	8.80(15)
<i>p</i> -Nitrobenzaldehyde	10.27(1)	Isopropyl methyl sulfide	8.7(2)
<i>m</i> -Nitroacetophenone	9.89(5)	Thiophenol	8.32(1)
<i>p</i> -Nitroacetophenone	10.07(2)	2-Ethylthiophene	8.8(2)
Methyl <i>p</i> -nitrobenzoate	10.20(3)	Dipropyl sulfide	8.5
F ₂	15.7	Methyl phenyl sulfide	8.9
HF	15.77(2)	2-Propylthiophene	8.6(2)
BF ₃	15.5	2-Butylthiophene	8.5(2)
C ₂ F ₄	10.12	Dimethyl disulfide	8.46(3)
Hexafluorobenzene	9.97	Diethyl disulfide	8.27(3)
<i>trans</i> -N ₂ F ₂	13.1(1)	COS	11.17(1)
NF ₃	13.2(2)	SO ₂ F ₂	13.3(1)
Methyl isothiocyanate	9.25(3)	<i>p</i> -Dichlorobenzene	8.95
Methyl thiocyanate	10.065(10)	Chloroform	11.42(3)
Ethyl isothiocyanate	9.14(3)	Trichloroethylene	9.45
Ethyl thiocyanate	9.89(1)	1,1,2,2-Tetrachloroethane	11.10(5)
Phenyl isothiocyanate	8.520(5)	CNCl	12.49(4)
Tolyl thiocyanate	9.06(5)	CF ₃ Cl	12.91(3)
Thiourea	8.50(5)	Chlorotrifluoroethylene	10.4(2)

TABLE 6.66A Ionization Potentials of Molecular Species (*continued*)

Species	Ionization potential, eV	Species	Ionization potential, eV
1-Methylthiourea	8.29(5)	Chloropentafluorobenzene	10.4(1)
1-Vinylthiourea	8.29(5)	Dichlorodifluoromethane	12.31(5)
1,1-Dimethylthiourea	8.34(5)	CF ₃ CCl=CClCF ₃	10.36(1)
1,3-Dimethylthiourea	8.17(5)	Trichlorofluoromethane	11.77(2)
1,1,3-Trimethylthiourea	7.93(5)	CF ₃ CCl ₃	11.78(3)
Tetramethylthiourea	7.95(5)	CFCl ₂ CF ₂ Cl	11.99(2)
CH ₃ COSH	10.00(2)	ClO ₃ F	13.6(2)
Cl ₂	11.48(1)	1-Bromo-1-propene	9.30(5)
HCl	12.74	1-Bromopropane	10.18(1)
CCl ₄	11.47(1)	2-Bromopropane	10.075(10)
Tetrachloroethylene	9.32(1)	1-Bromobutane	10.125(10)
PCl ₃	9.91	2-Bromobutane	9.98(1)
Chloromethane	11.3	1-Bromo-2-methylpropane	10.09(2)
Chloroethane	10.97	2-Bromo-2-methylpropane	9.89(3)
Chloroethylene	9.996	1-Bromopentane	10.10(2)
1-Chloro-1-propyne	9.9(1)	Bromobenzene	8.98(2)
1-Chloropropane	10.82(3)	<i>o</i> -Bromotoluene	8.78(1)
2-Chloropropane	10.78(2)	<i>m</i> -Bromotoluene	8.81(2)
1-Chlorobutane	10.67(3)	<i>p</i> -Bromotoluene	8.67(2)
2-Chlorobutane	10.65(3)	Dibromomethane	10.49(2)
1-Chloro-2-methylpropane	10.66(3)	<i>cis</i> -1,2-Dibromoethylene	9.45
2-Chloro-2-methylpropane	10.61(3)	<i>trans</i> -1,2-Dibromoethylene	9.46
Chlorobenzene	9.07	1,1-Dibromoethane	10.19(3)
α -Chlorotoluene	9.19(5)	1,3-Dibromopropane	10.07(2)
<i>o</i> -Chlorotoluene	8.83(2)	Bromoform	10.51(2)
<i>m</i> -Chlorotoluene	8.83(2)	Tribromoethylene	9.27
<i>p</i> -Chlorotoluene	8.69(2)	Cyanogen bromide	11.95(8)
<i>endo</i> -5-Chloro-2-norbornene	9.10(15)	Bromotrifluoromethane	11.89
<i>exo</i> -5-Chloro-2-norbornene	9.15(15)	2-Bromopyridine	9.65(5)
Dichloromethane	11.35(2)	4-Bromopyridine	9.94(5)
<i>cis</i> -1,2-Dichloroethylene	9.65	Acetyl bromide	10.55(5)
<i>trans</i> -1,2-Dichloroethylene	9.64	Methyl bromoacetate	10.37(5)
1,2-Dichloroethane	11.12(5)	CF ₂ BrCH ₂ Br	10.83(1)
2,3-Dichloro-1-propene	9.82(3)	Bromochloromethane	10.77(1)
1,2-Dichloropropane	10.87(5)	1-Bromo-2-chloroethane	10.63(3)
1,3-Dichloropropane	10.85(5)	Bromodichloromethane	10.88(5)
<i>o</i> -Dichlorobenzene	9.06	Bromotrimethylsilane	10.24(2)
<i>m</i> -Dichlorobenzene	9.12(1)	I ₂	9.28(2)
HI	10.39	CF ₃ CF ₂ CF ₂ CH ₂ Cl	11.84(2)
ICI	10.31(2)	Dichlorofluoromethane	12.39(20)
IBr	9.98(3)	Chlorotrimethylsilane	10.58(4)
Iodomethane	9.54	Trichloromethylsilane	11.36(3)
Iodoethane	9.33	Trichlorovinylsilane	10.79(2)
1-Iodopropane	9.26(1)	Trichloroethylsilane	10.74(4)
2-Iodopropane	9.17(2)	Trichloroisopropylsilane	10.28(10)
1-Iodobutane	9.21(1)	C ₂ H ₅ V(CO) ₄	8.2(3)
2-Iodobutane	9.09(2)	Cr(CO) ₆	8.03(3)
1-Iodo-2-methylpropane	9.18(2)	C ₂ H ₅ Mn(CO) ₃	8.3(4)

TABLE 6.66A Ionization Potentials of Molecular Species

Species	Ionization potential, eV	Species	Ionization potential, eV
2-Iodo-2-methylpropane	9.02(2)	Fe(CO) ₅	7.95(3)
1-Iodopentane	9.19(1)	Ni(CO) ₄	8.28(3)
Iodobenzene	8.73	Mo(CO) ₆	8.12(3)
<i>o</i> -Iodotoluene	8.62(1)	W(CO) ₆	8.18(3)
<i>m</i> -Iodotoluene	8.61(3)	As ₄	9.07(7)
<i>p</i> -Iodotoluene	8.50(1)	Arsine	10.03
RuO ₄	12.33(23)	AsCl ₃	11.7(1)
2-Chloropyridine	9.91(5)	Trimethylarsine	8.3(1)
4-Chloropyridine	10.15(5)	Triphenylarsine	7.34(7)
Acetyl chloride	11.02(5)	Br ₂	10.54(3)
1-Chloro-2-propanone	9.99	HBr	11.62(3)
2-Chlorophenol	9.28	BrCl	11.1(2)
4-Chlorophenol	9.07	Bromomethane	10.53
Benzoyl chloride	9.70(1)	Bromoethylene	9.80
4-Chlorobenzaldehyde	9.61(1)	Bromoethane	10.29
α -Chloroacetophenone	9.5	1-Bromo-1-propyne	10.1(1)
<i>p</i> -Chloroacetophenone	9.47(5)	OsO ₄	12.97(12)
Methyl chloroacetate	10.53(5)	Dimethylmercury	9.0
4-Methoxybenzoyl chloride	8.87(5)	Diethylmercury	8.5(1)
4-Chlorobenzoyl chloride	9.58(3)	Diisopropylmercury	7.6(1)
<i>cis</i> -Chlorofluoroethylene	9.86	CH ₃ HgCl	11.5(2)
<i>trans</i> -Chlorofluoroethylene	9.87	Triphenylbismuth	7.3(1)
<i>o</i> -Chlorofluorobenzene	9.155(10)	Stibine	9.58
<i>m</i> -Chlorofluorobenzene	9.21(1)	Triphenylstibine	7.3(1)
<i>p</i> -Chlorofluorobenzene	9.43(2)	Tetramethylstannane	8.25(15)
Chlorodifluoromethane	12.45(5)	Tetramethylplumbane	8.0(4)
1-Chloro-1,1-difluoroethane	11.98(1)	Tetramethylgermane	9.2(2)

TABLE 6.66B Alphabetical Listing of Ionization Potentials of Molecular Species

Species	IP (eV)	Species	IP (eV)
Acetylene	11.4	Butane	10.63(3)
Acetylene- <i>d</i> ₂ ; C ₂ D ₂	11.416	1-Butene	9.6
Allene	10.16	<i>cis</i> -2-Butene	9.13
Ammonia (NH ₃)	10.2	<i>trans</i> -2-Butene	9.13
Anthracene	7.55	1-Butyne	10.18(1)
Azine (N ₂ H ₂)	9.85(10)	2-Butyne	9.9(1)
Azulene	7.42	Butylbenzene	8.69(1)
1,2-Benzanthracene	8.01	<i>sec</i> -Butylbenzene	8.68(1)
Benzene	9.24	<i>tert</i> -Butylbenzene	8.68(1)
Bicyclo[2.2.1]heptane	8.67	Carbon dioxide, CO ₂	12.888
Bicyclo[3.2.0]heptane	9.37	Cubane	8.74(15)
Biphenyl	8.27(1)	Cyclobutane	10.58
1,2-Butadiene	9.57(2)	1,3-Cycloheptadiene	8.55
1,3-Butadiene	9.07	Cycloheptatriene	8.5

TABLE 6.66B Alphabetical Listing of Ionization Potentials of Molecular Species (*continued*)

Species	IP (eV)	Species	IP (eV)
Cyclohexane	9.8	4-Methylcyclohexene	8.91(1)
Cyclohexene	8.72	1-Methylcyclopentadiene	8.43(5)
Cyclooctatetraene	8	2-Methylcyclopentadiene	8.46(5)
Cyclopentadiene	8.97	1-Methylnaphthalene	7.96(1)
Cyclopentane	10.53(5)	2-Methylnaphthalene	7.955(10)
Cyclopentene	9.01(1)	2-Methylpentane	10.12
Cyclopropane	10.09	2-Methyl-1-propene	9.23(2)
Cyclopropene	9.95	1-Methylspiroheptadiene	8.02(10)
<i>cis</i> -Decalin	9.61(2)	6-Methylspiroheptadiene	8.4(1)
<i>trans</i> -Decalin	9.61(2)	β -Methylstyrene	8.35(1)
Diazomethane (C ₂ N ₂)	13.6	Naphthalene	8.12
Diborane	12	Neopentane	10.35
2,2-Dimethylbutane	10.06	Nitrogen (N ₂)	15.576
2,3-Dimethylbutane	10.02	Norbornene	8.95(15)
2,3-Dimethyl-2-butene	8.3	Pentaborane(9)	10.5
<i>cis</i> -1,2-Dimethylcyclohexane	10.08(2)	1,2-Pentadiene	9.42
<i>trans</i> -1,2-Dimethylcyclohexane	10.08(3)	1,3-Pentadiene	8.68
1,2-Dimethylcyclopentadiene	8.1(1)	1,4-Pentadiene	9.58
5,5-Dimethylcyclopentadiene	8.22(5)	2,3-Pentadiene	8.68
Diphenylacetylene	8.85(5)	Pentamethylbenzene	7.92(2)
Ethane	11.5	Pentane	10.35
Ethylbenzene	8.76(1)	1-Pentene	9.50(2)
3-Ethylbutane	10.08	<i>cis</i> -2-Pentene	9.11
Ethylene	10.5	<i>trans</i> -2-Pentene	9.06
Fluorene	8.63	Phenanthrene	8.1
Heptane	9.90(5)	Phenylacetylene	8.815(5)
Hexaborane	9.3	1-Phenyldodecane	9.05(10)
Hexa-1,3-diene-5-yne	9.5	3-Phenyldodecane	8.95(10)
1,3-Hexadiyne	9.25	1-Phenylicosane	9.34(10)
1,4-Hexadiyne	9.75	2-Phenylicosane	9.22(10)
1,5-Hexadiyne	10.35	3-Phenylicosane	8.95(10)
2,4-Hexadiyne	9.75	4-Phenylicosane	9.01(10)
Hexamethylbenzene	7.85(2)	5-Phenylicosane	9.04(10)
Hexamethylcyclopentadiene	7.74(5)	7-Phenylicosane	8.97(10)
Hexane	10.18	9-Phenylicosane	9.06(10)
1-Hexene	9.45(2)	7-Phenyltridecane	8.9100
Hydrazine (N ₂ H ₄)	8.74(6)	Propane	11.1
Hydrocyanic acid (HCN)	13.8	Propylbenzene	8.72(1)
Indene	8.81	Propyne	10.36
Isobutane	10.57	Styrene	8.47(2)
Isopentane	10.32	1,2,3,5-Tetramethylbenzene	8.47(5)
Isopropylbenzene	8.69(1)	1,2,4,5-Tetramethylbenzene	8.03
Methane	12.6	2,2,3,3-Tetramethylbutane	9.79
2-Methyl-1,4-butadiene	8.845(5)	Toluene	8.82(1)
3-Methyl-1-butane	9.51(3)	Triethylborane	9
2-Methyl-1-butene	9.12(2)	1,2,3-Trimethylbenzene	8.48
3-Methyl-2-butene	8.69(2)	1,2,4-Trimethylbenzene	8.27
7-Methylcycloheptatriene	8.39(10)	1,3,5-Trimethylbenzene	8.4
Methylcyclohexane	9.85(3)	Trimethylborane	8.8

TABLE 6.66B Alphabetical Listing of Ionization Potentials of Molecular Species (*continued*)

Species	IP (eV)	Species	IP (eV)
1,2,3-Trimethylcyclopentadiene	7.96(5)	<i>m</i> -Xylene	8.58
1,5,5-Trimethylcyclopentadiene	8.0(1)	<i>o</i> -Xylene	8.56
2,2,4-Trimethylpentane	9.86	<i>p</i> -Xylene	8.44
4-Vinylcyclohexene	8.93(2)		

TABLE 6.67 Ionization potentials of radical species
1 eV = 23.061 kcal·mol⁻¹

Values in parentheses are uncertainties in the final figure(s).

Species	Ionization potential, eV	Species	Ionization potential, eV
BH	9.77(5)	<i>tert</i> -Pentyl	7.1(1)
BH ₂	11.4(2)	Neopentyl	8.3(1)
BF	11.3	Benzyne	9.6
C ₂	12.0(6)	Cyclohexyl	7.7
C ₃	12.6	Benzyl	7.76(8)
CH	11.1(2)	Cycloheptatrienyl	6.24(1)
CH ₂	10.396(3)	1-Methylnaphthyl	7.35
CH ₃	9.83	2-Methylnaphthyl	7.56(5)
CD ₃	9.832(2)	(CH ₃) ₂ CCN	9.15(10)
C ₂ H ₃	9.4	<i>m</i> -Nitrobenzyl	8.56(10)
C ₂ H ₅	8.4	OH	13.17(10)
HC≡CCH ₂	8.25	HO ₂	11.53(2)
Allyl	8.15	CHO	9.8
Cyclopropyl	8.05	CH ₃ CO	10.3
C ₃ H ₆	9.73	C ₆ H ₅ O	8.84
Propyl	8.1	CF ₂	11.8
Isopropyl	7.5	NF ₂	11.9
C ₄ H ₂	10.2(1)	CH ₂ F	9.35
C ₄ H ₄	9.87	CHF ₂	9.45
Cyclobutyl	7.88(5)	HS	10.5(1)
CH ₃ CH=CHCH ₂	7.71(5)	CH ₃ S	8.06(10)
CH ₂ =C(CH ₃)CH ₂	8.03(5)	C ₆ H ₅ S	8.63(10)
Butyl	8.64(5)	CCl ₃	8.78(5)
<i>sec</i> -Butyl	7.93(5)	CH ₂ Cl	9.32
Isobutyl	8.35(5)	CHCl ₂	9.30
<i>tert</i> -Butyl	7.42(7)	NH ₂	11.3
Cyclopentyl	7.79(2)		

X-RAY DIFFRACTION

The X-ray diffraction method utilizes a monochromatic beam of X-rays to which a solid material is exposed. The beam of radiation interacts with the solid, and is both reflected and diffracted. The reflection pattern is recorded by a detector system sensitive to the X-radiation. Until recently, this involved an intricate mechanical device whose complex

motion permitted X-rays to be recorded over a range of positions, as the detector position changed. Automated instruments using this technology are often referred to as “4-circle diffractometers,” a term that refers to this complex detector motion. Newer X-ray instruments use charge coupled devices (CCDs) to simultaneously detect X-ray diffraction position and intensity over a much broader area. This enhanced detection technology reduces, often dramatically, the time required for data acquisition.

The Bragg equation describes the relationship between the impinging X-radiation, the diffraction angle, and the separation between lattice planes in the crystal under study. The Bragg equation is generally written as

$$\theta = \sin^{-1} (\lambda/2d)$$

where θ is the angle of the diffracted beam (usually called a reflection), λ is the wavelength of the incident X-ray beam, and d is the inter-planar spacing. From the diffraction pattern, both position and intensity, one can obtain structural information about the crystal under study.

Two types of X-ray studies are commonplace: X-ray powder analysis and crystal structure determination. Even in powders, the regular arrangement of atoms within the solid leads to characteristic diffraction patterns. X-ray powder patterns may therefore be used to characterize solids in much the same way that a UV or IR spectrum will give useful information but not necessarily a definitive structure.

The X-ray powder pattern obtained for the sodium salt of 2-propylpentanoic acid ($(\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{CHCOO}^-\text{Na}^+$) is shown in Figure 6.2. The X-ray powder pattern was detected over a range 2θ , in this case $2\text{--}40^\circ$ from the incident beam. This is a typical range although other ranges are used as well. The peak intensities are expressed in counts per second (cps) and may vary from experiment to experiment. However, the ratios of the peak heights are characteristic. Thus, X-ray powder patterns obtained from different samples of the same compound should give very similar, if not identical, patterns. Because the X-ray powder patterns are complex, the identity of two spectra suggests that the compounds producing them are also identical.

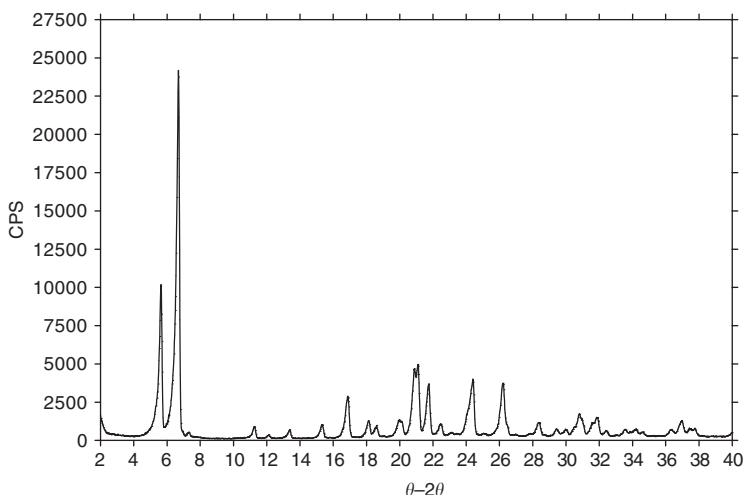


FIGURE 6.2 X-ray powder pattern of 2-propylpentanoic acid, $(\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{CHCOO}^-\text{Na}^+$.

The determination of a molecular structure from X-ray diffraction data is of critical importance to modern chemical and biological sciences. For small molecules, the structure is normally determined by direct methods. The X-ray diffraction pattern resulting from the interaction of X-rays with the electron clouds of different elements gives a pattern from which the elements present and their connectivity may be deduced. The expected diffraction pattern calculated for an apparent structure is then compared with the observed data to refine the result. Refinement factors (usually expressed as R_w) of 1–3% are common in modern small molecule structure determinations.

The Cambridge Structural Database is a repository for more than 250 000 (as of 2002) small molecule crystal structures. It is accessible at [http:// www.ccdc.cam.ac.uk/](http://www.ccdc.cam.ac.uk/) by subscription.

The process is more complex for such large molecules as proteins. Typically, a model of the amino acid backbone will be constructed first to obtain a general sense of the overall structure. Amino acid sidechains will then be added and the experimental data are again compared with the calculated diffraction pattern. This process is repeated until the complete structure is obtained. Because the uncertainties are larger in these systems, the resolution of the structure is typically reported in Ångstroms. Structures that have a resolution of 3 Å can and do give important information, especially when the gross structure of a protein was previously unknown. Recent improvements in chemical and biological techniques, computers, and X-ray instrumentation (especially in detectors) have made resolutions in the 1–2 Å range more common.

A database, called the Protein Data Bank or “PDB,” is a repository for protein structures. The database may be consulted at no charge and gives access to structures obtained by X-ray methods as well as by NMR and theoretical techniques. The Internet address is <http://www.rcsb.org/pdb>.

SECTION 7

PHYSICOCHEMICAL RELATIONSHIPS

LINEAR FREE ENERGY RELATIONSHIPS	7.2
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LINEAR FREE ENERGY RELATIONSHIPS

Organic chemists have studied the influence of substituents on various reactions for the better part of a century. Linear free energy relationships have played an important role in this pursuit by correlating equilibrium and rate processes. One of the earliest examples is now known as the Hammett equation. It emerged from the observation that the acidities of benzoic acids correlated with the rates at which ethyl esters of benzoic acids hydrolyzed. The relationship was expressed as follows in which K represents an equilibrium constant and k is a rate constant. The proportionality constant, m , is the slope of the log-log data plot for the two processes.

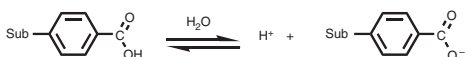
$$m \log \frac{K}{K_0} = \log \frac{k}{k_0}$$

When ΔH and ΔS vary linearly for two processes or when ΔH or ΔS is constant, the free energy relationship will be linear. The common form of the relationship is either

$$\log \frac{K}{K_0} = \sigma \rho \quad \text{or} \quad \log \frac{k}{k_0} = \sigma \rho$$

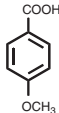
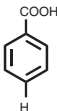
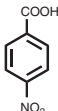
for equilibrium or rate processes, respectively. The Greek letters rho (ρ) and sigma (σ) symbolize the reaction and substituent constants, respectively. These equations may be used to describe and understand the influence of substituents on a reaction. Separate sigma values are defined by this reaction for *meta* and *para* substituents and provide a measure of the total electronic influence (polar, inductive, and resonance effects) in the absence of conjugation effects. The correlation is not as useful for *ortho*-substituted aromatic compounds because steric or other proximity effects intercede.

Typically in aromatic systems, the inductive effect is transmitted about equally to the *meta* and *para* positions. Consequently, σ_m is an approximate measure of a substituent's inductive effect whereas σ_p gives an approximate measure of a substituent's resonance effect. Consider the dissociation of benzoic acids in water. This process is assigned a reaction constant ρ of 1. The reaction is illustrated using "Sub" to represent a substituent.



We may compare three *para*-substituted benzoic acids. The reference point is *para*-hydrogen, which has a σ_p constant of 0, by definition. The methoxy group is electron donating and has a σ_p constant of -0.27 . Adding electrons to the benzoate anion (structure at right, above) should make the anion less stable. Thus, the ability to dissociate a cation (the acidity) should be diminished. The $\text{p}K_A$ is $-\log K_A$ so the higher the $\text{p}K_A$, the lower the acidity (the weaker the acid). In contrast, the nitro group is electron withdrawing. Its σ_p constant is $+0.78$ and its presence in the benzoate anion should be stabilizing. A more stable conjugate base implies a stronger acid and, indeed, the $\text{p}K_A$ for 4-nitrobenzoic acid is 3.44. Because these values are logarithmic, there is an order of magnitude difference in the acidities as a result of these substituents.

Comparison of acidities and sigma constants for three benzoic acids

Compound			
Substituent	OCH ₃	H	NO ₂
σ_p	-0.27	0.00	0.78
pK _A	4.49	4.20	3.44

Values of Hammett sigma constants are listed in Table 7.1. Taft sigma* (σ^*) values may be used similarly with respect to aliphatic and alicyclic systems. Values of σ^* constants are also listed in Table 7.1.

The reaction constant ρ is related to the reaction process rather than to the substituents present. A somewhat oversimplified way of considering ρ is to say that it indicates the demand the process makes on the substituents. The acidity of a benzoic acid, C₆H₅COOH, derivative is affected directly by substituents in the aromatic ring. Substituents exert somewhat less influence in phenylacetic acids, C₆H₅CH₂COOH, because the methylene group between carboxylate and the aromatic ring tends to insulate the latter from the former. This “insulation” is even greater for phenylpropanoic acids, C₆H₅CH₂CH₂COOH. The reaction constant ρ for dissociation of benzoic acid in water is set at 1.0. The reaction constants for dissociation of phenylacetic and phenylpropanoic acids are 0.49 and 0.21, respectively, under the same conditions. Values of the reaction parameter for some aromatic and aliphatic systems are given in Tables 7.2 and 7.3.

Since substituent effects in aliphatic systems and in *meta* positions in aromatic systems are essentially inductive in character, σ^* and σ_m values are related by the expression $\sigma_m = 0.217\sigma^* - 0.106$. Substituent effects fall off with increasing distance from the reaction center. The decline is generally a factor of 0.36 for the interposition of a —CH₂— group. This enables σ^* values to be estimated for R—CH₂— groups not otherwise available.

Modified sigma constants have been formulated for situations in which the substituent enters into resonance with the reaction center in an electron-demanding transition state (σ^+) or for an electron-rich transition state (σ^-). Generally, σ^- constants give better correlations in reactions involving phenols, anilines, pyridines, and in nucleophilic substitutions. Values for some modified sigma constants are given in Table 7.4.

TABLE 7.1 Hammett and Taft Substituent Constants

Substituent	Hammett constants		Taft constant σ^*
	σ_m	σ_p	
—AsO ₃ H	-0.09	-0.02	0.06
—B(OH) ₂	0.01	0.45	
—Br	0.39	0.23	2.84
—CH ₂ Br			1.00
<i>m</i> -BrC ₆ H ₄ —		0.09	

TABLE 7.1 Hammett and Taft Substituent Constants (*continued*)


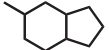
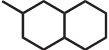





Substituent	Hammett constants		Taft constant σ^*
	σ_m	σ_p	
$p\text{-BrC}_6\text{H}_4\text{—}$		0.08	
—CH_3	−0.07	−0.17	0.0
$\text{—CH}_2\text{CH}_3$	−0.07	−0.15	−0.10
$\text{—CH}_2\text{CH}_2\text{CH}_3$	−0.05	−0.15	−0.12
$\text{—CH}(\text{CH}_3)_2$ (isopropyl)	−0.07	−0.15	−0.19
$\text{—CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	−0.07	−0.16	−0.13
$\text{—CH}_2\text{CH}(\text{CH}_3)_2$ (isobutyl)	−0.07	−0.12	−0.13
$\text{—CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (<i>sec</i> -butyl)		−0.12	−0.19
$\text{—C}(\text{CH}_3)_3$ (<i>t</i> -butyl)	−0.10	−0.20	−0.30
$\text{—CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (<i>n</i> -pentyl)			−0.25
$\text{—CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ (isopentyl)			−0.17
$\text{—CH}_2\text{C}(\text{CH}_3)_3$ (<i>t</i> -amyl)		−0.23	−0.12
$\text{—CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$			−0.37
$\text{—CH}(\text{CH}_2)_2$ (cyclopropyl)	−0.07	−0.21	
$\text{—CH}(\text{CH}_2)_5$ (cyclohexyl)			−0.15
		−0.26	
		−0.48	
	0.06	0.04	
—CH=CH_2 (vinyl, ethenyl)	0.02		0.56
$\text{—CH=C}(\text{CH}_3)_2$			0.19
—CH=CHCH_3 , <i>trans</i>			0.36
$\text{—CH}_2\text{CH=CH}_2$			0.0
$\text{—CH=CHC}_6\text{H}_5$	0.14	−0.05	0.41
$\text{—C}\equiv\text{CH}$	0.21	0.23	2.18
$\text{—C}\equiv\text{CC}_6\text{H}_5$	0.14	0.16	1.35
$\text{—CH}_2\text{C}\equiv\text{CH}$			0.81
$\text{—C}_6\text{H}_5$ (phenyl)	0.06	−0.01	0.60
$p\text{—CH}_3\text{C}_6\text{H}_4$ (<i>p</i> -tolyl)		−0.5	
 (1-naphthyl)			0.75
 (2-naphthyl)			0.75
$\text{—CH}_2\text{C}_6\text{H}_5$ (benzyl)		0.46	0.22
$\text{—CH}_2\text{CH}_2\text{C}_6\text{H}_5$ (2-phenylethyl)			−0.06
$\text{—CH}(\text{CH}_3)\text{C}_6\text{H}_5$ (α -phenylethyl)			0.37
$\text{—CH}(\text{C}_6\text{H}_5)_2$ (benzhydryl)			0.41
			0.44
 (2-furoyl)			0.25
 (3-indolyl)			−0.06

TABLE 7.1 Hammett and Taft Substituent Constants (*continued*)



Substituent	Hammett constants		Taft constant σ^*
	σ_m	σ_p	
 (2-thienyl)			1.31
 CH_2 — (2-thienylmethylene)			0.31
—CHO (formyl)	0.36	0.22	
—COCH ₃ (acetyl)	0.38	0.50	1.65
—COCH ₂ CH ₃ (propionyl)		0.48	
—COCH(CH ₃) ₂		0.47	
—COC(CH ₃) ₃		0.32	
—COCF ₃ (trifluoroacetyl)	0.65		3.7
—COC ₆ H ₅ (benzoyl)	0.34	0.46	2.2
—CONH ₂	0.28	0.36	1.68
—CONHC ₆ H ₅			1.56
—CH ₂ COCH ₃ (acetonyl)			0.60
—CH ₂ CONH ₂ (acetamido)			0.31
—CH ₂ CH ₂ CONH ₂			0.19
—CH ₂ CH ₂ CH ₂ CONH ₂			0.12
—CH ₂ CONHC ₆ H ₅			0.0
—COO [−] (carboxylate)	−0.1	0.0	−1.06
—COOH (carboxyl)	0.36	0.43	2.08
—CO—OCH ₃ (carbomethoxy)	0.32	0.39	2.00
—CO—OCH ₂ CH ₃ (carbethoxy)	0.37	0.45	2.12
—CH ₂ CO—OCH ₃			1.06
—CH ₂ CO—OCH ₂ CH ₃			0.82
—CH ₂ COOH			−0.06
—CH ₂ CH ₂ COOH	−0.03	−0.07	
—Cl	0.37	0.23	2.96
—CCl ₃ (trichloromethyl)	0.47		2.65
—CHCl ₂ (dichloromethyl)			1.94
—CH ₂ Cl (chloromethyl)	0.12	0.18	1.05
—CH ₂ CH ₂ Cl			0.38
—CH ₂ CCl ₃			0.75
—CH ₂ CH ₂ CCl ₃			0.25
—CH=CCl ₂			1.00
—CH ₂ CH=CCl ₂			0.19
<i>p</i> -ClC ₆ H ₄ — (<i>p</i> -chlorophenyl)		0.08	
—F	0.34	0.06	3.21
—CF ₃ (trifluoromethyl)	0.43	0.54	2.61
—CHF ₂ (difluoromethyl)			2.05
—CH ₂ F (fluoromethyl)			1.10
—CH ₂ CF ₃			0.90
—CH ₂ CF ₂ CF ₂ CF ₃			0.87
—C ₆ F ₅ (pentafluorophenyl)	−0.12	−0.03	
—Ge(CH ₃) ₃ (trimethylgermyl)		0.0	
—Ge(CH ₂ CH ₃) ₃ (triethylgermyl)		0.0	
—H	0.00	0.00	0.49
—I	0.35	0.28	2.46
—CH ₂ I (iodomethyl)			0.85
—N ₂ ⁺ (diazonio)	1.76	1.91	

TABLE 7.1 Hammett and Taft Substituent Constants (*continued*)


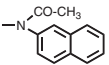
Substituent	Hammett constants		Taft constant σ^*
	σ_m	σ_p	
—N ₃ (azido)	0.33	0.08	2.62
—NH ₂ (amino)	−0.16	−0.66	0.62
—NH ₃ ⁺	1.13	1.70	3.76
—CH ₂ —NH ₂ (aminomethyl)			0.50
—CH ₂ —NH ₃ ⁺			2.24
—NH—CH ₃ (methylamino)	−0.30	−0.84	
—NH—C ₂ H ₅ (ethylamino)	−0.24	−0.61	
—NH—C ₄ H ₉ (butylamino)	−0.34	−0.51	
—NH(CH ₃) ₂ ⁺			4.36
—NH ₂ ⁺ —CH ₃	0.96		3.74
—NH ₂ ⁺ —C ₂ H ₅	0.96		3.74
—N(CH ₃) ₃ ⁺ (trimethylammonium)	0.88	0.82	4.55
—N(CH ₃) ₂ (dimethylamino)	−0.2	−0.83	0.32
—CH ₂ —N(CH ₃) ₃ ⁺			1.90
—N(CF ₃) ₂ [bis(trifluoromethyl)amino]	0.45	0.53	
<i>p</i> -H ₂ N—C ₆ H ₅ — (<i>p</i> -aminophenyl)		−0.30	
—NH—CO—CH ₃	0.21	0.00	1.40
—NH—CO—C ₂ H ₅			1.56
—NH—CO—C ₆ H ₅	0.22	0.08	1.68
—NH—CHO	0.25		1.62
—NH—CO—NH ₂	0.18		1.31
—NH—OH (hydroxylamino)	−0.04	−0.34	
—NH—CO—OC ₂ H ₅	0.33		1.99
—CH ₂ —NH—CO—CH ₃			0.43
—NH—SO ₂ —C ₆ H ₅			1.99
—NH—NH ₂ (hydrazido)	−0.02	−0.55	
—C≡N (cyano)	0.56	0.66	3.30
—CH ₂ —CN (cyanomethyl)	0.17	0.01	1.30
—N=O (nitroso)		0.12	
—NO ₂ (nitro)	0.71	0.78	4.0
—CH ₂ —NO ₂ (nitromethyl)			1.40
—CH ₂ —CH ₂ —NO ₂ (2-nitroethyl)			0.50
—CH=CHNO ₂ (2-nitroethenyl)	0.33	0.26	
<i>m</i> -O ₂ N—C ₆ H ₄ — (<i>m</i> -nitrophenyl)		0.18	
<i>p</i> -O ₂ N—C ₆ H ₄ — (<i>p</i> -nitrophenyl)		0.24	
 (picryl)	0.43	0.41	
—N ⁺ (CO-CH ₃)(CO-C ₆ H ₅)			1.37
—N ⁺ (CO-CH ₃)(CO-C ₆ H ₅)			1.65
			
—O [−]	−0.71	−0.52	
—OH (hydroxy)	0.12	−0.37	1.34
—O—CH ₃ (methoxy)	0.12	−0.27	1.81
—O—C ₂ H ₅ (ethoxy)	0.10	−0.24	1.68

TABLE 7.1 Hammett and Taft Substituent Constants (*continued*)



Substituent	Hammett constants		Taft constant σ^*
	σ_μ	σ_p	
—O—C ₃ H ₇ (propoxy)	0.00	—0.25	1.68
—O—CH(CH ₃) ₂ (isopropoxy)	0.05	—0.45	1.62
—O—C ₄ H ₉ (butoxy)	—0.05	—0.32	1.68
—O—C ₅ H ₉ (cyclopentyloxy)			1.62
—O—C ₆ H ₁₁ (cyclohexyloxy)	0.29		1.81
—O—CH ₂ —C ₆ H ₁₁ (cyclohexylmethoxy)	0.18		1.31
—O—C ₆ H ₅ (phenoxy)	0.25	—0.32	2.43
—O—CH ₂ —C ₆ H ₅ (phenylmethoxy)		—0.42	
—OCF ₃ (trifluoromethoxy)	0.40	0.35	
 (3,4-methylenedioxyphenyl, piperonyl)		—0.27	
 (3,4-ethylenedioxyphenyl)		—0.12	
—O—CO—CH ₃ (acetoxo)	0.39	0.31	
—ONO ₂ (nitrate ester)			3.86
—O—N=C(CH ₃) ₂			1.81
—ONH ₃ ⁺			2.92
—CH ₂ —O [—]			0.27
—CH ₂ —OH	0.08	0.08	0.31
—CH ₂ —O—CH ₃			0.52
—CH(OH)—CH ₃			0.12
—CH(OH)—C ₆ H ₅			0.50
<i>p</i> -HO—C ₆ H ₄ — (<i>p</i> -hydroxyphenyl)		—0.24	
<i>p</i> -CH ₃ O—C ₆ H ₄ — (<i>p</i> -methoxyphenyl)		—0.10	
—CH ₂ —CH(OH)—CH ₃			—0.06
—CH ₂ —C(OH)(CH ₃) ₂			—0.25
—P(CH ₃) ₂ (dimethylphosphino)	0.1	0.05	
—P(CH ₃) ₃ ⁺ (trimethylphosphino)	0.8	0.9	
—P(CF ₃) ₂	0.6	0.7	
—PO ₃ H [—]	0.2	0.26	
—PO(OC ₂ H ₅) ₂	0.55	0.60	
—SH (thio, mercapto)	0.25	0.15	1.68
—SCH ₃ (methylthio)	0.15	0.00	1.56
—S(CH ₃) ₂ ⁺ (dimethylsulfonium)	1.0	0.9	
—SCH ₂ CH ₃ (ethylthio)	0.23	0.03	1.56
—SCH ₂ CH ₂ CH ₃ (propylthio)			1.49
—SCH ₂ CH ₂ CH ₂ CH ₃ (butylthio)			1.44
—SC ₆ H ₁₁ (cyclohexylthio)			1.93
—SC ₆ H ₅ (phenylthio)	0.30		1.87
—SC(C ₆ H ₅) ₃ (triphenylmethylthio)			0.69
—SCH ₂ C ₆ H ₅ (benzylthio)			1.56
—SCH ₂ CH ₂ C ₆ H ₅ (phenethylthio)			1.44
—CH ₂ SH (thiomethyl)	0.03		0.62
—CH ₂ SCH ₂ C ₆ H ₅			0.37
—SCF ₃ (trifluoromethylthio)	0.40	0.50	
—SCN (thiocyanato)	0.63	0.52	3.43

TABLE 7.1 Hammett and Taft Substituent Constants (continued)

Substituent	Hammett constants		Taft constant σ^*
	σ_μ	σ_p	
—S—CO—CH ₃	0.39	0.44	
—S—CO—NH ₂	0.34		2.07
—SO—CH ₃ (methylsulfoxy)	0.52	0.49	
—SO—C ₆ H ₅ (phenylsulfoxy)			3.24
—CH ₂ —SO—CH ₃			1.33
—SO ₂ —CH ₃ (methylsulfonyl)	0.60	0.68	3.68
—SO ₂ —CH ₂ CH ₃ (ethylsulfonyl)			3.74
—SO ₂ —CH ₂ CH ₂ CH ₃ (propylsulfonyl)			3.68
—SO ₂ —C ₆ H ₅ (phenylsulfonyl)	0.67		3.55
—SO ₂ —CF ₃ (trifluoromethylsulfonyl)	0.79	0.93	
—SO ₂ —NH ₂	0.46	0.57	
—CH ₂ —SO ₂ —CH ₃			1.38
—SO ₃ [−]	0.05	0.09	0.81
—SO ₃ H		0.50	
—SeCH ₃	0.1	0.0	
—Se—C ₆ H ₁₁ (cyclohexylselenyl)			2.37
—SeCN	0.67	0.66	3.61
—Si(CH ₃) ₃	−0.04	−0.07	−0.81
—Si(CH ₂ CH ₃) ₃		0.0	
—Si(CH ₃) ₂ C ₆ H ₅			−0.87
—Si(CH ₃) ₂ —O—Si(CH ₃) ₃			−0.81
—CH ₃ Si(CH ₃) ₃	−0.16	−0.22	−0.25
—CH ₂ CH ₂ Si(CH ₃) ₃			−0.25
—Sn(CH ₃) ₃		0.0	
—Sn(CH ₂ CH ₃) ₃		0.0	

TABLE 7.2 pK_A and Rho (ρ) Values for the Hammett Equation

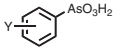
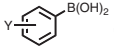
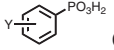
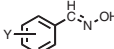
Acid	pK _A	ρ
 (arenearsonic acids) pK ₁ pK ₂	3.54 8.49	1.05 0.87
 (areneboronic acids, in aqueous 25% ethanol)	9.70	2.15
 (arenephosphonic acids) pK ₁ pK ₂	1.84 6.97	0.76 0.95
 (α-aryldoximes)	10.70	0.86
Ar—Se(O)OH (benzeneseleninic acids)	4.78	1.03
Ar—SO ₂ —NH ₂ (benzenesulfonamides, 20 °C)	10.00	1.06
Ar ¹ —SO ₂ —NHA ² r (benzenesulfonanilides, 20 °C)		
Y—C ₆ H ₄ —SO ₂ —NH—C ₆ H ₅	8.31	1.16

TABLE 7.2 pK_A and ρ (ρ) Values for the Hammett Equation (*continued*)















Acid	pK_A	ρ
$C_6H_5-SO_2-NH-C_6H_4-Y$	8.31	1.74
$Ar-CO-OH$ (benzoic acids)	4.21	1.00
 (cinnamic acids)	4.45	0.47
$Ar-OH$ (phenols)	9.92	2.23
 (phenylacetic acids)	4.30	0.49
 (phenylpropionic acids, in aqueous 35% dioxane)	3.24	0.81
 (phenylpropionic acids)	4.45	0.21
$Ar-CHOH-CF_3$ (phenyltrifluoromethylcarbinols)	11.90	1.01
 (pyridine-1-oxides, pyridine- <i>N</i> -oxides)	0.94	2.09
 (2-pyridones, 2-hydroxypyridines)	11.65	4.28
 (4-pyridones, 4-hydroxypyridines)	11.12	4.28
 (pyrroles)	17.00	4.28
 (5-substituted pyrrole-2-carboxylic acids)	2.82	1.40
$Ar-CO-SH$ (thiobenzoic acids)	2.61	1.0
$Ar-SH$ (thiophenols)	6.50	2.2
 (trifluoroacetophenone hydrates)	10.00	1.11
 (5-substituted tropolones)	6.42	3.10
Cations resulting from protonation of		
$Ar-CO-CH_3$ (acetophenones)	-6.0	2.6
$Ar-NH_2$ (anilines)	4.60	2.90
 (C-aryl- <i>N,N'</i> -dibutylamidines, in aqueous 50% ethanol)	11.14	1.41
<i>N,N</i> -Dimethylanilines	5.07	3.46
 (isoquinolines)	5.32	5.90
1-Naphthylamines	3.85	2.81
2-Naphthylamines	4.29	2.81
Pyridines	5.18	5.90
 (quinolines)	4.88	5.90

TABLE 7.3 pK_A and Rho (ρ) Values for the Taft Equation

Acid	pK_A	Rho (ρ)
RCOOH	4.66	1.62
RCH_2COOH	4.76	0.67
$\text{RC}\equiv\text{C}-\text{COOH}$	2.39	1.89
$\text{H}_2\text{C}=\text{C}(\text{R})-\text{COOH}$	4.39	0.64
$(\text{CH}_3)_2\text{C}=\text{C}(\text{R})-\text{COOH}$	4.65	0.47
$\text{Z}-\text{C}_6\text{H}_5-\text{CH}=\text{C}(\text{R})-\text{COOH}$	3.77	0.63
$\text{E}-\text{C}_6\text{H}_5-\text{CH}=\text{C}(\text{R})-\text{COOH}$	4.61	0.47
$\text{R}-\text{CO}-\text{CH}_2-\text{COOH}$	4.12	0.43
$\text{HO}-\text{N}=\text{CR}-\text{COOH}$	4.84	0.34
RCH_2OH	15.9	1.42
$\text{RCH}(\text{OH})_2$	14.4	1.42
$\text{R}^1\text{CO}-\text{NHR}^2$	22.0	3.1*
$\text{CH}_3\text{CO}-\text{CR}=\text{C}(\text{OH})\text{CH}_3$	9.25	1.78
$\text{CH}_3\text{CO}-\text{CHR}-\text{CO}-\text{OC}_2\text{H}_5$	12.59	3.44
$\text{R}-\text{CO}-\text{NHOH}$	9.48	0.98
$\text{R}^1\text{R}^2\text{C}=\text{N}-\text{OH}$ (R^1, R^2 are not acyl groups)	12.35	1.18
<div>$\text{HO}-\text{N}$ $\quad \diagup$ $\text{R}-\text{C}-\text{C}-\text{CH}_3$ $\quad \parallel \quad \diagdown$ $\quad \text{O} \quad \text{O}$</div>	9.00	0.94
$\text{RCH}(\text{NO}_2)_2$	5.24	3.60
RSH	10.22	3.50
RCH_2SH	10.54	1.47
$\text{R}-\text{CO}-\text{SH}$	3.52	1.62
Cations resulting from protonation of		
RNH_2	10.15	3.14
$\text{R}^1\text{R}^2\text{NH}$	10.59	3.23
$\text{R}^1\text{R}^2\text{R}^3\text{N}$	9.61	3.30
$\text{R}^1\text{R}^2\text{PH}$	3.59	2.61
$\text{R}^1\text{R}^2\text{R}^3\text{P}$	7.85	2.67

* σ^* for R^1CO and R^2

TABLE 7.4 Special Hammett Sigma Constants

Substituent	σ_m^+	σ_p^+	σ_p^-
$-\text{CH}_3$	-0.07	-0.31	-0.17
$-\text{C}(\text{CH}_3)_3$	-0.06	-0.26	
$-\text{C}_6\text{H}_5$	0.11	-0.18	
$-\text{CF}_3$	0.52	0.61	0.74
$-\text{F}$	0.35	-0.07	0.02
$-\text{Cl}$	0.40	0.11	0.23
$-\text{Br}$	0.41	0.15	0.26
$-\text{I}$	0.36	0.14	
$-\text{C}\equiv\text{N}$	0.56	0.66	0.88
$-\text{CH}=\text{O}$			1.13

TABLE 7.4 Special Hammett Sigma Constants (*continued*)

Substituent	σ_m^+	σ_p^+	σ_p^-
—CO—NH ₂			0.63
—CO—CH ₃			0.85
—COOH	0.32	0.42	0.73
—CO—OCH ₃	0.37	0.49	0.66
—CO—OCH ₂ CH ₃	0.37	0.48	0.68
—N ₂ ⁺			3.2
—NH ₂	0.16	−1.3	−0.66
—N(CH ₃) ₂		−1.7	
—N(CH ₃) ₃ ⁺	0.36	0.41	
—NH—CO—CH ₃		−0.60	
—NO ₂	0.67	0.79	1.25
—OH		−0.92	
—O [−]			−0.81
—OCH ₃	0.05	−0.78	−0.27
—SF ₅			0.70
—SCF ₃			0.57
—SO ₂ CH ₃			1.05
—SO ₂ CF ₃			1.36

SECTION 8

ELECTROLYTES, ELECTROMOTIVE FORCE, AND CHEMICAL EQUILIBRIUM

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EQUILIBRIUM CONSTANTS

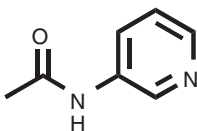
The acidities of organic compounds are typically expressed by citing their pK_A values. These are defined as $-\log_{10} K_A$ for the reaction



The equilibrium constant K_A is defined as

$$K_A = \frac{[H^+][A^-]}{[HA]}$$

Thus, for example, the pK_A of water is $-\log_{10} ([H^{\oplus}][HO^{\ominus}]/[H_2O])$ or $(10^{-7}) \cdot (10^{-7})/55.5$. The concentration of protons or hydroxide ions in water is $10^{-7} M$ and the concentration of water in water is $55.5 M$. The equilibrium constant K_A is therefore $10^{-15.74}$. The operator “p” means “ $-\log$ ” so the pK_A of water is 15.7. The equilibrium constant K_w for water is 10^{-14} and is simply the product of $[H^{\oplus}] \cdot [HO^{\ominus}]$.



3-acetamidopyridine

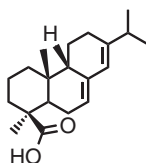
Acidity constants are given for a range of compounds in Table 8.1. When more than one ionizable proton is present, pK_1 , pK_2 , etc. values are given. Cations formed from the indicated compound by protonation are indicated by “(+1)” or “(+2)” for a dication. For example, the dissociation of 3-acetamidopyridine is reported in Table 8.1 as “4.37(+1).” This means dissociation of the compound that is protonated (at the pyridine nitrogen atom).

Temperature values different from $25^{\circ}C$ are given in parentheses as are other relevant variations. For example, the dissociation constant for acetic acid- d_1 is reported in D_2O .

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C

Ionic strength μ is zero unless otherwise indicated. The protonation state of cations is designated by a value (+1), (+2), etc. that follows the pK_A value. Neutral species are indicated by (0), if it is not obvious otherwise. The charge state of anionic species is designated by (−1), (−2), etc.

Substance	pK_1	pK_2	pK_3	pK_4
Abietic acid	7.62			
Acetamide	−0.37(+1)			
Acetamidine	1.60(+1)			
<i>N</i> -(2-Acetamido)-2-aminoethanesulfonic acid (20 °C)	6.88			
2-Acetamidobenzoic acid	3.63			
3-Acetamidobenzoic acid	4.07			
4-Acetamidobenzoic acid	4.28			
2-(Acetamido)butanoic acid	3.716			
<i>N</i> -(2-Acetamido)iminodiacetic acid (20 °C)	6.62			
3-Acetamidopyridine	4.37(+1)			
Acetanilide	0.4(+1)	13.39(0) ^{40 °C}		
Acetic acid	4.756			
Acetic acid- <i>d</i> (in D ₂ O)	5.32			
Acetoacetic acid (18 °C)	3.58			
Acetohydrazine	3.24(+1)			
Acetone oxime	12.2			
2-Acetoxybenzoic acid (acetylsalicylic acid)	3.48			
3-Acetoxybenzoic acid	4.00			
4-Acetoxybenzoic acid	4.38			
Acetylacetic acid (18 °C)	3.58			
<i>N</i> -Acetyl- α -alanine	3.715			
<i>N</i> -Acetyl- β -alanine	4.455			
2-Acetylaminobutanoic acid	3.72			
3-Acetylaminopropionic acid	4.445			
2-Acetylbenzoic acid	4.13			
3-Acetylbenzoic acid	3.83			
4-Acetylbenzoic acid	3.70			
2-Acetylcyclohexanone	14.1			
<i>N</i> -Acetylcysteine (30 °C)	9.52			
Acetylenedicarboxylic acid	1.75	4.40		
<i>N</i> -Acetyl glycine	3.670			



Abietic acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK ₁	pK ₂	pK ₃	pK ₄
<i>N</i> -Acetylguanidine	8.23(+1)			
<i>N</i> - α -Acetyl-L-histidine	7.08			
Acetylhydroxamic acid (20 °C)	9.40			
<i>N</i> -Acetyl-2-mercaptoethylamine	9.92(SH)			
4-Acetyl- β -mercaptoisoleucine (30 °C)	10.30			
2-Acetyl-1-naphthol (30 °C)	13.40			
<i>N</i> -Acetylpenicillamine (30 °C)	9.90			
2-Acetylphenol	9.19			
4-Acetylphenol	8.05			
2-Acetylpyridine	2.643(+1)			
3-Acetylpyridine	3.256(+1)			
4-Acetylpyridine	3.505(+1)			
Aconitine	8.11(+1)			
Acridine	5.60(+1)			
Acrylic acid	4.26			
Adenine	4.17(+1)	9.75(0)		
Adeninedeoxyriboside-5'-phosphoric acid		4.4	6.4	
Adenine- <i>N</i> -oxide	2.69(+1)	8.49(0)		
Adenosine	3.5(+1)	12.34(0)		
Adenosine-5'-diphosphoric acid		4.2(−1)	7.20(−2)	
Adenosine-2'-phosphoric acid	3.81(+1)	6.17(0)		
Adenosine-3'-phosphoric acid	3.65(0)	5.88(−1)		
Adenosine-5'-phosphoric acid	3.74(0)	6.05(−1)	13.06(−2)	
Adenosine-5'-triphosphoric acid		4.00(−1)	6.48(−2)	
Adipamic acid (adipic acid monoamide)	4.629			
Adipic acid	4.418	5.412		
α -Alanine	2.34(+1)	9.87(0)		
β -Alanine	3.55(+1)	10.238(0)		
α -Alanine, methyl ester ($\mu = 0.10$)	7.743(+1)			
β -Alanine, methyl ester ($\mu = 0.10$)	9.170(+1)			
<i>N</i> -D-Alanyl- α -D-alanine ($\mu = 0.1$)	3.32(+1)	8.13(0)		
<i>N</i> -L-Alanyl- α -L-alanine ($\mu = 0.1$)	3.32(+1)	8.13(0)		
<i>N</i> -L-Alanyl- α -D-alanine	3.12(+1)	8.30(0)		
<i>N</i> - α -Alanylglycine	3.11(+1)	8.11(0)		

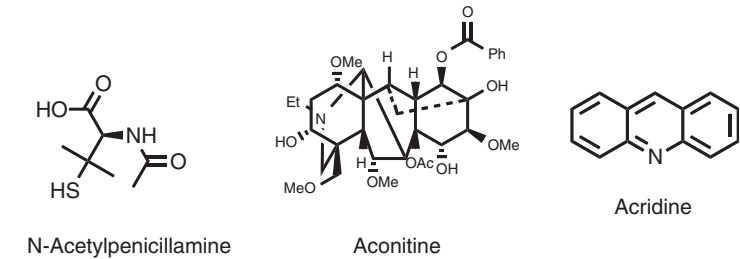
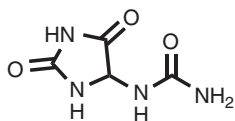
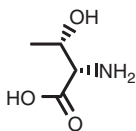


TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

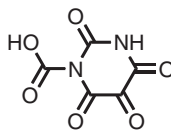
Substance	pK_1	pK_2	pK_3	pK_4
Alanylglycylglycine	3.190(+1)	8.15(0)	9.40	
β -Alanylhistidine	2.64	6.86		
Albumin (bovine serum, $\mu = 0.15$)	10–10.3			
2-Aldoxime pyridine	3.42(+1)	10.22(0)		
Alizarin Black SN	5.79	12.8		
Alizarin-3-sulfonic acid	5.54	11.01		
Allantoin	8.96			
Allothreonine	2.108(+1)	9.096(0)		
Alloxanic acid	6.64			
Allylactic acid	4.68			
Allylamine	9.69(+1)			
5-Allylbarbituric acid	4.78(+1)			
5-Allyl-5-(-methylbutyl)barbituric acid	8.08			
2-Allylphenol	10.28			
1-Allylpiperidine	9.65(+1)			
2-Allylpropionic acid	4.72			
3-Amidotetrazoline	3.95(+1)			
2-Aminoacetamide	7.95(+1)			
Aminoacetonitrile	5.34(+1)			
9-Aminoacridine (20°C)	9.95(+1)			
4-Aminoantipyrine	4.94(+1)			
2-Aminobenzenesulfonic acid	2.459(0)			
3-Aminobenzenesulfonic acid	3.738(0)			
4-Aminobenzenesulfonic acid	3.227(0)			
2-Aminobenzoic acid	2.09(+1)	4.79(0)		
3-Aminobenzoic acid	3.07(+1)	4.79(0)		
4-Aminobenzoic acid	2.41(+1)	4.85(0)		
2-Aminobenzoic acid, methyl ester	2.36(+1)			
3-Aminobenzoic acid, methyl ester	3.58(+1)			
4-Aminobenzoic acid, methyl ester	2.45(+1)			



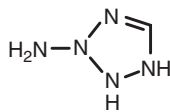
Allantoin



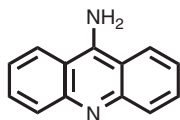
Allothreonine



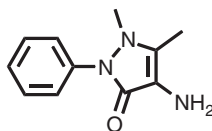
Alloxanic acid



3-Aminotetrazoline



9-Aminoacridine



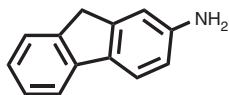
4-Aminoantipyrine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

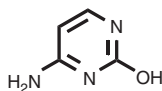
Substance	pK_1	pK_2	pK_3	pK_4
3-Aminobenzonitrile	2.75(+1)			
4-Aminobenzonitrile	1.74(+1)			
4-Aminobenzophenone	2.15(+1)			
2-Aminobenzothiazole (20 °C)	4.48(+1)			
2-Aminobenzoylhydrazide	1.85	3.47	12.80	
2-Aminobiphenyl	3.78(+1)			
3-Aminobiphenyl	4.18(+1)			
4-Aminobiphenyl	4.27(+1)			
4-Amino-3-bromomethylpyridine	7.47(+1)			
4-Amino-3-bromopyridine (20 °C)	7.04(+1)			
2-Aminobutanoic acid	2.286(+1)	9.830(0)		
3-Aminobutanoic acid		10.14(0)		
4-Aminobutanoic acid	4.031(+1)	10.556(0)		
2-Aminobutanoic acid, methyl ester ($\mu = 0.1$)	7.640(+1)			
4-Aminobutanoic acid, methyl ester ($\mu = 0.1$)	9.838(+1)			
D-(+)-2-Amino-1-butanol	9.52(+1)			
3-Amino- <i>N</i> -butyl-3-methyl-2- butanone oxime	9.09(+1)			
4-Aminobutylphosphonic acid	2.55	7.55	10.9	
2-Amino- <i>N</i> -carbamoylbutanoic acid	3.886(+1)			
4-Amino- <i>N</i> -carbamoylbutanoic acid	4.683(+1)			
2-Amino- <i>N</i> -carbamoyl-2- methylpropanoic acid	4.463			
1-Amino-1-cycloheptanecarboxylic acid	2.59(+1)	10.46(0)		
1-Amino-1-cyclohexanecarboxylic acid	2.65(+1)	10.03(0)		
2-Amino-1-cyclohexanecarboxylic acid	3.56(+1)	10.21(0)		
1-Aminocyclopentane	10.65(+1)			
1-Aminocyclopropane	9.10(+1)			
10-Aminodecylphosphonic acid		8.0	11.25	
10-Aminodecylsulfonic acid	2.65(+1)			
1-Amino-2-di(aminomethyl)butane	3.58(+3)	8.59(+2)	9.66(+1)	
2-Amino- <i>N,N</i> -dihydroxyethyl- 2-hydroxyl-1,3-propanediol	6.484(+1)			
2-Amino- <i>N,N</i> -dimethylbenzoic acid	1.63(+1)	8.42(0)		
4-Amino-2,5-dimethylphenol	5.28(+1)	10.40(0)		
4-Amino-3,5-dimethylpyridine (20 °C)	9.54(+1)			
12-Aminododecanoic acid	4.648(+1)			
2-Aminoethane-1-phosphoric acid	5.838	10.64		
1-Aminoethanesulfonic acid	−0.33	9.06		
2-Aminoethanesulfonic acid	1.5	9.061		
2-Aminoethanethiol (cysteamine) ($\mu = 0.01$)	8.23(+1)			
2-Aminoethanol (ethanolamine)	9.50(+1)			
2-[2-(2-Aminoethyl) aminoethyl] pyridine	3.50	6.59	9.51	

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
2-Amino-2-ethyl-1-butanol	9.82(+1)			
3-(2-Aminoethyl)indole		10.2		
3-Amino- <i>N</i> -ethyl-3-methyl-2-butanone oxime	9.23(+1)			
<i>N</i> -(2-Aminoethyl)morpholine	4.06(+2)	9.15(+1)		
<i>p</i> -(2-Aminoethyl)phenol	9.3	10.9		
2-Aminoethylphosphonic acid	2.45(+1)	7.0(0)	10.8(−1)	
<i>N</i> -(2-Aminoethyl)piperidine (30°C)	6.38	9.89		
2-(2-Aminoethyl)pyridine ($\mu = 0.5$)	4.24(+2)	9.78(+1)		
4-Amino-3-ethylpyridine (20°C)	9.51(+1)			
<i>N</i> -(2-Aminoethyl)pyrrolidine (30°C)	6.56(+2)	9.74(+1)		
2-Aminofluorine	10.34(+1)			
2-Amino-D- β -glucose ($\mu = 0.05$)	2.20(+1)	9.08(0)		
2-Amino- <i>N</i> -glycylbutanoic acid	3.155(+1)	8.331(0)		
7-Aminoheptanoic acid	4.502			
2-Aminohexanoic acid	2.335(+1)	9.834(0)		
6-Aminohexanoic acid	4.373(+1)	10.804(0)		
<i>C</i> -Amino- <i>C</i> -hydrazine carbonylmethane	2.38(+2)	7.69(+1)		
2-Amino-3-hydroxybenzoic acid	2.5(+1)	5.192(0)	10.118(OH)	
L-2-Amino-3-hydroxybutanoic acid (threonine)	2.088(+1)	9.100(0)		
DL-2-Amino-4-hydroxybutanoic acid ($\mu = 0.1$)	2.265(+1)	9.257(0)		
DL-4-Amino-3-hydroxybutanoic acid ($\mu = 0.1$)	3.834(+1)	9.487(0)		
2-Amino-2'-hydroxydiethyl sulfide	9.27(+1)			
4-Amino-2-hydroxypyrimidine (cytosine)	4.58(+1)	12.15(0)		
3-Amino- <i>N</i> -isopropyl-3-methyl-2-butanone oxime	9.09(+1)			
4-Amino-3-isopropylpyridine (20°C)	9.54(+1)			
1-Aminoisoquinoline (20°C, $\mu = 0.01$)	7.62(+1)			
3-Aminoisoquinoline (20°C, $\mu = 0.005$)	5.05(+1)			
4-Aminoisoxazolidine-3-one	7.4(+1)			
Aminomalonic acid	3.32(+1)	9.83(0)		
DL-2-Amino-4-mercaptoputanoic acid	2.22(+1)	8.87(0)	10.86(SH)	



2-Aminofluorene



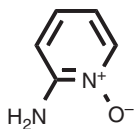
4-Amino-2-hydroxypyrimidine (cytosine)

TABLE 8.1 pK_a Values of Organic Materials in Water at 25 °C (*continued*)

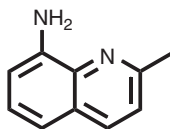
Substance	pK_1	pK_2	pK_3	pK_4
2-Amino-3-mercapto-3-Methylbutanoic acid	1.8(+1)	7.9(0)	10.5(SH)	
2-Amino-6-methoxybenzothiazole	4.50(+1)			
3-Amino-4-methylbenzenesulfonic acid	3.633			
4-Amino-3-methylbenzenesulfonic acid	3.125			
2-Amino-4-methylbenzothiazole	4.7(+1)			
1-Amino-3-methylbutane	10.64(+1)			
3-Amino-3-methyl-2-butanone oxime	9.09(+1)			
3-Amino- <i>N</i> -methyl-3-methyl-2-butanone oxime	9.23(+1)			
2-Amino-3-methylpentanoic acid	2.320(+1)	9.758(0)		
3-Aminomethyl-6-methylpyridine (30 °C)	8.70(+1)			
Aminomethylphosphonic acid	2.35	5.9	10.8	
2-Amino-2-methyl-1,3-propanediol	8.801			
2-Amino-2-methyl-1-propanol	9.694(+1)			
2-Amino-2-methylpropanoic acid	2.357(+1)	10.205(0)		
(2-Aminomethyl)pyridine ($\mu = 0.5$)	2.31(+2)	8.79(+1)		
2-Amino-3-methylpyridine	7.24(+1)			
4-Amino-3-methylpyridine	9.43(+1)			
2-Amino-4-methylpyridine	7.48(+1)			
2-Amino-5-methylpyridine	7.22(+1)			
2-Amino-6-methylpyridine	7.41(+1)			
2-Amino-4-methylpyrimidine (20 °C)	4.11(+1)			
Aminomethylsulfonic acid	5.75(+1)			
<i>N</i> -Aminomorpholine	4.19(+1)			
4-Amino-1-naphthalenesulfonic acid	2.81			
1-Amino-2-naphthalenesulfonic acid	1.71			
1-Amino-3-naphthalenesulfonic acid	3.20			
1-Amino-5-naphthalenesulfonic acid	3.69			
1-Amino-6-naphthalenesulfonic acid	3.80			
1-Amino-7-naphthalenesulfonic acid	3.66			
1-Amino-8-naphthalenesulfonic acid	5.03			
2-Amino-1-naphthalenesulfonic acid	2.35			
2-Amino-4-naphthalenesulfonic acid	3.79			
2-Amino-6-naphthalenesulfonic acid	3.79	8.94		
2-Amino-8-naphthalenesulfonic acid	3.89			
3-Amino-1-naphthoic acid	2.61	4.39		
4-Amino-2-naphthoic acid	2.89	4.46		
8-Amino-2-naphthol	4.20(+1)			
DL-2-Aminopentanoic acid (DL-norvaline)	2.318(+1)	9.808		
3-Aminopentanoic acid	4.02(+1)	10.399(0)		
4-Aminopentanoic acid	3.97(+1)	10.46(0)		
5-Aminopentanoic acid	4.20(+1)	9.758(0)		
5-Aminopentanoic acid, ethyl ester	10.151			
2-Aminophenol	9.28	9.72		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3-Aminophenol	9.83	9.87		
4-Aminophenol	8.50	10.30		
4-Aminophenylacetic acid (20°C)	3.60	5.26		
2-Aminophenylarsonic acid	ca 2	3.77	8.66	
3-Aminophenylarsonic acid	ca 2	4.02	8.92	
4-Aminophenylarsonic acid	ca 2	4.02	8.62	
3-Aminophenylboric acid	4.46	8.81		
4-Aminophenylboric acid	3.71	9.17		
4-Aminophenyl (4-chlorophenyl) sulfone	1.38			
2-Aminophenylphosphonic acid		4.10	7.29	
3-Aminophenylphosphonic acid			7.16	
4-Aminophenylphosphonic acid			7.53	
1-Amino-1,2,3-propanetricarboxylic acid ($\mu = 2.2$)	2.10(+1)	3.60(0)	4.60(-1)	9.82(-2)
3-Aminopropanoic acid	3.551(+1)	10.235(0)		
1-Amino-1-propanol	9.96(+1)			
DL-2-Amino-1-propanol	9.469(+1)			
3-Amino-1-propanol	9.96(+1)			
3-Aminopropene	9.691(+1)			
3-Amino- <i>N</i> -propyl-3-methyl- 2-butanone oxime	9.09(+1)			
2-Aminopropylsulfonic acid		9.15		
2-Aminopyridine	6.71(+1)			
3-Aminopyridine	6.03(+1)			
4-Aminopyridine	9.114(+1)			
2-Aminopyridine-1-oxide	2.58(+1)			
3-Aminopyridine-1-oxide	1.47(+1)			
4-Aminopyridine-1-oxide	3.54(+1)			
8-Aminoquinaldine	4.86(+1)			
2-Aminoquinoline (20°C, $\mu = 0.01$)	7.34(+1)			
3-Aminoquinoline (20°C, $\mu = 0.01$)	4.95(+1)			
4-Aminoquinoline (20°C, $\mu = 0.01$)	9.17(+1)			
5-Aminoquinoline (20°C, $\mu = 0.01$)	5.46(+1)			
6-Aminoquinoline (20°C, $\mu = 0.01$)	5.63(+1)			
8-Aminoquinoline (20°C, $\mu = 0.01$)	3.99(+1)			
4-Aminosalicylic acid	1.991(+1)	3.917(0)	13.74	
5-Aminosalicylic acid	2.74(+1)	5.84(0)		
2-Amino-3-sulfopropanoic acid	1.89(+1)	8.70(0)		
4-Amino-2,3,5,6- tetramethylpyridine (20°C)	10.58(+1)			



2-Aminopyridine-1-oxide



8-Aminoquinaldine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (continued)

Substance	pK ₁	pK ₂	pK ₃	pK ₄
5-Amino-1,2,3,4-tetrazole (20 °C)	1.76	6.07		
2-Aminothiazole (20 °C)	5.36(+ 1)			
1-Amino-3-thiobutane (30 °C)	9.18(+ 1)			
5-Amino-3-thio-1-pentanol (30 °C)	9.12(+ 1)			
2-Aminothiophenol	< 2(+ 1)	7.90(0)		
2-Amino-4,4,4-trifluorobutanoic acid		8.171(0)		
3-Amino-4,4,4-trifluorobutanoic acid		5.831(0)		
3-Amino-2,4,6-trinitrotoluene		9.5(+ 1)		
Angiotensin II	10.37			
Anhydroplatynecine	9.40			
Aniline	4.60(+ 1)			
2-Anilinoethylsulfonic acid	3.80(+ 1)			
3-Anilinoethylsulfonic acid	4.85(+ 1)			
Anthracene-1-carboxylic acid	3.68			
Anthracene-2-carboxylic acid	4.18			
Anthracene-9-carboxylic acid	3.65			
Anthraquinone-1-carboxylic acid (20 °C)	3.37			
Anthraquinone-2-carboxylic acid (20 °C)	3.42			
9,10-Anthraquinone monoxime	9.78			
9,10-Anthraquinone-1-sulfonic acid	0.27			
9,10-Anthraquinone-2-sulfonic acid	0.38			
Antipyrine	1.45(+ 1)			
Apomorphine (15 °C)		8.92		
D-(−)-Arabinose	12.34			
L-(+)-Arginine		8.994(+ 1)	12.47(− 1)	
Arsenazo III [pK ₅ = 10.5(− 4); pK ₆ = 12.0(− 5)]		1.2	2.7	7.9(− 3)
Arsenoacetic acid		4.67	7.68	
Arsenoacrylic acid		4.23	8.60	
Arsenobutanoic acid		4.92	7.64	
2-Arsenocrotonic acid		4.61	8.75	
3-Arsenocrotonic acid		4.03	8.81	
Arsenopentanoic acid		4.89	7.75	
L-(+)-Ascorbic acid (vitamin C)	4.17	11.57		
L-(+)-Asparagine		8.80(0)		
L-Asparaginylglycine		4.53	9.07	
D-Aspartic acid		3.87(0)	10.00(−)	
Aspartic diamide (μ = 0.2)	7.00			

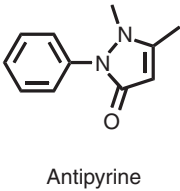
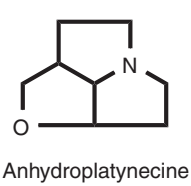


TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Aspartylaspartic acid		3.40	4.70	8.26
α -Aspartylhistidine (38°C, $\mu = 0.1$)		3.02	6.82	7.98
β -Aspartylhistidine (38°C, $\mu = 0.1$)		2.95	6.93	8.72
<i>N</i> -Aspartyl- <i>p</i> -tyrosine ($\mu = 0.01$)		3.57	8.92	10.23(OH)
Aspidospermine	7.65			
Atropine (17°C)	4.35(+1)			
1-Azacycloheptane	11.11(+1)			
1-Azacyclooctane	11.1(+1)			
Azetidine	11.29(+1)			
Aziridine	8.04(+1)			
Barbituric acid		8.372(0)		
<i>m</i> -Benzbetaine	3.217(+1)			
<i>p</i> -Benzbetaine	3.245(+1)			
Benzenearsonic acid (22°C)		8.48(−1)		
Benzene-1-arsonic acid-4-carboxylic acid		4.22 (COOH)	5.59	
Benzeneboronic acid	13.7			
Benzene-1-carboxylic acid- 2-phosphoric acid		3.78	9.17	
Benzene-1-carboxylic acid- 3-phosphoric acid		4.03	7.03	
Benzene-1-carboxylic acid- 4-phosphoric acid	1.50	3.95	6.89	
Benzenediazine	11.08(+1)			
1,3-Benzenedicarboxylic acid (isophthalic acid)	3.62(0)	4.60(−1)		
1,4-Benzenedicarboxylic acid (terephthalic acid)	3.54(0)	4.46(−1)		
1,3-Benzenedicarboxylic acid mononitrile	3.60(0)			
1,4-Benzenedicarboxylic acid mononitrile	3.55(0)			
Benzenehexacarboxylic acid ($pK_5 = 6.32$; $pK_6 = 7.49$)	0.68	2.21	3.52	5.09
Benzenepentacarboxylic acid ($pK_5 = 6.46$)	1.80	2.73	3.96	5.25
Benzenesulfinic acid	1.50			
Benzenesulfonic acid	2.554			
1,2,3,4-Benzenetetracarboxylic acid	2.05	3.25	4.73	6.21



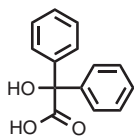
Azetidine



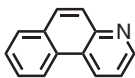
Aziridine (ethyleneimine)

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

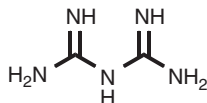
Substance	pK_1	pK_2	pK_3	pK_4
1,2,3,5-Benzenetetracarboxylic acid	2.38	3.51	4.44	5.81
1,2,4,5-Benzenetetracarboxylic acid	1.92	2.87	4.49	5.63
1,2,3-Benzenetricarboxylic acid	2.88	4.75	7.13	
1,2,4-Benzenetricarboxylic acid	2.52	3.84	5.20	
1,3,5-Benzenetricarboxylic acid	2.12	4.10	5.18	
Benzil- α -dioxime	12.0			
Benzilic acid	3.09			
Benzimidazole	5.53(+1)	12.3(0)		
Benzohydroxamic acid (20 °C)	8.89(0)			
Benzoic acid	4.204			
5,6-Benzoquinoline (20 °C)	5.00(+1)			
7,8-Benzoquinoline (20 °C)	4.15(+1)			
1,4-Benzoquinone monoxime	6.20			
Benzosulfonic acid	0.70			
1,2,3-Benzotriazole	8.38(+1)			
1-Benzoylacetone	8.23			
Benzoylamine	9.34(+1)			
2-Benzoylbenzoic acid	3.54			
Benzoylglutamic acid	3.49	4.99		
<i>N</i> -Benzoylglycine (hippuric acid)	3.65			
Benzoylhydrazine	3.03(+2)	12.45(+1)		
Benzoylpyruvic acid	6.40	12.10		
3-Benzoyl-1,1,1-trifluoroacetone	6.35			
Benzylamine	9.35(+1)			
Benzylamine-4-carboxylic acid	3.59	9.64		
2-Benzyl-2-phenylsuccinic acid (20 °C)	3.69	6.47		
2-Benzylpyridine	5.13(+1)			
4-Benzylpyridine-1-oxide	-1.018(+)			
1-Benzylpyrrolidine	9.51(+1)			
2-Benzylpyrrolidine	10.31(+1)			
Benzylsuccinic acid (20 °C)	4.11	5.65		
3-(Benzylthio)propanoic acid	4.463			
Berberine (18 °C)	11.73(+1)			
Betaine	1.832(+1)			
Biguanide	2.96(+2)	11.51(+1)		
2,2'-Biimidazoly ($\mu = 0.3$)	5.01(+1)			
2-Biphenylcarboxylic acid	3.46			



Benzilic acid



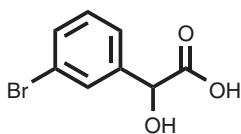
5,6-Benzoquinoline



Biguanide

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
(1,1'-Biphenyl)-4,4'-diamine	3.63(+2)	4.70(+1)		
Bis(2-aminoethyl) ether (30°C)	8.62(+2)	9.59(+1)		
<i>N,N'</i> -Bis(2-aminoethyl)- ethylenediamine (20°C)	3.32(+4)	6.67(+3)	9.20(+2)	9.92(+1)
<i>N,N</i> -Bis(2-hydroxyethyl)-2- aminoethane sulfonic acid (BES) (20°C)	7.15			
<i>N,N</i> -Bis(2-hydroxyethyl)glycine (bicine) (20°C)	8.35			
Bis(2-hydroxyethyl)iminotris (hydroxymethyl)- methane (bis-tris)	6.46(+1)			
1,3-Bis[tris(hydroxymethyl) methylamino]propane (20°C)	6.80(+1)			
Bromoacetic acid	2.902			
2-Bromoaniline	2.53(+1)			
3-Bromoaniline	3.53(+1)			
4-Bromoaniline	3.88(+1)			
2-Bromobenzoic acid	2.85			
3-Bromobenzoic acid	3.810			
4-Bromobenzoic acid	3.99			
2-Bromobutanoic acid (35°C)	2.939			
<i>erythro</i> -2-Bromo-3-chlorosuccinic acid (19°C, $\mu = 0.1$)	1.4	2.6		
<i>threo</i> -2-Bromo-chlorosuccinic acid (19°C, $\mu = 0.1$)	1.5	2.8		
<i>trans</i> -2-Bromocinnamic acid	4.41			
3-Bromo-4-(dimethylamino)pyridine (20°C)	6.52(+1)			
2-Bromo-4,6-dinitroaniline	-6.94(+1)			
3-Bromo-2-hydroxymethylbenzoic acid (20°C)	3.28			
6-Bromo-2-hydroxymethylbenzoic acid (20°C)	2.25			
7-Bromo-8-hydroxyquinoline- 5-sulfonic acid	2.51	6.70		
3-Bromomandelic acid	3.13			
3-Bromo-4-methylaminopyridine (20°C)	7.49(+1)			
(2-Bromomethyl)butanoic acid	3.92			
Bromomethylphosphonic acid	1.14	6.52		



3-Bromomandelic acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

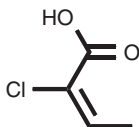
Substance	pK_1	pK_2	pK_3	pK_4
2-Bromo-6-nitrobenzoic acid	1.37			
2-Bromophenol	8.452			
3-Bromophenol	9.031			
4-Bromophenol	9.34			
2-(2'-Bromophenoxy)acetic acid	3.12			
2-(3'-Bromophenoxy)acetic acid	3.09			
2-(4'-Bromophenoxy)acetic acid	3.13			
2-Bromo-2-phenylacetic acid	2.21			
2-(Bromophenyl)acetic acid	4.054			
4-(Bromophenyl)acetic acid	4.188			
4-Bromophenylarsonic acid	3.25	8.19		
4-Bromophenylphosphinic acid (17 °C)	2.1			
2-Bromophenylphosphonic acid	1.64	7.00		
3-Bromophenylphosphonic acid	1.45	6.69		
4-Bromophenylphosphonic acid	1.60	6.83		
3-Bromophenylselenic acid	4.43			
4-Bromophenylselenic acid	4.50			
2-Bromopropanoic acid	2.971			
3-Bromopropanoic acid	3.992			
Bromopropynoic acid	1.855			
2-Bromopyridine	0.71(+1)			
3-Bromopyridine	2.85(+1)			
4-Bromopyridine	3.71(+1)			
3-Bromoquinoline	2.69(+1)			
Bromosuccinic acid	2.55	4.41		
2-Bromo- <i>p</i> -tolylphosphonic acid	1.81	7.15		
Brucine (15 °C)	2.50(+2)	8.16(+1)		
2-Butanamine (<i>sec</i> -butylamine)	10.56(+1)			
1,2-Butanediamine	6.399(+2)	9.388(+1)		
1,4-Butanediamine	9.35(+2)	10.82(+1)		
2,3-Butanediamine	6.91(+2)	10.00(+1)		
1,2,3,4-Butanetetra-carboxylic acid	3.43	4.58	5.85	7.16
<i>cis</i> -2-Butenoic acid (isocrotonic acid)	4.44			
<i>trans</i> -2-Butenoic acid (<i>trans</i> - crotonic acid) (35 °C)	4.676			
3-Butenoic acid (vinylacetic acid)	4.68			
3-Butoxybenzoic acid (20 °C)	4.25			
Butylamine	10.64(+1)			
<i>tert</i> -Butylamine	10.685(+1)			
4- <i>tert</i> -Butylaniline	3.78(+1)			
<i>N</i> - <i>tert</i> -Butylaniline	7.10(+1)			
Butylarsonic acid (18 °C)	4.23	8.91		
2- <i>tert</i> -Butylbenzoic acid	3.57			
3- <i>tert</i> -Butylbenzoic acid	4.199			
4- <i>tert</i> -Butylbenzoic acid	4.389			
<i>N</i> -Butylethylenediamine	7.53(+2)	10.30(+1)		
<i>N</i> -Butylglycine	2.35(+1)	10.25(0)		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
<i>tert</i> -Butylhydroperoxide	12.80			
1-(<i>tert</i> -Butyl)-2-hydroxybenzene	10.62			
1-(<i>tert</i> -Butyl)-3-hydroxybenzene	10.119			
1-(<i>tert</i> -Butyl)-4-hydroxybenzene	10.23			
Butylmethylamine	10.90(+1)			
2-Butyl-1-methyl-2-pyrroline	11.84(+1)			
4- <i>tert</i> -Butylphenylactic acid	4.417			
Butylphosphinic acid	3.41			
<i>tert</i> -Butylphosphinic acid	4.24			
<i>tert</i> -Butylphosphonic acid	2.79	8.88		
1-Butylpiperidine ($\mu = 0.02$)	10.43(+1)			
2- <i>tert</i> -Butylpyridine	5.76(+1)			
3- <i>tert</i> -Butylpyridine	5.82(+1)			
4- <i>tert</i> -Butylpyridine	5.99(+1)			
2- <i>tert</i> -Butylthiazole ($\mu = 0.1$)	3.00(+1)			
4- <i>tert</i> -Butylthiazole ($\mu = 0.1$)	3.04(+1)			
2-Butyn-1,4-dioic acid	1.75	4.40		
2-Butynoic acid (tetrolic acid)	2.620			
Butyric acid	4.817			
4-Butyrobetaine (20°C)	3.94(+1)			
Caffeine (40°C)	10.4			
Calcein ($pK_5 > 12$)	< 4	5.4	9.0	10.5
Calmagite	8.14	12.35		
D-Camphoric acid	4.57	5.10		
Canaline	2.40	3.70	9.20	
Canavanine	2.50(+2)	6.60(+1)	9.25(0)	
<i>N</i> -Carbamoylactic acid	3.64			
<i>N</i> -Carbamoyl- α -D-alanine	3.89(+1)			
<i>N</i> -Carbamoyl- β -alanine	4.99(+1)			
DL- <i>N</i> -Carbamoylalanine	3.892(+1)			
<i>N</i> -Carbamoylglycine	3.876			
2-Carbamoylpyridine (20°C)	2.10(+1)			
3-Carbamoylpyridine	3.328(+1)			
4-Carbamoylpyridine (20°C)	3.61(+1)			
β -Carboxymethylaminopropanoic acid	3.61(+1)	9.46(0)		
Chloroacetic acid	2.867			
<i>N</i> -(2'-Chloroacetyl)glycine	3.38(0)			
<i>cis</i> -3-Chloroacrylic acid (18°C, $\mu = 0.1$)	3.32			
<i>trans</i> -3-chloroacrylic acid (18°C, $\mu = 0.1$)	3.65			
2-Chloroaniline	2.64(+1)			
3-Chloroaniline	3.52(+1)			
4-Chloroaniline	3.99(+1)			
2-Chlorobenzoic acid	2.877			
3-Chlorobenzoic acid	3.83			
4-Chlorobenzoic acid	3.986			
2-Chlorobutanoic acid	2.86			

TABLE 8.1 pK_a Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3-Chlorobutanoic acid	4.05			
4-Chlorobutanoic acid	4.50			
2-Chloro-3-butenic acid	2.54			
3-Chlorobutylarsonic acid (18 °C)	3.95	8.85		
<i>trans</i> -2'-Chlorocinnamic acid	4.234			
<i>trans</i> -3'-Chlorocinnamic acid	4.294			
<i>trans</i> -4'-Chlorocinnamic acid	4.413			
2-Chlorocrotonic acid	3.14			
3-Chlorocrotonic acid	3.84			
Chlorodifluoroacetic acid	0.46			
1-Chloro-1,2-dihydroxybenzene	8.522			
1-Chloro-2,6-dimethyl-4-hydroxybenzene	9.549			
4-Chloro-2,6-dinitrophenol	2.97			
2-Chloroethylarsonic acid	3.68	8.37		
3-Chlorohexyl-1-arsonic acid (18 °C)	3.51	8.31		
2-Chloro-3-hydroxybutanoic acid	2.59			
3-Chloro-2-(hydroxymethyl)benzoic acid (20 °C)	3.27			
6-Chloro-2-(hydroxymethyl)benzoic acid (20 °C)	2.26			
7-Chloro-8-hydroxyquinoline-5-sulfonic acid	2.92	6.80		
2-Chloroisocrotonic acid	2.80			
3-Chloroisocrotonic acid	4.02			
3-Chlorolactic acid	3.12			
3-Chloromandelic acid	3.237			
3-Chloro-4-methoxyphenylphosphonic acid	2.25	6.7		
3-Chloro-4-methylaniline	4.05(+1)			
4-Chloro- <i>N</i> -methylaniline	3.9(+1)			
4-Chloro-3-methylphenol	9.549			
Chloromethylphosphonic acid	1.40	6.30		
2-Chloro-2-methylpropanoic acid	2.975			
2-Chloro-6-nitroaniline	-2.41(+1)			
4-Chloro-2-nitroaniline	-1.10(+1)			
2-Chloro-3-nitrobenzoic acid	2.02			
2-Chloro-4-nitrobenzoic acid	1.96			
2-Chloro-5-nitrobenzoic acid	2.17			
2-Chloro-6-nitrobenzoic acid	1.342			
4-Chloro-2-nitrophenol	6.48			



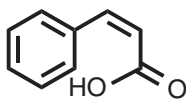
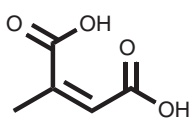
2-Chloroisocrotonic acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

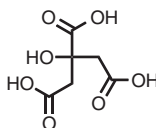
Substance	pK_1	pK_2	pK_3	pK_4
2-Chlorophenol	8.55			
3-Chlorophenol	9.10			
4-Chlorophenol	9.43			
(4-Chloro-3-nitrophenoxy)acetic acid	2.959			
2-Chloro-4-nitrophenylphosphonic acid	1.12	6.14		
3-Chloropentyl-1-arsonic acid (18°C)	3.71	8.77		
2-Chlorophenoxyacetic acid	3.05			
3-Chlorophenoxyacetic acid	3.07			
4-Chlorophenoxyacetic acid	3.10			
4-Chlorophenoxy-2-methylacetic acid	3.26			
2-Chlorophenylacetic acid	4.066			
3-Chlorophenylacetic acid	4.140			
4-Chlorophenylacetic acid	4.190			
2-Chlorophenylalanine	2.23(+1)	8.94(0)		
3-Chlorophenylalanine	2.17(+1)	8.91(0)		
DL-4-Chlorophenylalanine	2.08(+1)	8.96(0)		
4-Chlorophenylarsonic acid	3.33	8.25		
2-Chlorophenylphosphonic acid	1.63	6.98		
3-Chlorophenylphosphonic acid	1.55	6.65		
4-Chlorophenylphosphonic acid	1.66	6.75		
3-(2'-Chlorophenyl)propanoic acid	4.577			
3-(3'-Chlorophenyl)propanoic acid	4.585			
3-(4'-Chlorophenyl)propanoic acid	4.607			
3-Chlorophenylselenic acid	4.47			
4-Chlorophenylselenic acid	4.48			
4-Chloro-1,2-phthalic acid	1.60			
2-Chloropropanoic acid	2.84			
3-Chloropropanoic acid	3.992			
2-Chloropropylarsonic acid (18°C)	3.76	8.39		
3-Chloropropylarsonic acid (18°C)	3.63	8.53		
Chloropropynoic acid	1.845			
2-Chloropyridine	0.49(+1)			
3-Chloropyridine	2.84(+1)			
4-Chloropyridine	3.83(+1)			
7-Chlorotetracycline	3.30(+1)	7.44	9.27	
4-Chloro-2-(2'-thiazolylazo)phenol	7.09			
4-Chlorothiophenol	5.9			
N-Chloro- <i>p</i> -toluenesulfonamide	4.54(+1)			
3-Chloro- <i>o</i> -toluidine	2.49(+1)			
4-Chloro- <i>o</i> -toluidine	3.385(+1)			
5-Chloro- <i>o</i> -toluidine	3.85(+1)			
6-Chloro- <i>o</i> -toluidine	3.62(+1)			
Chrome Azurol S	2.45	4.86	11.47	
Chrome Dark Blue	7.56	9.3	12.4	
Cinchonine	5.85(+2)	9.92(+1)		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
<i>cis</i> -Cinnamic acid	3.879			
<i>trans</i> -Cinnamic acid	4.438			
Citraconic acid	2.29(0)	6.15(−1)		
Citric acid	3.128	4.761	6.396	
L-(+)-Citrulline	2.43(+1)	9.41(0)		
Cocaine	8.41(+1)			
Codeine	7.95(+1)			
Colchicine	1.65(+1)			
Coniine ($\mu = 0.5$)	11.24(+1)			
Creatine (40 °C)	3.28(+1)			
Creatinine	3.57(+1)			
<i>o</i> -Cresol	10.26			
<i>m</i> -Cresol	10.00			
<i>p</i> -Cresol	10.26			
Cumene hydroperoxide	12.60			
Cupreine	7.63(+1)			
Cyanamide	10.27			
Cyanoacetic acid	2.460			
Cyanoacetohydrazide	2.34(+2)	11.17(+1)		
2-Cyanobenzoic acid	3.14			
3-Cyanobenzoic acid	3.60			
4-Cyanobenzoic acid	3.55			
4-Cyanobutanoic acid	4.44			
<i>trans</i> -1-Cyanocyclohexane-2-carboxylic acid	3.865			
4-Cyano-2,6-dimethylphenol	8.27			
4-Cyano-3,5-dimethylphenol	8.21			
2-Cyanoethylamine	7.7(+1)			
<i>N</i> -(2-Cyano)ethylnorcodeine	5.68(+1)			
Cyanomethylamine	5.34(+1)			
2-Cyano-2-methyl-2-phenylacetic acid	2.290			
1-Cyanomethylpiperidine	4.55(+1)			
2-Cyano-2-methylpropanoic acid	2.422			
3-Cyanophenol	8.61			
<i>o</i> -Cyanophenoxyacetic acid	2.98			
<i>m</i> -Cyanophenoxyacetic acid	3.03			
<i>p</i> -Cyanophenoxyacetic acid	2.93			
2-Cyanopropanoic acid	2.37			
3-Cyanopropanoic acid	3.99			
2-Cyanopyridine	−0.26(+1)			

*cis*-Cinnamic acid

Citraconic acid



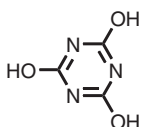
Citric acid



Cumene hydroperoxide

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

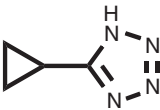
Substance	pK_1	pK_2	pK_3	pK_4
3-Cyanopyridine	1.45(+1)			
4-Cyanopyridine	1.90(+1)			
Cyanuric acid	6.78			
Cyclobutanecarboxylic acid	4.785			
1,1-Cyclobutanedicarboxylic acid	3.13	5.88		
<i>cis</i> -1,2-Cyclobutanedicarboxylic acid	3.90	5.89		
<i>trans</i> -1,2-Cyclobutanedicarboxylic acid	3.79	5.61		
<i>cis</i> -1,3-Cyclobutanedicarboxylic acid	4.04	5.31		
<i>trans</i> -1,3-Cyclobutanedicarboxylic acid	3.81	5.28		
Cyclohexanecarboxylic acid	4.90			
1,1-Cyclohexanediactic acid	3.49	6.96		
<i>cis</i> -1,2-Cyclohexanediactic acid (20°C)	4.42	5.45		
<i>trans</i> -1,2-Cyclohexanediactic acid (20°C)	4.38	5.42		
<i>cis</i> -1,2-Cyclohexanediamine	6.43(+2)	9.93(+1)		
<i>trans</i> -1,2-Cyclohexanediamine	6.34(+2)	9.74(+1)		
1,1-Cyclohexanedicarboxylic acid	3.45	4.11		
<i>cis</i> -1,2-Cyclohexanedicarboxylic acid (20°C)	4.34	6.76		
<i>trans</i> -1,2-Cyclohexanedicarboxylic acid (20°C)	4.18	5.93		
<i>cis</i> -1,3-Cyclohexanedicarboxylic acid (16°C)	4.10	5.46		
<i>trans</i> -1,3-Cyclohexanedicarboxylic acid (19°C)	4.31	5.73		
<i>trans</i> -1,4-Cyclohexanedicarboxylic acid (16°C)	4.18	5.42		
1,3-Cyclohexanedione	5.26			
<i>cis,cis</i> -1,3,5-Cyclohexanetriamine	6.9(+3)	8.7(+2)	10.4(+1)	
Cyclohexanonimine	9.15			
<i>cis</i> -4-Cyclohexene-1,2-dicarboxylic acid (20°C)	3.89	6.79		
<i>trans</i> -4-Cyclohexene-1,2-dicarboxylic acid (20°C)	3.95	5.81		
Cyclohexylacetic acid	4.51			
Cyclohexylamine	10.64(+1)			
2-(Cyclohexylamino)ethanesulfonic acid (CHES) (20°C)	9.55			



Cyanuric acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

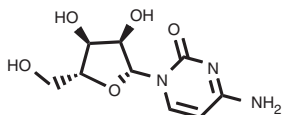
Substance	pK ₁	pK ₂	pK ₃	pK ₄
3-Cyclohexylamino- 1-propanesulfonic acid (CAPS) (20 °C)	10.40			
4-Cyclohexylbutanoic acid	4.95			
Cyclohexylcyanoacetic acid	2.367			
1,2-Cyclohexylenedinitriloacetic acid (μ = 0.1)	2.4	3.5	6.16	12.35
3-Cyclohexylpropanoic acid	4.91			
2-Cyclohexylpyrrolidine	10.76(+1)			
2-Cyclohexyl-2-pyrroline	7.91(+1)			
Cyclohexylthioacetic acid	3.488			
Cyclopentanecarboxylic acid	4.905			
cis-Cyclopentane-1-carboxylic acid- 2-acetic acid	4.40	5.79		
trans-Cyclopentane-1-carboxylic acid-2-acetic acid	4.39	5.67		
Cyclopentane-1,2-diamine- <i>N,N',N'</i> - tetraacetic acid (μ = 0.1)				10.20
Cyclopentane-1,1-dicarboxylic acid	3.23	4.08		
cis-Cyclopentane-1,2-dicarboxylic acid	4.43	6.67		
trans-Cyclopentane-1,2-dicarboxylic acid	3.96	5.85		
cis-Cyclopentane-1,3-dicarboxylic acid	4.26	5.51		
trans-Cyclopentane-1,3-dicarboxylic acid	4.32	5.42		
Cyclopentylamine	10.65(+1)			
1,1-Cyclopentyldiacetic acid	3.80	6.77		
cis-Cyclopentyl-1,2-diacetic acid	4.42	5.42		
trans-Cyclopentyl-1,2-diacetic acid	4.43	5.43		
Cyclopropanecarboxylic acid	4.827			
Cyclopropane-1,1-dicarboxylic acid	1.82	5.43		
cis-Cyclopropane-1,2-dicarboxylic acid	3.33	6.47		
trans-Cyclopropane-1,2-dicarboxylic acid	3.65	5.13		
Cyclopropylamine	9.10(+1)			
5-Cyclopropyl-1,2,3,4-tetrazole	4.90(+1)			
L-Cysteic acid (3-sulfo-L-alanine)	1.89(+1)	8.7(0)		
L-(+)-Cysteine	1.71(+1)	8.39(0)	10.70(SH)	



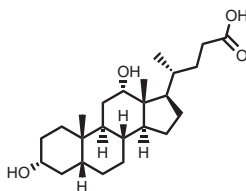
5-Cyclopropyl-1,2,3,4-tetrazole

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
L-(+)-Cysteine, ethyl ester	6.69 (NH_3^+)	9.17(SH)		
L-(+)-Cysteine, methyl ester	6.56 (NH_3^+)	8.99(SH)		
L-Cysteinyl-L-asparagine	2.97	7.09	8.47	
L-Cystine (35°C)	1.6(+2)	2.1(+1)	8.02(0)	8.71(-1)
Cystinylglycylglycine (35°C)	3.12	3.21	6.01	6.87
Cytidine	4.08(+1)	12.24(0)		
Cytidine-2'-phosphoric acid	0.8(+1)	4.36(0)	6.17(-1)	
Cytidine-3'-phosphoric acid	0.80(+1)	4.31(0)	6.04(-1)	13.2(sugar)
Cytidine-5'-phosphoric acid		4.39(0)	6.62(-1)	
Cytosine	4.58(+1)	12.15(0)		
Decanedioic acid (sebacic acid)	4.59	5.59		
Dehydroascorbic acid (20°C)	3.21	7.92	10.3	
2'-Deoxyadenosine ($\mu = 0.1$)	3.8(+1)			
Deoxycholic acid	6.58			
2-Deoxyglucose	12.52			
2-Deoxyguanosine ($\mu = 0.1$)	2.5(+1)			
5-Desoxypyridoxal ($\mu = 0$)	4.17(+1)	8.14(OH)		
1,1-Diacetic acid semicarbazide (30°C, $\mu = 0.1$)	2.96	4.04		
Diacetylacetone	7.42			
Diallylamine ($\mu = 0.02$)	9.29(+1)			
5,5-Diallylbarbituric acid	7.78(0)			
1,3-Diamino-2-aminomethylpropane	6.44(+3)	8.56(+2)	10.38(+1)	
3,5-Diaminobenzoic acid	5.30			
1,3-Diamino- <i>N,N'</i> -bis- (2-aminoethyl)propane ($\mu = 0.5$)	6.01(+4)	7.26(+3)	9.49(+2)	10.23(+1)
2,4-Diaminobutanoic acid (20°C)	1.85(+2)	8.24(+1)	10.40(0)	
2,2'-Diaminodithiethyl sulfide (30°C)	8.84(+2)	9.64(+1)		
1,8-Diamino-3,6-dithiooctane (30°C)	8.43(+2)	9.31(+1)		
2,7-Diaminooctanedioic acid (20°C, $\mu = 0.1$)	1.84(+2)	2.64(+1)	9.23(0)	9.89(-1)
1,8-Diamino-3,6-octanedione (30°C)	8.60(+2)	9.57(+1)		
1,8-Diamino-3-oxa-6-thiooctane	8.54(+2)	9.46(+1)		
2,3-Diaminopropanoic acid ($\mu = 0.1$)	1.33(+2)	6.674(+1)	9.623(0)	
2,3-Diaminopropanoic acid, methyl ester ($\mu = 0.1$)	4.412(+1)	8.250(0)		



Cytidine



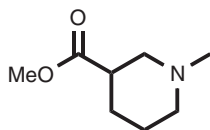
Deoxycholic acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
1,3-Diamino-2-propanol (20 °C)	7.93(+2)	9.69(+1)	7.60(−1)	
2,5-Diaminopyridine (20 °C)	2.13(+2)	6.48(+1)		
1,4-Diazabicyclo[2.2.2]octane	2.90(+2)	8.60(+1)		
Dibenzylamine	8.52(+1)			
Dibenzylsuccinic acid (20 °C)	3.96	6.66		
Dibromoacetic acid	1.39			
3,5-Dibromoaniline	2.35(+1)			
3,5-Dibromophenol	8.056			
2,2-Dibromopropanoic acid	1.48			
2,3-Dibromopropanoic acid	2.33			
<i>rac</i> -2,3-Dibromosuccinic acid (20 °C)	1.43	2.24		
<i>meso</i> -2,3-Dibromosuccinic acid (20 °C)	1.51	2.71		
3,5-Dibromo- <i>p</i> -L-tyrosine	2.17(+1)	6.45(0)		
Dibutylamine	11.25(+1)			
Di- <i>sec</i> -butylamine	10.91(+1)			
2,6-Di- <i>tert</i> -butylpyridine	3.58(+1)			
<i>rac</i> -2,3-Di- <i>tert</i> -butylsuccinic acid ($\mu = 0.1$)	3.58	10.2		
1,12-Dicarboxydodecaborane	9.07	10.23		
Dichloroacetic acid	1.26			
Dichloroacetylacetic acid	2.11			
3,5-Dichloroaniline	2.37(+1)			
1,3-Dichloro-2,5-dihydroxybenzene ($\mu = 0.65$)	7.30	9.99		
2,5-Dichloro-3,6-dihydroxy- <i>p</i> -benzoquinone	1.09	2.42		
Dichloromethylphosphonic acid	1.14	5.61		
2,4-Dichloro-6-nitroaniline	−3.00(+1)			
2,5-Dichloro-4-nitroaniline	−1.74(+1)			
2,6-Dichloro-4-nitroaniline	−3.31(+1)			
2,3-Dichlorophenol	7.44			
2,4-Dichlorophenol	7.85			
2,6-Dichlorophenol	6.78			
3,4-Dichlorophenol	8.630			
3,5-Dichlorophenol	8.179			
2,4-Dichlorophenoxyacetic acid (2,4-D)	2.64			
4,6-Dichlorophenoxy-2-methylacetic acid	3.13			
3,6-Dichlorophthalic acid	1.46			
2,2-Dichloropropanoic acid	2.06			
2,3-Dichloropropanoic acid	2.85			
<i>rac</i> -2,3-Dichlorosuccinic acid (20 °C)	1.43	2.81		
<i>meso</i> -2,3-Dichlorosuccinic acid	1.49	2.97		
3,5-Dichloro- <i>p</i> -tyrosine	2.12	6.47	7.62	
2-Dicyanoethylamine	5.14(+1)			
2,2-Dicyanopropanoic acid	−2.8			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Dicyclohexylamine	11.25(+1)			
Dicyclopentylamine	10.93(+1)			
Didodecylamine	10.99(+)			
Diethanolamine	8.88(+1)			
Di(ethoxyethyl)amine	8.47(+1)			
3,5-Diethoxyphenol	9.370			
3-(Diethoxyphosphinyl)benzoic acid	3.65			
4-(Diethoxyphosphinyl)benzoic acid	3.60			
3-(Diethoxyphosphinyl)phenol	8.66			
4-(Diethoxyphosphinyl)phenol	8.28			
Diethylamine	10.8(+1)			
2-(Diethylamino)ethyl- 4-aminobenzoate	8.85(+1)			
α -(Diethylamino)toluene	9.44(+1)			
<i>N,N</i> -Diethylaniline	6.56(+1)			
5,5-Diethylbarbituric acid (veronal)	8.020(0)			
<i>N,N</i> -Diethylbenzylamine	9.48(+1)			
Diethylbiguanide (30°C)	2.53(+1)	11.68(0)		
Diethylenetriamine	4.42(+3)	9.21(+2)	10.02(+1)	
Diethylenetriaminepentaacetic acid ($pK_5 = 10.58$)	1.80(0)	2.55(-1)	4.33(-2)	8.60(-3)
<i>N,N</i> -Diethylethylenediamine	7.70(+2)	10.46(+1)		
2,2-Diethylglutaric acid	3.62	7.12		
<i>N,N</i> -Diethylglycine	2.04(+1)	10.47(0)		
Diethylglycolic acid (18°C)	3.804			
Diethylmalonic acid	2.151	7.417		
Diethylmethylamine	10.43(+1)			
<i>rac</i> -2,3-Diethylsuccinic acid	3.63	6.46		
<i>meso</i> -2,3-Diethylsuccinic acid	3.54	6.59		
<i>N,N</i> -Diethyl- <i>o</i> -toluidine	7.18(+1)			
Difluoroacetic acid	1.33			
3,3-Difluoroacrylic acid	3.17			
Diglycolic acid	2.96			
Diguanidine	12.8			
Dihexylamine	11.0(+1)			
Dihydroarecaidine	9.70			
Dihydroarecaidine, methyl ester	8.39			
Dihydrocodeine	8.75(+1)			
Dihydroergonovine	7.38(+1)			
α -Dihydrolysergic acid	3.57	8.45		



Dihydroarecaidine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

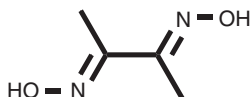
Substance	pK_1	pK_2	pK_3	pK_4
γ -Dihydrolysergic acid	3.60	8.71		
α -Dihydrolysergol	8.30			
β -Dihydrolysergol	8.23			
Dihydromorphine	9.35			
3,4-Dihydroxyalanine	2.32(+1)	8.68(0)	9.87(−1)	
1,2-Dihydroxyanthraquinone-3-sulfonic acid (alizarin-3-sulfonic acid)		5.54(−1)	11.01(−2)	
3,4-Dihydroxybenzaldehyde	7.55			
1,2-Dihydroxybenzene (pyrocatechol) ($\mu = 0.1$)	9.356(0)	12.98(−1)		
1,3-Dihydroxybenzene (resorcinol)	9.44(0)	12.32(−1)		
1,4-Dihydroxybenzene (hydroquinone)	9.91(0)	12.04(−1)		
4,5-Dihydroxybenzene-1,3-disulfonic acid			7.66(−2)	12.6(−3)
2,3-Dihydroxybenzoic acid (30 °C)	2.98	10.14		
2,4-Dihydroxybenzoic acid (β -resorcylic acid)	3.29	8.98		
2,5-Dihydroxybenzoic acid	2.97	10.50		
2,6-Dihydroxybenzoic acid	1.30			
3,4-Dihydroxybenzoic acid	4.48	8.67	11.74	
3,5-Dihydroxybenzoic acid	4.04			
2,5-Dihydroxy- <i>p</i> -benzoquinone	2.71	5.18		
3,4-Dihydroxy-3-cyclobutene-1,2-dione	0.541	3.480		
2,3-Dihydroxy-2-cyclopenten-1-one (20 °C)	4.72			
1,4-Dihydroxy-2,6-dinitrobenzene	4.42	9.14		
Di(2,2'-hydroxyethyl)amine	8.8(+1)			
<i>N,N</i> -Di(2-hydroxyethyl)glycine	8.333			
Dihydroxymaleic acid	1.10			
Dihydroxymalic acid	1.92			
1,3-Dihydroxy-2-methylbenzene ($\mu = 0.65$)	10.05	11.64		
2,2-Di(hydroxymethyl)-3-hydroxypropanoic acid	4.460			
2,4-Dihydroxy-5-methylpyrimidine	9.90			
2,4-Dihydroxy-6-methylpyrimidine	9.52			
1,4-Dihydroxynaphthalene (26 °C, $\mu = 0.65$)	9.37	10.93		
1,2-Dihydroxy-3-nitrobenzene	6.68			
1,2-Dihydroxy-4-nitrobenzene ($\mu = 0.1$)	6.701			
2,4-Dihydroxy-1-phenylazobenzene ($\mu = 0.1$)	11.98			
2,4-Dihydroxyoxazolidine	6.11(+1)			
2,4-Dihydroxypteridine	< 1.3	7.92		
2,6-Dihydroxypurine	7.53(0)	11.84(−1)		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
2,4-Dihydroxypyridine (20°C)	1.37(+1)	6.45(0)	13(−1)	
Dihydroxytartaric acid	1.95	4.00		
1,4-Dihydroxy-2,3,5,6-tetramethylbenzene ($\mu = 0.65$)	11.25	12.70		
3,5-Diiodoaniline	2.37(+1)			
2,5-Diiodohistamine	2.31(+2)	8.20(+1)	10.11(0)	
2,5-Diiodohistidine ($\mu = 0.1$)	2.72	8.18	9.76	
3,5-Diiodophenol	8.103			
3,5-Diiodotyrosine	2.117(+1)	6.479(0)	7.821(−1)	
Diisopropylmalonic acid	2.124	8.848		
Dilactic acid	2.955			
<i>threo</i> -1,4-Dimercapto-2,3-butanediol	8.9			
<i>meso</i> -2,3-Dimercaptosuccinic acid	2.71	3.48	8.89(SH)	10.79(SH)
3,5-Dimethoxyaniline	3.86(+1)			
2,6-Dimethoxybenzoic acid	3.44			
1,10-Dimethoxy-3,8-dimethyl-4,7-phenanthroline	7.21			
Di(2-methoxyethyl)amine	9.51(+1)			
3,5-Dimethoxyphenol	9.345			
(3,4-Dimethoxy)phenylacetic acid	4.333			
Dimethylamine	10.77(+1)			
4-Dimethylaminobenzaldehyde	1.647(+1)			
<i>N,N</i> -Dimethylaminocyclohexane	10.72(+1)			
4-Dimethylamino-1-phenyl-3-pyrazolin-5-one	4.18(+1)			
4-Dimethylamino-3,5-dimethylpyridine (20°C)	8.15(+1)			
2-(Dimethylamino)ethanol	9.26(+1)			
2-[2-(Dimethylamino)ethyl]pyridine	3.46(+2)	8.75(+1)		
3-(Dimethylaminoethyl)pyridine	4.30(+2)	8.86(+1)		
4-(Dimethylaminoethyl)pyridine	4.66(+2)	8.70(+1)		
4-(Dimethylamino)-3-ethylpyridine (20°C)	8.66(+1)			
4-(Dimethylamino)-3-isopropylpyridine (20°C)	8.27(+1)			
2-(Dimethylaminomethyl)pyridine	2.58(+2)	8.12(+1)		
3-(Dimethylaminomethyl)pyridine	3.17(+2)	8.00(+1)		
4-(Dimethylaminomethyl)pyridine	3.39(+2)	7.66(+1)		
4-(Dimethylamino)-3-methylpyridine (20°C)	8.68(+1)			
4-(Dimethylaminophenyl)phosphonic acid	2.0(+1)	4.2	7.35	
3-(Dimethylamino)propanoic acid	9.85(+1)			
4-(Dimethylamino)pyridine (20°C)	6.09(+1)			
<i>N,N</i> -Dimethylaniline	5.15(+1)			
2,3-Dimethylaniline	4.70(+1)			
2,4-Dimethylaniline	4.89(+1)			
2,5-Dimethylaniline	4.53(+1)			
2,6-Dimethylaniline	3.95(+1)			

TABLE 8.1 pK_a Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3,4-Dimethylaniline	5.17(+1)			
3,5-Dimethylaniline	4.765(+1)			
<i>N,N</i> -Dimethylaniline-4-phosphonic acid (17°C)	2.0(+1)	4.2	7.39	
Dimethylarsinic acid (cacodylic acid)	6.273			
1,3-Dimethylbarbituric acid	4.68(+1)			
2,3-Dimethylbenzoic acid	3.771			
2,4-Dimethylbenzoic acid	4.217			
2,5-Dimethylbenzoic acid	3.990			
2,6-Dimethylbenzoic acid	3.362			
3,4-Dimethylbenzoic acid	4.41			
3,5-Dimethylbenzoic acid	4.302			
<i>N,N</i> -Dimethylbenzylamine	9.02(+1)			
Dimethylbiguanide	2.77(+1)	11.52		
2,2-Dimethylbutanoic acid (18°C)	5.03			
Dimethylchlorotetracycline ($\mu = 0.01$)	3.30(+1)			
2,6-Dimethyl-4-cyanophenol	8.27			
3,5-Dimethyl-4-cyanophenol	8.21			
5,5-Dimethyl-1,3-cyclohexanedione	5.15			
<i>cis</i> -3,3-Dimethyl-1,2-cyclopropanedicarboxylic acid	2.34	8.31		
<i>trans</i> -3,3-Dimethyl-1,2-cyclopropanedicarboxylic acid	3.92	5.32		
3,5-Dimethyl-4-(dimethylamino)-pyridine (20°C)	8.12(+1)			
2,2-Dimethyl-1,3-dioxane-4,6-dione	5.1			
1,1-Dimethylethanethiol ($\mu = 0.1$)	11.22			
<i>N,N</i> -Dimethylethylenediamine- <i>N,N</i> -diacetic acid	6.63	9.53		
<i>N,N'</i> -Dimethylethylenediamine- <i>N,N'</i> -diacetic acid	7.40	10.16		
<i>N,N</i> -Dimethylethylenediamine- <i>N,N'</i> -diacetic acid	5.99	9.97		
<i>N,N</i> -Dimethylglycine	2.146(+1)	9.940(0)		
Dimethylglycolic acid (18°C)	4.04			
<i>N,N</i> -Dimethylglycylglycine	3.11(+1)	8.09(0)		
Dimethylglyoxime	10.60			
5,5-Dimethyl-2,4-hexanedione	10.01			
5,5-Dimethylhydantoin	9.19			
2,4-Dimethyl-8-hydroxyquinoline	6.20(+1)	10.60(0)		
3,4-Dimethyl-8-hydroxyquinoline	5.80(+1)	10.05(0)		



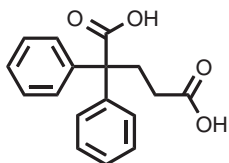
Dimethylglyoxime

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

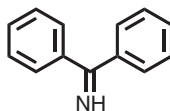
Substance	pK_1	pK_2	pK_3	pK_4
2,4-Dimethyl-8-hydroxyquinoline-7-sulfonic acid	3.20 (NH ⁺)	10.14(OH)		
Dimethylhydroxytetracycline	7.5	9.4		
2,4-Dimethylimidazole	8.38(+1)			
Dimethylmalic acid	3.17	6.06		
2,2-Dimethylmalonic acid	3.17	6.06		
3,5-Dimethyl-4-(methylamino)pyridine (20°C)	9.96(+1)			
2,3-Dimethylnaphthalene-1-carboxylic acid	3.33			
2,6-Dimethyl-4-nitrophenol	7.190			
3,5-Dimethyl-4-nitrophenol	8.245			
α,α -Dimethyloxaloacetic acid	1.77	4.62		
3,3-Dimethylpentanedioic acid	3.70	6.34		
2,2-Dimethylpentanoic acid	4.969			
4,4-Dimethylpentanoic acid (18°C)	4.79			
2,3-Dimethylphenol	10.50			
2,4-Dimethylphenol	10.58			
2,5-Dimethylphenol	10.22			
2,6-Dimethylphenol	10.59			
3,4-Dimethylphenol	10.32			
3,5-Dimethylphenol	10.15			
2,6-Dimethylphenoxyacetic acid	3.356			
Dimethylphenylsilylacetic acid	5.27			
<i>N,N'</i> -Dimethylpiperazine	4.630(+2)	8.539(+1)		
1,2-Dimethylpiperidine	10.22			
<i>cis</i> -2,6-Dimethylpiperidine	11.07(+1)			
2,2-Dimethylpropanoic acid (pivalic acid)	5.031			
2,2'-Dimethylpropylphosphonic acid	2.84	8.65		
2,4-Dimethylpyridine (2,4-lutidine)	6.74(+1)			
2,5-Dimethylpyridine (2,5-lutidine)	6.43(+1)			
2,6-Dimethylpyridine (2,6-lutidine)	6.71(+1)			
3,4-Dimethylpyridine (3,4-lutidine)	6.47(+1)			
3,5-Dimethylpyridine (3,5-lutidine)	6.09(+1)			
2,4-Dimethylpyridine-1-oxide	1.627(+1)			
2,5-Dimethylpyridine-1-oxide	1.208(+1)			
2,6-Dimethylpyridine-1-oxide	1.366(+1)			
3,4-Dimethylpyridine-1-oxide	1.493(+1)			
3,5-Dimethylpyridine-1-oxide	1.181(+1)			
2,3-Dimethylquinoline	4.94(+1)			
2,6-Dimethylquinoline	5.46(+1)			
<i>meso</i> -2,2-Dimethylsuccinic acid	3.77	5.936		
<i>rac</i> -2,2-Dimethylsuccinic acid	3.93	6.20		
<i>D</i> -2,3-Dimethylsuccinic acid	3.82	5.93		
<i>meso</i> -2,3-Dimethylsuccinic acid	3.67	5.30		
<i>rac</i> -2,3-Dimethylsuccinic acid	3.94	6.20		
2,4-Dimethylthiazole ($\mu = 0.1$)	3.98			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
2,5-Dimethylthiazole ($\mu = 0.1$)	3.91			
4,5-Dimethylthiazole ($\mu = 0.1$)	3.73			
<i>N,N</i> -Dimethyl- <i>o</i> -toluidine	5.86(+1)			
<i>N,N</i> -Dimethyl- <i>p</i> -toluidine	7.24(+1)			
2,4-Dinitroaniline	-4.25(+1)			
2,6-Dinitroaniline	-5.23(+1)			
3,5-Dinitroaniline	0.229(+1)			
2,3-Dinitrobenzoic acid	1.85			
2,4-Dinitrobenzoic acid	1.43			
2,5-Dinitrobenzoic acid	1.62			
2,6-Dinitrobenzoic acid	1.14			
3,4-Dinitrobenzoic acid	2.82			
3,5-Dinitrobenzoic acid	2.85			
1,1-Dinitrobutane (20 °C)	5.90			
1,1-Dinitrodecane	3.60			
1,1-Dinitroethane (20 °C)	5.21			
Dinitromethane (20 °C)	3.60			
1,1-Dinitropentane	5.337			
2,4-Dinitrophenol	4.08			
2,5-Dinitrophenol	5.216			
2,6-Dinitrophenol	3.713			
3,4-Dinitrophenol	5.424			
3,5-Dinitrophenol	6.732			
2,4-Dinitrophenylacetic acid	3.50			
1,1-Dinitropropane (20 °C)	5.5			
2,6-Dioxo-1,2,3,6-tetrahydro-4-pyrimidinecarboxylic acid (orotic acid)	1.8(+1)	9.55(0)		
Diphenylacetic acid	3.939			
Diphenylamine	0.9(+1)			
2,2-Diphenylglutaric acid (20 °C)	3.91	5.38		
1,3-Diphenylguanidine	10.12			
2,2-Diphenylheptanedioic acid (20 °C)	4.28	5.39		
2,2-Diphenylhexanedioic acid (20 °C)	4.17	5.40		
3,3-Diphenylhexanedioic acid	4.22	5.19		
Diphenylhydroxyacetic acid (35 °C)	3.05			
Diphenylketimine	6.82			
2,2-Diphenylnonanedioic acid (20 °C)	4.33	5.38		



2,2-Diphenylglutaric acid



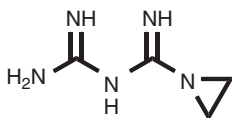
Diphenylketimine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

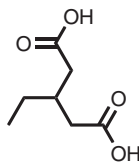
Substance	pK_1	pK_2	pK_3	pK_4
<i>meso</i> -2,2-Diphenylsuccinic acid	3.48			
<i>rac</i> -2,2-Diphenylsuccinic acid	3.58			
2,2-Diphenylsuccinic acid, 1-methyl ester (20°C)	4.47			
2,2-Diphenylsuccinic acid, 4-methyl ester (20°C)	3.900			
Diphenylthiocarbazon	4.50	15		
Dipropylamine	10.91(+1)			
Dipropylenetriamine	7.72(+3)	9.56(+2)	10.65(+1)	
2,2-Dipropylglutaric acid	3.688	7.31		
Dipropylmalonic acid	2.04	7.51		
2,2'-Dipyridyl	-0.52(+2)	4.352(+1)		
2,3'-Dipyridyl (20°C)	1.52(+2)	4.42(+1)		
2,4'-Dipyridyl (20°C)	1.19(+2)	4.77(+1)		
3,3'-Dipyridyl (20°C, $\mu = 0.2$)	3.0(+2)	4.60(+1)		
3,4'-Dipyridyl (20°C, $\mu = 0.2$)	3.0(+2)	4.85(+1)		
4,4'-Dipyridyl	3.17(+2)	4.82(+1)		
Dithiodiacetic acid (18°C)	3.075	4.201		
1,4-Dithioerythritol	9.5			
Dithiooxamide (rubeanic acid)	10.89			
Dulcitol	13.46			
Ecgonine	10.91			
Emetine	7.36(+1)	8.23(0)		
Epinephrine enantiomorph	9.39(+1)			
Epinephrine, pseudo	9.53(+1)			
Ergometrine	7.32(+1)			
Ergonovine	6.73(+1)			
Eriochrome Black T	6.3	11.55		
1,2-Ethanediamine	6.85(+2)	9.92(+1)		
Ethane-1,2-diamino- <i>N,N'</i> -dimethyl- <i>N,N'</i> -diacetic acid (20°C)	6.047(0)	10.068(-1)		
1,2-Ethanedithiol	8.96	10.54		
Ethanethiol ($\mu = 0.015$)	10.61			
Ethoxyacetic acid (18°C)	3.65			
2-Ethoxyaniline (<i>o</i> -phenetidine)	4.47(+1)			
3-Ethoxyaniline	4.17(+1)			
4-Ethoxyaniline	5.25(+1)			
2-Ethoxybenzoic acid (20°C)	4.21			
3-Ethoxybenzoic acid (20°C)	4.17			
4-Ethoxybenzoic acid (20°C)	4.80			
Ethoxycarbonyl ethylamine	9.13(+1)			
2-Ethoxyethanethiol	9.38			
2-Ethoxyethylamine	6.26(+1)			
2-Ethoxyphenol	10.109			
3-Ethoxyphenol	9.655			
(4-Ethoxyphenyl)phosphonic acid	2.06	7.28		
4-Ethoxypyridine	6.67(+1)			
Ethyl acetoacetate	10.68			
3-Ethylacrylic acid	4.695			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
<i>N</i> -Ethylalanine	2.22(+1)	10.22(0)		
Ethylamine	10.63(+1)			
(3-Ethylamino)phenylphosphonic acid	1.1(+1)	4.90(0)	7.24(−1)	
<i>N</i> -Ethylaniline	5.11(+1)			
2-Ethylaniline	4.42(+1)			
3-Ethylaniline	4.70(+1)			
4-Ethylaniline	5.00(+1)			
Ethylarsonic acid (18 °C)	3.89	8.35		
Ethylbarbituric acid	3.69(+1)			
2-Ethylbenzimidazole ($\mu = 0.16$)	6.27(+1)			
2-Ethylbenzoic acid	3.79			
4-Ethylbenzoic acid	4.35			
Ethylbiguanide	2.09(+1)	11.47(0)		
2-Ethylbutanoic acid (20 °C)	4.710			
<i>S</i> -Ethyl-L-cysteine ($\mu = 0.1$)	2.03(+1)	8.60(0)		
Ethylenebiguanide (30 °C)	1.74	2.88	11.34	11.76
Ethylenebis(thioacetic acid) (18 °C)	3.382(0)	4.352(−1)		
Ethylenediamine- <i>N,N'</i> -diacetic acid	6.42	9.46		
Ethylenediamine- <i>N,N</i> -dimethyl- <i>N',N'</i> -diacetic acid	6.047	10.068		
Ethylenediamine- <i>N',N</i> -dipropanoic acid (30 °C)	6.87	9.60		
Ethylenediamine- <i>N,N,N',N'</i> -tetraacetic acid ($\mu = 0.1$)	1.99	2.67	6.16	10.26
Ethylenediamine- <i>N,N,N',N'</i> -tetrapropanoic acid (30 °C)	3.00	3.43	6.77	9.60
Ethylene glycol	14.22			
Ethyleneimine	8.04(+1)			
<i>cis</i> -Ethylene oxide dicarboxylic acid	1.93	3.92		
<i>trans</i> -Ethylene oxide dicarboxylic acid	1.93	3.25		
<i>N</i> -Ethylethylenediamine	7.63(+2)	10.56(+1)		
<i>N</i> -Ethylglycine ($\mu = 0.1$)	2.34(+1)	10.23(0)		
3-Ethylglutaric acid	4.28	5.33		
Ethyl hydroperoxide	11.80			
Ethyl hydrogen malonate	3.55			
3-Ethyl-2-hydroxypyridine	5.00(+1)			
Ethylmalonic acid	2.90(0)	5.55(−1)		



Ethylenebiguanide



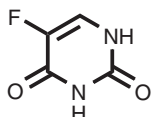
3-Ethylglutaric acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

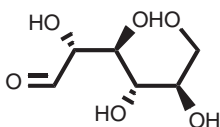
Substance	pK_1	pK_2	pK_3	pK_4
<i>N</i> -Ethyl mercaptoacetamide	8.14(SH)			
Ethyl 2-mercaptoacetate	7.95(SH)			
Ethyl 3-mercaptopropanoate	9.48(SH)			
3-Ethyl-4-(methylamino)pyridine (20°C)	9.90(+1)			
5-Ethyl-5-(1-methylbutyl)barbituric acid	8.11(0)			
Ethyl methyl ketoxime	12.45			
Ethylmethylmalonic acid	2.86(0)	6.41(−1)		
1-Ethyl-2-methylpiperidine	10.66(+1)			
3-Ethyl-6-methylpyridine (20°C)	6.51(+1)			
3-Ethyl-4-methylpyridine-1-oxide	−1.534(+1)			
5-Ethyl-2-methylpyridine-1-oxide	−1.288(+1)			
1-Ethyl-2-methyl-2-pyrroline	11.84(+1)			
Ethylmorphine (15°C)	8.08			
Ethyl nitroacetate	5.85			
3-Ethylpentane-2,4-dione	11.34			
2-Ethylpentanoic acid (18°C)	4.71			
5-Ethyl-5-pentylbarbituric acid	7.960			
2-Ethylphenol	10.2			
3-Ethylphenol	10.07			
4-Ethylphenol	10.0			
4-Ethylphenylacetic acid	4.373			
5-Ethyl-5-phenylbarbituric acid	7.445			
Ethylphosphinic acid	3.29			
Ethylphosphonic acid	2.43	8.05		
1-Ethylpiperidine ($\mu = 0.01$)	10.45(+1)			
2,2-Ethylpropylglutaric acid	3.511			
Ethylpropylmalonic acid	3.14	7.43		
2-Ethylpyridine	5.89(+1)			
3-Ethylpyridine (20°C)	5.80(+1)			
4-Ethylpyridine	5.87(+1)			
Ethyl 3-pyridinecarboxylate	3.35(+1)			
Ethyl 4-pyridinecarboxylate	3.45(+1)			
2-Ethylpyridine-1-oxide	−1.19(+1)			
3-Ethylpyridine-1-oxide	−0.965(+1)			
Ethylpyrrolidine	10.43(+1)			
2-Ethyl-2-pyrroline	7.87(+1)			
Ethylsuccinic acid	4.08(0)			
<i>S</i> -Ethylthioacetic acid	5.06			
<i>N</i> -Ethyl- <i>o</i> -toluidine	4.92(+1)			
<i>N</i> -Ethylveratramine	7.40(+1)			
β -Eucaine	9.35(+1)			
Fluoroacetic acid	2.586			
2-Fluoroacrylic acid	2.55			
2-Fluoroaniline	3.20(+1)			
3-Fluoroaniline	3.58(+1)			
4-Fluoroaniline	4.65(+1)			
2-Fluorobenzoic acid	3.27			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

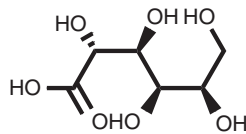
Substance	pK_1	pK_2	pK_3	pK_4
3-Fluorobenzoic acid	3.865			
4-Fluorobenzoic acid	4.14			
Fluoromandelic acid	4.244			
2-Fluorophenol	8.73			
3-Fluorophenol	9.29			
4-Fluorophenol	9.89			
2-Fluorophenoxyacetic acid	3.08			
3-Fluorophenoxyacetic acid	3.08			
4-Fluorophenoxyacetic acid	3.13			
4-Fluorophenylacetic acid	4.25			
2'-Fluorophenylalanine	2.14(+1)	9.01(0)		
3'-Fluorophenylalanine	2.10(+1)	8.98(0)		
4-Fluorophenylalanine	2.13(+1)	9.05(0)		
2-Fluorophenylphosphonic acid	1.64	6.80		
3-Fluorophenylselenic acid	4.34			
4-Fluorophenylselenic acid	4.50			
2-Fluoropyridine	-0.44(+1)			
3-Fluoropyridine	2.97(+1)			
5-Fluorouracil	8.00(0)	ca 13(-1)		
Folic acid (pteroylglutamic acid)	8.26			
Formic acid	3.751			
N-Formylglycine	3.43			
2-Formyl-3-hydroxypyridine (20 °C)	3.40(+1)	6.95(OH)		
4-Formyl-3-hydroxypyridine	4.05(+1)	6.77(OH)		
2-Formyl-3-methoxypyridine (20 °C)	3.89(+1)	12.95		
Formyl-3-methoxypyridine (20 °C)	4.45(+1)	11.7		
D-(-)-Fructose	12.03			
Fumaric acid	3.10	4.60		
2-Furancarboxylic acid (2-furoic acid)	3.164			
D-(+)-Galactose	12.35			
Galactose-1-phosphoric acid	1.00	6.17		
Glucoascorbic acid	4.26	11.58		
D-Gluconic acid	3.86			
α -D-(+)-Glucose	12.28			
α -D-Glucose-1-phosphate	1.11(0)	6.504(-1)		
trans-Glutaconic acid	3.77	5.08		
D-(-)-Glutamic acid	2.162(+1)	4.272(0)	9.358(-1)	
L-Glutamic acid	2.13(+1)	4.31(0)	9.76(-1)	
Glutamic acid, 1-ethyl ester	3.85(+1)	7.84(0)		



5-Fluorouracil



D-(+)-Galactose



D-Gluconic acid

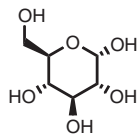
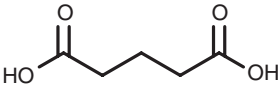
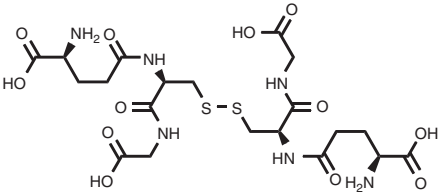
 α -D-(+)-Glucose

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Glutamic acid, 5-ethyl ester	2.15(+1)	9.19(0)		
L-Glutamine ($\mu = 0.2$)	2.15(+1)	9.00(0)		
Glutaric acid	3.77	6.08		
Glutaric acid monoamide	4.600(0)			
Glutarimide	11.43			
Glutathione	2.12(+1)	3.53(0)	8.66	9.12
DL-Glyceric acid	3.64			
Glycerol	14.15			
Glyceryl-1-phosphoric acid		6.656(−1)		
Glyceryl-2-phosphoric acid	1.335(0)	6.650(−1)		
Glycine	2.351(+1)	9.70(0)		
Glycine amide	8.03(+1)			
Glycine, ethyl ester	7.66(+1)			
Glycine hydroxamic acid	7.10	9.10		
Glycine, methyl ester	7.59(+1)			
Glycine- <i>O</i> -phenylphosphorylserine	2.96	8.07		
Glycolic acid	3.831			
<i>N</i> -Glycyl- α -alanine	3.15(+1)	8.33(0)		
Glycylalanylalalanine	3.38(+1)	8.10(0)		
<i>N</i> -Glycylasparagine	2.942			
Glycylaspartic acid	2.81(+1)	4.45(0)	8.60(−1)	
Glycyl-DL-glutamine (18°C)	2.88(+1)	8.33(0)		
<i>N</i> -Glycylglycine	3.126(+1)	8.252(0)		
Glycylglycylcysteine (35°C)	2.71	2.71	7.94	7.94
Glycylglycylglycine	3.225(+1)	8.090(0)		
Glycyl-L-histidine ($\mu = 0.16$)	6.79	8.20		
Glycylisoleucine	8.00			
<i>N</i> -Glycyl-L-leucine	3.180(+1)	8.327(0)		
Glycyl- <i>O</i> -phosphorylserine	2.90	6.02	8.43	
L-Glycylproline ($\mu = 0.1$)	2.81(+1)	8.65(0)		
<i>N</i> -Glycylsarcosine ($\mu = 0.1$)	2.98(+1)	8.55(0)		
<i>N</i> -Glycylserine	2.98(+1)	8.38(0)		
Glycylserylglycine	3.32	7.99		
Glycyltyrosine	2.93	8.45	10.49	
Glycylvaline	3.15	8.18		
Glyoxaline	7.03(+1)			
Glyoxylic acid	3.30(0)			
Guanidineacetic acid	2.82(+1)			



Glutaric acid



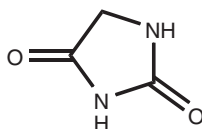
Glutathione

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Guanine	3.3(+1)	9.2	12.3	
Guanine deoxyriboside- 3'-phosphoric acid		2.9	6.4	9.7
Guanosine	1.9(+1)	9.25(0)	12.33 (OH)	
Guanosine-5'-diphosphoric acid ($\mu = 0.1$; $pK_5 = 59.6$)			2.9	6.3
Guanosine-3'-phosphoric acid	0.7	2.3	5.92	9.38
Guanosine-5'-phosphoric acid ($\mu = 0.1$)		2.4	6.1	9.4
Guanosine-5'-triphosphoric acid [$\mu = 0.1$; $pK_5 = 7.10(-3)$; $pK_6 = 9.3(-4)$]				3.0(-2)
Guanylurea	1.80	8.20		
Harmine (20 °C)	7.61(+1)			
Heptafluorobutanoic acid	0.17			
4,4,5,5,6,6,6-Heptafluorohexanoic acid	4.18			
4,4,5,5,6,6,6-Heptafluoro-2-hexenoic acid	3.23			
Heptanedioic acid (pimelic acid)	4.484	5.424		
2,4-Heptanedione	8.43(keto); 9.15(enol)			
Heptanoic acid	4.893			
Heroin	7.6(+1)			
2,4-Hexadienoic acid (sorbic acid)	4.77			
1,1,1,3,3,3-Hexafluoro- 2,2-propanediol	8.801			
1,1,1,3,3,3-Hexafluoro-2-propanol	9.42			
Hexahydroazepine	11.07			
Hexamethyldisilazine	7.55			
1,2,3,8,9,10-Hexamethyl- 4,7-phenanthroline (20 °C)	7.26			
1,6-Hexanediamine	9.830(+2)	10.930(+1)		
1,6-Hexanedioic acid	4.418	5.412		
2,4-Hexanedione	8.49 (enol); 9.32 (keto)			
2,2',4,4',6,6'-Hexanitrodiphenylamine	5.42 (+1)			
Hexanoic acid (20 °C)	4.849			
<i>trans</i> -2-Hexenoic acid	4.74			
<i>trans</i> -3-Hexenoic acid	4.72			
3-Hexen-4-oic acid	4.58			
4-Hexen-5-oic acid	4.74			
Hexylamine	10.64(+1)			
Hexylarsonic acid	4.16	9.19		
Hexylphosphonic acid	2.6	7.9		
DL-Histidine	1.82(+2)	6.00(+1)	9.16(0)	

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Histidine amide ($\mu = 0.2$)	5.78(+2)	7.64(+1)		
Histidine, methyl ester ($\mu = 0.1$)	5.01(+2)	7.23(+1)		
Histidylglycine	2.40(+2)	5.80(+1)	7.82(0)	
Histidylhistidine ($\mu = 0.16$)	5.40(+2)	6.80(+1)	7.95(0)	
DL-Homatropine	9.7(+1)			
DL-Homocysteine	2.222(+1)	8.87	10.86	
Homocysteine ($\mu = 0.1$)	1.593(+2)	2.523(+1)	8.676(0)	9.413(−1)
Hydantoin	9.12			
Hydrastine	6.23(+1)			
Hydrazine- <i>N,N</i> -diacetic acid	< 0.1	2.8	3.8	
Hydrazine- <i>N',N'</i> -diacetic acid	2.40	3.12	7.32	
4-Hydrazinocarbonylpyridine (20°C)	1.82	3.52	10.79	
<i>N</i> -Hydroxyacetamide	9.40			
2'-Hydroxyacetophenone	9.90			
3'-Hydroxyacetophenone	9.19			
4'-Hydroxyacetophenone	8.05			
1-Hydroxyacridine (15°C)	5.72			
2-Hydroxyacridine (15°C)	5.62			
3-Hydroxyacridine (15°C)	5.30			
α -Hydroxyasparagine	2.28(+1)	7.20(0)		
β -Hydroxyasparagine	2.09(+1)	8.29(0)		
Hydroxyaspartic acid	1.91(+1)	3.51(0)	9.11(−1)	
2-Hydroxybenzaldehyde (salicylaldehyde)	8.34			
3-Hydroxybenzaldehyde	9.00			
4-Hydroxybenzaldehyde	7.620			
2-Hydroxybenzaldehyde oxime	1.37(+1)	9.18	12.11	
2-Hydroxybenzamide	8.36			
2-Hydroxybenzenemethanol (2-hydroxybenzyl alcohol)	9.92			
3-Hydroxybenzenemethanol	9.83			
4-Hydroxybenzenemethanol	9.82			
4-Hydroxybenzenesulfonic acid		9.055(−1)		
2-Hydroxybenzohydroxamic acid	5.19			
2-Hydroxybenzoic acid (salicylic acid)	2.98	12.38		
3-Hydroxybenzoic acid	4.076	9.85		
4-Hydroxybenzoic acid	4.582	9.23		
4-Hydroxybenzonitrile	7.95			
2-Hydroxy-5-bromobenzoic acid	2.61			
2-Hydroxybutanoic acid (30°C)	3.65			



Hydantoin

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

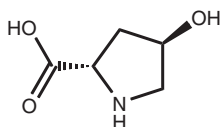
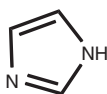
Substance	pK_1	pK_2	pK_3	pK_4
L-3-Hydroxybutanoic acid (30 °C)	4.41			
4-Hydroxybutanoic acid (30 °C)	4.71			
2-Hydroxy-5-chlorobenzoic acid	2.63			
<i>trans</i> -2'-Hydroxycinnamic acid	4.614			
<i>trans</i> -3'-Hydroxycinnamic acid	4.40			
10-Hydroxycodeine	7.12			
<i>cis</i> -2-Hydroxycyclohexane-1-carboxylic acid	4.796			
<i>trans</i> -2-Hydroxycyclohexane-1-carboxylic acid	4.682			
<i>cis</i> -3-Hydroxycyclohexane-1-carboxylic acid	4.602			
<i>trans</i> -3-Hydroxycyclohexane-1-carboxylic acid	4.815			
<i>cis</i> -4-Hydroxycyclohexane-1-carboxylic acid	4.836			
<i>trans</i> -4-Hydroxycyclohexane-1-carboxylic acid	4.687			
1-Hydroxy-2,4-dihydroxymethylbenzene	9.79			
<i>N</i> -(Hydroxyethyl)biguanide	2.8(+2)	11.53(+1)		
<i>N</i> -(2-Hydroxyethyl)ethylenediamine	7.21(+2)	10.12(+1)		
<i>N'</i> -(2-Hydroxyethyl)ethylene-diamine- <i>N,N'</i> -triacetic acid	2.39	5.37	9.93	
<i>N</i> -(2-Hydroxyethyl)iminodiacetic acid ($\mu = 0.1$)	2.2	8.65		
<i>N</i> -(2-Hydroxyethyl)piperazine- <i>N'</i> -ethanesulfonic acid (20 °C)	7.55			
4'-(2-Hydroxyethyl)-1'-piperazine-propanesulfonic acid (20 °C)	8.00			
2-Hydroxyethyltrimethylamine	8.94(+1)			
L- β -Hydroxyglutamic acid	2.09	4.18	9.20	
1-Hydroxy-4-hydroxymethylbenzene	9.84			
5-Hydroxy-2-(hydroxymethyl)-4 <i>H</i> -pyran-4-one	7.90	8.03		
3-Hydroxy-2-hydroxymethylpyridine (20 °C, $\mu = 0.2$)	5.00(+1)	9.07(OH)		
3-Hydroxy-4-hydroxymethylpyridine (20 °C, $\mu = 0.2$)	5.00(+1)	8.95(OH)		
8-Hydroxy-7-iodoquinoline-5-sulfonic acid	2.51(0)	7.417(-1)		
Hydroxylysine (38 °C, $\mu = 0.1$)	2.13(+2)	8.62(+1)	9.67(0)	
2-Hydroxy-3-methoxybenzaldehyde	7.912			
3-Hydroxy-4-methoxybenzaldehyde (isovanillin)	8.889			
4-Hydroxy-3-methoxybenzaldehyde (vanillin)	7.396			
4-Hydroxy-3-methoxybenzoic acid	4.355			
1-Hydroxy-2-methoxybenzylamine	8.70(+1)	10.52(0)		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
2-Hydroxy-1-methoxybenzylamine	8.89(+1)	10.52(0)		
3-Hydroxy-2-methoxybenzylamine	8.94(+1)	10.42(0)		
2-Hydroxymethyl-2-benzeneacetic acid	4.12			
(2-Hydroxy-5-methylbenzene)-methanol	10.15			
2-Hydroxy-3-methylbenzoic acid	2.99			
2-Hydroxy-4-methylbenzoic acid	3.17			
2-Hydroxy-5-methylbenzoic acid	4.08			
2-Hydroxy-6-methylbenzoic acid	3.32			
2-Hydroxy-2-methylbutanoic acid (18°C)	3.991			
3-Hydroxy-2-methylbutanoic acid (18°C)	4.648			
4-Hydroxy-4-methylpentanoic acid (18°C)	4.873			
1-Hydroxymethylphenol	9.95			
Hydroxymethylphosphoric acid	1.91	7.15		
2-Hydroxy-2-methylpropanoic acid ($\mu = 0.1$)	3.717			
2-Hydroxy-4-methylpyridine	4.529(+1)			
8-Hydroxy-2-methylquinoline	5.55(+1)	10.31(0)		
8-Hydroxy-4-methylquinoline	5.56(+1)	10.00(0)		
8-Hydroxy-2-methylquinoline-5-sulfonic acid	4.80(0)	9.30(-1)		
8-Hydroxy-4-methylquinoline-7-sulfonic acid	4.78(0)	10.01(-1)		
8-Hydroxy-6-methylquinoline-5-sulfonic acid	4.20(0)	8.7(-1)		
2-Hydroxy-1-naphthoic acid (20°C)	3.29	9.68		
2-Hydroxy-2-nitrobenzoic acid	2.23			
2-Hydroxy-3-nitrobenzoic acid	1.87			
2-Hydroxy-5-nitrobenzoic acid	2.12			
2-Hydroxy-6-nitrobenzoic acid	2.24			
2-Hydroxy-4-nitrophenylphosphonic acid	1.22	5.39		
8-Hydroxy-7-nitroquinoline-5-sulfonic acid	1.94(0)	5.750(-1)		
3-Hydroxy-4-nitrotoluene ($\mu = 0.1$)	7.41			
4-Hydroxypentanoic acid (18°C)	4.686			
4-Hydroxy-3-pentenoic acid	4.30			
3-Hydroxyphenazine (15°C)	2.67			
4-Hydroxyphenylarsonic acid	3.89	8.37	10.05 (phenol)	
3-Hydroxyphenylboric acid	8.55	10.84		
2-Hydroxy-2-phenylpropanoic acid	3.532			
2-(2-Hydroxyphenyl)pyridine (20°C)	4.19(+1)	10.64		

TABLE 8.1 pK_a Values of Organic Materials in Water at 25 °C (*continued*)

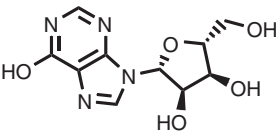
Substance	pK_1	pK_2	pK_3	pK_4
<i>trans</i> -4-Hydroxyproline	1.818(+1)	9.662(0)		
Hydroxypropanedioic acid (tartronic acid)	2.37	4.74		
2-Hydroxypropanoic acid	3.858			
1-Hydroxy-2-propylbenzene	10.50			
4-Hydroxypteridine	1.3(+1)	7.89(0)		
2-Hydroxypyridine	1.25(+1)	11.62(0)		
3-Hydroxypyridine	4.80(+1)	8.72(0)		
4-Hydroxypyridine	3.23(+1)	11.09(0)		
2-Hydroxypyridine- <i>N</i> -oxide	−0.62(+1)	5.97(0)		
2-Hydroxypyrimidine	2.24(+1)	9.17(0)		
4-Hydroxypyrimidine	1.85(+1)	8.59(0)		
8-Hydroxyquinazoline	3.41(+1)	8.65(0)		
2-Hydroxyquinoline (20 °C)	−0.31(+1)	11.74		
3-Hydroxyquinoline (20 °C)	4.30(+1)	8.06(0)		
4-Hydroxyquinoline (20 °C)	2.27(+1)	11.25(0)		
5-Hydroxyquinoline (20 °C)	5.20(+1)	8.54(0)		
6-Hydroxyquinoline (20 °C)	5.17(+1)	8.88(0)		
7-Hydroxyquinoline (20 °C)	5.48(+1)	8.85(0)		
8-Hydroxyquinoline (20 °C)	4.91(+1)	9.81(0)		
8-Hydroxyquinoline-5-sulfonic acid	4.092(+1)	8.776(0)		
DL-Hydroxysuccinic acid (malic acid)	3.458	5.097		
L-Hydroxysuccinic acid	3.40	5.05		
Hydroxytetracycline	3.27(+1)	7.32(0)	9.11(−1)	
5-Hydroxy-1,2,3,4-tetrazole	3.32			
4-Hydroxy-3-(2'-thiazolyazo)toluene	8.36			
2-Hydroxytoluene	10.33			
3-Hydroxytoluene	10.10			
4-Hydroxytoluene	10.276			
4-Hydroxy- α,α,α -trifluorotoluene	8.675			
1-Hydroxy-2,4,6-trihydroxymethylbenzene	9.56			
Hydroxyuracil	8.64			
Hydroxyvaline	2.55(+1)	9.77(0)		
Hyoscyamine	9.68(+1)			
Hypoxanthene	1.79(+1)	8.91(0)	12.07(−1)	
Hypoxanthine	5.3			
Imidazole	6.993(+1)	10.58(0)		
Imidazolidinetrione (parabanic acid)	6.10			

*trans*-4-Hydroxyproline

Imidazole

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

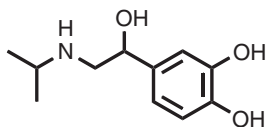
Substance	pK_1	pK_2	pK_3	pK_4
4-(4-Imidazolyl)butanoic acid ($\mu = 0.1$)	4.26(+1)	7.62(0)		
2-(4-Imidazolyl)ethylamine	5.784(+2)	9.756(+1)		
3-(4-Imidazolyl)propanoic acid ($\mu = 0.16$)	3.96(+1)	7.57(0)		
3,3'-Iminobispropanoic acid	4.11(0)	9.61(-1)		
3,3'-Iminobispropylamine (30°C)	8.02(+2)	9.70(+1)	10.70(0)	
2,2'-Iminodiacetic acid (diglycine) (30°C, $\mu = 0.1$)	2.54(0)	9.12(-1)		
4-Indanol	10.32			
Indole-3-acetic acid	4.75			
Inosine	ca 1.5(+1)	8.96(0)	12.36	
Inosine-5'-phosphoric acid	1.54(0)	6.66(-1)		
Inosine-5'-triphosphoric acid [$pK_5 = 7.68(-4)$]			2.2(-2)	6.92(-3)
Iodoacetic acid	3.175			
2-Iodoaniline	2.54(+1)			
3-Iodoaniline	3.58(+1)			
4-Iodoaniline	3.82(+1)			
2-Iodobenzoic acid	2.86			
3-Iodobenzoic acid	3.86			
4-Iodobenzoic acid	4.00			
5-Iodohistamine	4.06(+2) (imidazole)	9.20(+1) (NH_3^+)	11.88(0) (imino)	
7-Iodo-8-hydroxyquinoline-5-sulfonic acid	2.514	7.417		
Iodomandelic acid	3.264			
Iodomethylphosphoric acid	1.30	6.72		
2-Iodophenol	8.464			
3-Iodophenol	8.879			
4-Iodophenol	9.200			
2-Iodophenoxyacetic acid	3.17			
3-Iodophenoxyacetic acid	3.13			
4-Iodophenoxyacetic acid	3.16			
2-Iodophenylacetic acid	4.038			
3-Iodophenylacetic acid	4.159			
4-Iodophenylacetic acid	4.178			
2-Iodophenylphosphoric acid	1.74	7.06		
2-Iodopropanoic acid	3.11			
3-Iodopropanoic acid	4.08			
2-Iodopyridine	1.82(+1)			



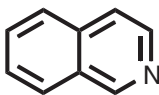
Inosine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

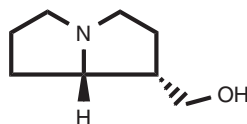
Substance	pK_1	pK_2	pK_3	pK_4
3-Iodopyridine	3.25(+1)			
4-Iodopyridine (20 °C)	4.02(+1)			
Isoasparagine	2.97(+1)	8.02(0)		
Isobutylic acid (18 °C)	4.79			
Isobutylamine	10.41(+1)			
Isochlorotetracycline	3.1(+1)	6.7(0)	8.3(−1)	
Isocreatine	2.84(+1)			
Isoglutamine	3.81(+1)	7.88(0)		
Isohistamine ($\mu = 0.1$)	6.036(+2)	9.274(+1)		
L-Isoleucine	2.318(+1)	9.758(0)		
Isoxysergic acid	3.33(0)	8.46(NH)		
Isopilocarpine (15 °C)	7.18(+1)			
2-(Isopropoxy)benzoic acid (20 °C)	4.24			
3-(Isopropoxy)benzoic acid (20 °C)	4.15			
4-(Isopropoxy)benzoic acid (20 °C)	4.68			
Isopropylamine	10.64(+1)			
N-Isopropylaniline	5.50(+1)			
5-Isopropylbarbituric acid	4.907(+1)			
2-Isopropylbenzene acid	3.64			
4-Isopropylbenzoic acid	4.36			
N-Isopropylglycine ($\mu = 0.1$)	2.36(+1)	10.06(0)		
Isopropylmalonic acid	2.94	5.88		
Isopropylmalonic acid mononitrile	2.401			
3-Isopropyl-4-(methylamino)pyridine (20 °C)	9.96(+1)			
3-Isopropylpentanedioic acid	4.30	5.51		
4-Isopropylphenylacetic acid	4.391			
Isopropylphosphinic acid	3.56			
Isopropylphosphonic acid	2.66	8.44		
2-Isopropylpyridine	5.83(+1)			
3-Isopropylpyridine (20 °C)	5.72(+1)			
4-Isopropylpyridine	6.02(+1)			
DL-Isoproterenol	8.64(+1)			
Isoquinoline	5.40(+1)			
Isoretronecanol	10.83			
L-Isoserine ($\mu = 0.16$)	2.72(+1)	9.25(0)		
Isothiocyanatoacetic acid	6.62			
L-(+)-Lactic acid	3.858			
L-Leucine	2.328(+1)	9.744(0)		
Leucine amide	7.80(+1)			



DL-Isoproterenol



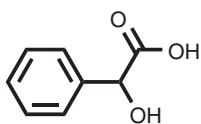
Isoquinoline



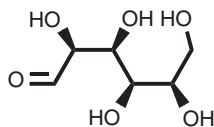
Isoretronecanol

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Leucine, ethyl ester ($\mu = 0.1$)	7.57(+1)			
L-Leucyl-L-asparagine	3.00(+1)	8.12(0)		
L-Leucyl-L-glutamine	2.99(+1)	8.11(0)		
DL-Leucylglycine	3.25(+1)	8.28(0)		
Leucylisoserine (20°C)	3.188(+1)	8.207(0)		
D-Leucyl-L-tyrosine	3.12(+1)	8.38(0)	10.35(−1)	
L-Leucyl-L-tyrosine	3.46(+1)	7.84(0)	10.09(−1)	
Lysergic acid	3.44(+1)	7.68(0)		
L-(+)-Lysine	2.18(+2)	8.95(+1)	10.53(0)	
Lysine, methyl ester ($\mu = 0.1$)	6.965(+1)	10.251(0)		
L-Lysyl-L-alanine	3.22(+1)	7.62(0)	10.70(−1)	
L-Lysyl-D-alanine	3.00(+1)	7.74(0)	10.63(−1)	
Lysylglutamic acid	2.93(+2)	4.47(+1)	7.75(0)	10.50(+1)
L-Lysyl-L-lysine ($\mu = 0.1$)	3.01(+2)	7.53(+1)	10.05(0)	10.01(−1)
L-Lysyl-D-lysine ($\mu = 0.1$)	2.85(+2)	7.53(+1)	9.92(0)	10.89(−1)
L-Lysyl-L-lysyl-L-lysine ($\mu = 0.1$)	3.08(+2)	7.34(+1)	9.80(0)	10.54(−1)
L-Lysyl-D-lysyl-L-lysine ($\mu = 0.1$)	2.91(+2)	7.29(+1)	9.79(0)	10.54(−1)
L-Lysyl-D-lysyl-lysine ($\mu = 0.1$)	2.94(+2)	7.15(+1)	9.60(0)	10.38(−1)
α -D-Lyxose	12.11			
Maleic acid	1.910	6.33		
Malonamic acid	3.641(0)			
Malonic acid	2.826	5.696		
Malonitrile (cyanoacetic acid)	2.460			
Mandelic acid	3.411			
D-(+)-Mannose	12.08			
Mercaptoacetic acid (thioglycolic acid)	3.60(0)	10.56(SH)		
2-Mercaptobenzoic acid (20°C)	4.05(0)			
2-Mercaptobutanoic acid	3.53(0)			
Mercaptodiacetic acid	3.32	4.29		
2-Mercaptoethanesulfonic acid (20°C)		9.5(−1)		
2-Mercaptoethanol	9.88			
2-Mercaptoethylamine	8.27(+1)	10.53(0)		
2-Mercaptohistidine	1.84(+1)	8.47(0)	11.4(SH)	
Mercapto-S-phenylacetic acid ($\mu = 0.1$)	3.9			
2-Mercaptopropane ($\mu = 0.1$)	10.86			
3-Mercapto-1,2-propanediol ($\mu = 0.5$)	9.43			
2-Mercaptopropanoic acid	4.32(0)	10.20(SH)		
3-Mercaptopropanoic acid		10.84(SH)		



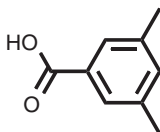
Mandelic acid



D-(+)-Mannose

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
2-Mercaptopyridine (20 °C)	-1.07(+1)	10.00(0)	10.94(SH)	
3-Mercaptopyridine (20 °C)	2.26(+1)	7.03(0)		
4-Mercaptopyridine (20 °C)	1.43(+1)	8.86(0)		
2-Mercaptoquinoline (20 °C)	-1.44(+1)	10.21(0)		
3-Mercaptoquinoline (20 °C)	2.33(+1)	6.13(0)		
4-Mercaptoquinoline (20 °C)	0.77(+1)	8.83(0)		
Mercaptosuccinic acid	3.30(0)	4.94(-1)		
Mesitylenic acid	4.32			
Mesoxaldialdehyde	3.60			
Methacrylic acid	4.66			
Methanethiol	10.70			
DL-Methionine	2.13(+1)	9.28(0)	9.176(0)	
2-(<i>N</i> -Methoxyacetamido)pyridine	2.01(+1)			
3-(<i>N</i> -Methoxyacetamido)pyridine	3.52(+1)			
4-(<i>N</i> -Methoxyacetamido)pyridine	4.62(+1)			
Methoxyacetic acid	3.570			
3-Methoxy-D- α -alanine	2.037(+1)	9.176(0)		
2-Methoxyaniline	4.53(+1)			
3-Methoxyaniline	4.20(+1)			
4-Methoxyaniline	5.36(+1)			
2-Methoxybenzoic acid	4.09			
3-Methoxybenzoic acid	4.08		6.96	
4-Methoxybenzoic acid	4.49			
<i>N,N</i> -Methoxybenzylamine	9.68(+1)			
2-Methoxycarbonylaniline	2.23(+1)			
3-Methoxycarbonylaniline	3.64(+1)			
4-Methoxycarbonylaniline	2.38(+1)			
Methoxycarbonylmethylamine	7.66(+1)			
2-Methoxycarbonylpyridine	2.21(+1)			
3-Methoxycarbonylpyridine	3.13(+1)			
4-Methoxycarbonylpyridine	3.26(+1)			
<i>trans</i> -2-Methoxycinnamic acid	4.462		3.231	
<i>trans</i> -3-Methoxycinnamic acid	4.376			
<i>trans</i> -4-Methoxycinnamic acid	4.539			
2-Methoxyethylamine	9.45(+1)			
2-Methoxy-4-nitrophenylphosphonic acid	1.53	6.96		
2-Methoxyphenol	9.99			
3-Methoxyphenol	9.652			
4-Methoxyphenol	10.20			
(2'-Methoxy)phenoxyacetic acid	3.231			



Mesitylenic acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
(3'-Methoxy)phenoxyacetic acid	3.141			
(4'-Methoxy)phenoxyacetic acid	3.213			
4'-Methoxyphenylacetic acid	4.358			
(4-Methoxyphenyl)phosphinic acid (17°C)	2.35			
(2-Methoxyphenyl)phosphonic acid	2.16	7.77		
(4-Methoxyphenyl)phosphonic acid (17°C)	2.4	7.15		
3-(2'-Methoxyphenyl)propanoic acid	4.804			
3-(3'-Methoxyphenyl)propanoic acid	4.654			
3-(4'-Methoxyphenyl)propanoic acid	4.689			
3-Methoxyphenylselenic acid	4.65			
4-Methoxyphenylselenic acid	5.05			
2-Methoxy-4-(2-propenyl)phenol	10.0			
2-Methoxypyridine	3.06(+1)			
3-Methoxypyridine	4.91(+1)			
4-Methoxypyridine	6.47(+1)			
4-Methoxy-2-(2'-thiazoylazo)phenol	7.83			
2-Methylacrylic acid (18°C)	4.66			
<i>N</i> -Methylalanine	2.22(+1)	10.19(0)		
<i>O</i> -Methylallothreonine ($\mu = 0.1$)	1.92(+1)	8.90(0)		
Methylamine	10.62(+1)			
2-(<i>N</i> -Methylamino)benzoic acid	1.93(+1)	5.34(0)		
3-(<i>N</i> -Methylamino)benzoic acid		5.10(0)		
4-(<i>N</i> -Methylamino)benzoic acid		5.05		
Methylaminodiacetic acid (20°C)	2.146	10.088		
2-(Methylamino)ethanol	9.88(+1)			
2-(2-Methylaminoethyl)pyridine (30°C)	3.58(+2)	9.65(+1)		
2-(Methylaminomethyl)-6-methyl- pyridine ($\mu = 0.5$)	3.03(+2)	9.15(+1)		
2-(Methylaminomethyl)pyridine (30°C)	2.92(+2)	8.82(+1)		
4-Methylamino-3-methylpyridine (20°C)	9.83(+1)			
(3-Methylamino)phenylphosphonic acid	1.1(+1)	4.72(+1)	7.30(-1)	
(4-Methylamino)phenylphosphonic acid			7.85(-1)	
3-(Methylamino)pyridine (30°C)	8.70(+1)			
4-(Methylamino)pyridine (20°C)	9.65(+1)			
4-(Methylamino)-2,3,5,6-tetramethyl- pyridine (20°C)	10.06(+1)			
<i>N</i> -Methylaniline	4.85(+1)			
Methylarsonic acid (18°C)	3.41	8.18		
1-Methylbarbituric acid	4.35(+1)			
5-Methylbarbituric acid	3.386(+1)			
2-(<i>N</i> -Methylbenzamido)pyridine	1.44(+1)			

TABLE 8.1 pK_a Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3-(<i>N</i> -Methylbenzamido)pyridine	3.66(+1)			
4-(<i>N</i> -Methylbenzamido)pyridine	4.68(+1)			
2-Methylbenzimidazole ($\mu = 0.16$)	6.29(+1)			
2-Methylbenzoic acid (<i>o</i> -toluic acid)	3.90			
3-Methylbenzoic acid	4.269			
4-Methylbenzoic acid	4.362			
<i>N</i> -Methyl-1-benzoylecgonine	8.65			
Methylbiguanidine	3.00(+2)	11.44(+1)		
2-Methyl-2-butanethiol	11.35			
2-Methylbutanoic acid	4.761			
3-Methylbutanoic acid (20 °C)	4.767			
(<i>E</i>)-2-Methyl-2-butendioic acid (mesaconic acid)	3.09	4.75		
3-Methyl-2-butenic acid	5.12			
(<i>E</i>)-2-Methyl-2-butenic acid (tiglic acid)	4.96			
(<i>Z</i>)-2-Methyl-2-butenic acid (angelic acid)	4.30			
4-Methylcarboxylphenol	8.47			
(<i>E</i>)-2-Methylcinnamic acid	4.500			
(<i>E</i>)-3-Methylcinnamic acid	4.442			
(<i>E</i>)-4-Methylcinnamic acid	4.564			
1-Methylcyclohexane-1-carboxylic acid	5.13			
<i>cis</i> -2-Methylcyclohexane- 1-carboxylic acid	5.03			
<i>trans</i> -2-methylcyclohexane- 1-carboxylic acid	5.73			
<i>cis</i> -3-methylcyclohexane- 1-carboxylic acid	4.88			
<i>trans</i> -3-Methylcyclohexane- 1-carboxylic acid	5.02			
<i>cis</i> -4-Methylcyclohexane- 1-carboxylic acid	5.04			
<i>trans</i> -4-Methylcyclohexane- 1-carboxylic acid	4.89			
2-Methylcyclohexyl-1,1-diacetic acid	3.53	6.89		
3-Methylcyclohexyl-1,1-diacetic acid	3.49	6.08		
4-Methylcyclohexyl-1,1,1-diacetic acid	3.49	6.10		
3-Methylcyclopentyl-1,1-diacetic acid	3.79	6.74		
5-Methyl-L-cysteine	8.97			
<i>N</i> -Methylcytidine	3.88			
5-Methylcytidine	4.21			
<i>N</i> -Methyl-2'-deoxycytidine	3.97			
5-Methyl-2'-deoxycytidine	4.33			
2-Methyl-3,5-dinitrobenzoic acid	2.97			
5-Methyldipropylenetriamine (30 °C)	6.32(+3)	9.19(+2)	10.33(+1)	
2,2'-Methylenebis(4-chlorophenol)	7.6	11.5		

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

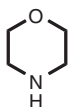
Substance	pK_1	pK_2	pK_3	pK_4
2,2'-Methylenebis(4,6-dichloro-phenol)	5.6	10.56		
Methylenebis(thioacetic acid) (18°C)	3.310	4.345		
3,3'-(Methylenedithio)dialanine	2.200(+1)	8.16(0)		
Methylenesuccinic acid	3.85	5.45		
<i>N</i> -Methylethylamine	4.23(+1)			
<i>N</i> -Methylethylenediamine	6.86(+1)	10.15(+1)		
α -Methylglucoside	13.71			
3-Methylglutaric acid	4.24	5.41		
<i>N</i> -Methylglycine (sarcosine)	2.12(+1)	10.20(0)		
5-Methyl-2,4-heptanedione	8.52(enol); 9.10(keto)			
5-Methyl-2,4-hexanedione	8.66(enol); 9.31(keto)			
5-Methyl-4-hexenoic acid	4.80			
3-Methylhistamine	5.80(+1)	9.90(0)		
1-Methylhistidine	1.69	6.48	8.85	
2-Methylhistidine (18°C)	1.7	7.2	9.5	
2-Methyl-8-hydroxyquinoline ($\mu = 0.005$)	4.58(+1)	11.71(0)		
4-Methyl-8-hydroxyquinoline	4.67(+1)	11.62(0)		
1-Methylimidazole	7.06(+1)			
4-Methylimidazole	7.55(+1)			
<i>N</i> -Methyliminodiacetic acid	2.15	10.09		
<i>S</i> -Methylisothiurea	9.83(+1)			
<i>O</i> -Methylisourea	9.72(+1)			
Methylmalonic acid	3.07	5.87		
2-(<i>N</i> -Methylmethane-sulfonamido)pyridine	1.73(+1)			
3-(<i>N</i> -Methylmethane-sulfonamido)pyridine	3.94(+1)			
4-(<i>N</i> -Methylmethane-sulfonamido)pyridine	5.14(+1)			
2-Methyl-6-methyl-aminopyridine (20°C)	3.17(+1)	8.84(0)		
3-Methyl-4-methyl-aminopyridine (20°C)		9.84(0)		
4-Methyl-2,2'-(4-methylpyridyl)pyridine	5.32(+1)			
<i>N</i> -Methylmorpholine	7.13(+1)			
2-Methyl-1-naphthoic acid	3.11			
<i>N</i> -Methyl-1-naphthylamine	3.70(+1)			
2-Methyl-4-nitrobenzoic acid	1.86			
2-Methyl-6-nitrobenzoic acid	1.87			
1-Methyl-2-nitroterephthalic acid	3.11			
4-Methyl-2-nitroterephthalic acid	1.82			
3-Methylpentanedioic acid	4.25	5.41		
3-Methylpentane-2,4-dione	10.87			
2-Methylpentanoic acid	4.782			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

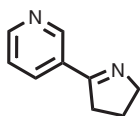
Substance	pK_1	pK_2	pK_3	pK_4
3-Methylpentanoic acid	4.766			
4-Methylpentanoic acid	4.845			
<i>cis</i> -3-Methyl-2-pentenoic acid	5.15			
<i>trans</i> -3-Methyl-2-pentenoic acid	5.13			
4-Methyl-2-pentenoic acid	4.70			
4-Methyl-3-pentenoic acid	4.60			
6-Methyl-1,10-phenanthroline	5.11(+1)			
(2-Methylphenoxy)acetic acid	3.227			
(3-Methylphenoxy)acetic acid	3.203			
(4-Methylphenoxy)acetic acid	3.215			
(2-Methylphenyl)acetic acid (18 °C)	4.35			
(4-Methylphenyl)acetic acid	4.370			
5-Methyl-5-phenylbarbituric acid	8.011(0)			
3-(2-Methylphenyl)propanoic acid	4.66			
3-(3-Methylphenyl)propanoic acid	4.677			
3-(4-Methylphenyl)propanoic acid	4.684			
1-Methyl-2-phenylpyrrolidine	8.80			
5-Methyl-1-phenyl-1,2,3-triazole-4-carboxylic acid	3.73			
Methylphosphinic acid	3.08			
Methylphosphonic acid	2.38	7.74		
3-Methyl- <i>o</i> -phthalic acid	3.18			
4-Methyl- <i>o</i> -phthalic acid	3.89			
<i>N</i> -Methylpiperazine ($\mu = 0.1$)	4.94(+2)	9.09(+1)		
2-Methylpiperazine	5.62(+2)	9.60(+1)		
<i>N</i> -Methylpiperidine	10.19(+1)			
2-Methylpiperidine	10.95(+1)			
3-Methylpiperidine	11.07(+1)			
4-Methylpiperidine ($\mu = 0.5$)	11.23(+1)			
2-Methyl-1,2-propanediamine	6.178(+2)	9.420(+1)		
2-Methyl-2-propanethiol	11.2			
2-Methylpropanoic acid	4.853			
2-Methyl-2-propylamine	10.682(+1)			
2-Methyl-2-propylglutaric acid	3.626			
2-Methylpyridine	5.96(+1)			
3-Methylpyridine	5.68(+1)			
4-Methylpyridine	6.00(+1)			
Methyl 4-pyridinecarboxylate	3.26(+1)			
6-Methylpyridine-2-carboxylic acid	5.83			
2-Methylpyridine-1-oxide	1.029(+1)			
3-Methylpyridine-1-oxide	10.921(+1)			
4-Methylpyridine-1-oxide	1.258(+1)			
<i>O</i> -Methylpyridoxal ($\mu = 0.16$)	4.74			
Methyl-2-pyridyl ketoxime	9.97			
1-Methyl-2-(3-pyridyl)pyrrolidine	3.41	7.94		
1-Methylpyrrolidine	10.46(+1)			
1-Methyl-3-pyrroline	9.88(+1)			
5-Methylquinoline	4.62(+1)			
Methylsuccinic acid	4.13	5.64		
Methylsulfonylacetic acid	2.36			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

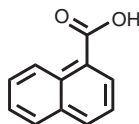
Substance	pK_1	pK_2	pK_3	pK_4
3-Methylsulfonylaniline	2.68(+1)			
4-Methylsulfonylaniline	1.48(+1)			
3-Methylsulfonylbenzoic acid	3.52			
4-Methylsulfonylbenzoic acid	3.64			
4-Methylsulfonyl-3,5-dimethylphenol	8.13			
3-Methylsulfonylphenol	9.33			
4-Methylsulfonylphenol	7.83			
1-Methyl-1,2,3,4-tetrahydro-3-pyridinecarboxylic acid (arecaidine; isoguvacine)	9.07			
5-Methyl-1,2,3,4-tetrazole	3.32			
2-Methylthiazole ($\mu = 0.1$)	3.40(+1)			
4-Methylthiazole ($\mu = 0.1$)	3.16(+1)			
5-Methylthiazole ($\mu = 0.1$)	3.03(+1)			
Methylthioacetic acid	3.72			
4-Methylthioaniline	4.40(+1)			
2-Methylthioethylamine (30°C)	9.18(+1)			
Methylthioglycolic acid	7.68			
3-(<i>S</i> -Methylthio)phenol	9.53			
4-(<i>S</i> -Methylthio)phenol	9.53			
2-Methylthiopyridine (20°C)	3.59(+1)			
3-Methylthiopyridine (20°C)	4.42(+1)			
4-Methylthiopyridine (20°C)	5.94(+1)			
5-Methylthio-1,2,3,4-tetrazole	4.00(+1)			
<i>O</i> -Methylthreonine	2.02(+1)	9.00(0)		
<i>O</i> -Methyltyrosine	2.21(+1)	9.35(0)		
1-Methylxanthine	7.70	12.0		
3-Methylxanthine	8.10	11.3		
7-Methylxanthine	8.33	ca 13		
9-Methylxanthine	6.25			
Morphine (20°C)	7.87(+1)	9.85(0)		
Morpholine	8.492(+1)			
2-(<i>N</i> -Morpholino)ethanesulfonic acid (MES) (20°C)	6.15			
3-(<i>N</i> -Morpholino)-2-hydroxypropanesulfonic acid (37°C)	6.75			
3-(<i>N</i> -Morpholino)propanesulfonic acid (20°C)	7.20			
Murexide	0.0	9.20	10.50	
Myosmine	5.26			
1-Naphthalenecarboxylic acid (1-naphthoic acid)	3.695			



Morpholine



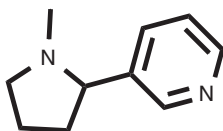
Myosmine



1-Naphthalenecarboxylic acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
2-Naphthalenecarboxylic acid	4.161			
1-Naphthol (20 °C)	9.30			
2-Naphthol (20 °C)	9.57			
Naphthoquinone monoxime	8.01			
1-Naphthylacetic acid	4.236			
2-Naphthylacetic acid	4.256			
1-Naphthylamine	3.92(+1)			
2-Naphthylamine	4.11(+1)			
1-Naphthylarsonic acid	3.66	8.66		
1-Naphthylsulfonic acid	0.57			
Narceine (15 °C)	3.5(+1)	9.3		
Narcotine	6.18(+1)			
Nicotine	3.15(+1)	7.87(0)		
Nicotyrine	4.76(+1)			
Nitrilotriacetic acid (NTA) (20 °C)	1.65	2.94	10.33	
Nitroacetic acid	1.68			
2-Nitroaniline	-0.28(+1)			
3-Nitroaniline	2.46(+1)			
4-Nitroaniline	1.01(+1)			
2-Nitrobenzene-1,4-dicarboxylic acid	1.73			
3-Nitrobenzene-1,2-dicarboxylic acid	1.88			
4-Nitrobenzene-1,2-dicarboxylic acid	2.11			
2-Nitrobenzoic acid	2.18			
3-Nitrobenzoic acid	3.46			
4-Nitrobenzoic acid	3.441			
<i>trans</i> -2-Nitrocinnamic acid	4.15			
<i>trans</i> -3-Nitrocinnamic acid	4.12			
<i>trans</i> -4-Nitrocinnamic acid	4.05			
Nitroethane	8.57			
2-Nitrohydroquinone	7.63	10.06		
<i>N</i> -Nitroiminodiacetic acid	2.21	3.33		
3-Nitromesitol	8.984			
Nitromethane	10.21			
1-Nitro-6,7-phenanthroline ($\mu = 0.2$)	3.23(+1)			
5-Nitro-1,10-phenanthroline	3.232(+1)			
6-Nitro-1,10-phenanthroline	3.23(+1)			
2-Nitrophenol	7.222			
3-Nitrophenol	8.360			
4-Nitrophenol	7.150			
(2-Nitrophenoxy)acetic acid	2.896			



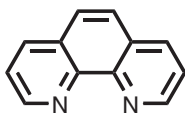
Nicotine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
(3-Nitrophenoxy)acetic acid	2.951			
(4-Nitrophenoxy)acetic acid	2.893			
2-Nitrophenylacetic acid	4.00			
3-Nitrophenylacetic acid	3.97			
4-Nitrophenylacetic acid	3.85			
2-Nitrophenylarsonic acid	3.37	8.54		
3-Nitrophenylarsonic acid	3.41	7.80		
4-Nitrophenylarsonic acid	2.90	7.80		
7-(4-Nitrophenylazo)-8-hydroxy-5-quinolinesulfonic acid	3.14(0)	7.495(−1)		
3-Nitrophenylphosphonic acid	1.30	6.27		
4-Nitrophenylphosphonic acid	1.24	6.23		
3-(2'-Nitrophenyl)propanoic acid	4.504			
3-(4'-Nitrophenyl)propanoic acid	4.473			
3-Nitrophenylselenic acid	4.07			
4-Nitrophenylselenic acid	4.00			
1-Nitropropane	8.98			
2-Nitropropane	7.675			
2-Nitropropanoic acid	3.79			
2-Nitropyridine ($\mu = 0.02$)	−2.06(+1)			
3-Nitropyridine ($\mu = 0.02$)	0.79(+1)			
4-Nitropyridine ($\mu = 0.02$)	1.23(+1)			
<i>N</i> -Nitrosoiminodiacetic acid	2.28	3.38		
4-Nitrosophenol	6.48			
Nitrourea	4.15(+1)			
1,9-Nonanedioic acid (azelaic acid)	4.53	5.40		
Nonanoic acid (pelargonic acid)	4.95			
DL-Norleucine	2.335(+1)	9.834(0)		
Novocaine	8.85(+1)			
2,2,3,3,4,4,5,5-Octafluoropentanoic acid	2.65			
1,8-Octanedioic acid (suberic acid)	4.512	5.404		
Octanoic acid (caprylic acid)	4.895			
Octopine-DD	1.35	2.30	8.68	11.25
Octopine-LD	1.40	2.30	8.72	11.34
Octylamine	10.65(+1)			
L-(+)-Ornithine	1.94(+2)	8.65(+1)	10.76(0)	
Oxalic acid	1.271	4.272		
3,6-Oxaoctanedioic acid ($\mu = 1.0$)	3.055	3.676		
Oxoacetic acid	3.46			
2-Oxabutanedioic acid (oxaloacetic acid)	2.56	4.37		
2-Oxobutanoic acid	2.50			
5-Oxohexanoic acid (5-ketohexanoic acid) (18°C)	4.662			
3-Oxo-1,5-pentanedioic acid	3.10			
4-Oxopentanoic acid (levulinic acid)	4.59			
2-Oxopropanoic acid (pyruvic acid)	2.49			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Oxytetracycline	3.10(+1)	7.26	9.11	
Papaverine	5.90(+1)			
Pentamethylenebis(thioacetic acid) (18 °C)	3.485	4.413		
3,3-Pentamethylenepentanedioic acid	3.49	6.96		
1,5-Pentanediamine	10.05(+2)	10.916(+1)		
2,4-Pentanedione	8.24(enol); 8.95(keto)			
1-Pentanoic acid (valeric acid)	4.842			
2-Pentenoic acid	4.70			
3-Pentenoic acid	4.52			
4-Pentenoic acid	4.677			
Pentylarsonic acid	4.14	9.07		
<i>N</i> -Pentylveratramine	7.28(+1)			
Perhydrodiphenic acid (20 °C)	4.96	6.68		
Perlididine (18 °C)	4.01	11.39		
Peroxyacetic acid	8.20			
1,7-Phenanthroline	4.30(+1)			
1,10-Phenanthroline	4.857(+1)			
6,7-Phenanthroline	4.857(+1)			
Phenazine	1.2(+1)			
Phenethylthioacetic acid	3.795			
Phenol	9.99			
Phenol-3-phosphoric acid	1.78	7.03	10.2	
Phenol-4-phosphoric acid	1.99	7.25	9.9	
Phenolphthalein	9.4			
3-Phenolsulfonic acid		9.05(−1)		
Phenolsulfonephthalein	7.9			
Phenoxyacetic acid	3.171			
2-Phenoxybenzoic acid	3.53			
3-Phenoxybenzoic acid	3.95			
4-Phenoxybenzoic acid	4.52			
5-Phenoxy-1,2,3,4-tetrazole	3.49(+1)			
Phenylacetic acid	4.312			
L-3-Phenyl- α -alanine	2.16(+1)	9.31(0)		
3-Phenyl- α -alanine, methyl ester	7.05(+1)			
Phenylalanylarginine ($\mu = 0.01$)	2.66(+1)	7.57(0)	12.40(−1)	
Phenylalanylglycine ($\mu = 0.01$)	3.10(+1)	7.71(0)		
7-Phenylazo-8-hydroxy- 5-quinolinesulfonic acid	3.41(0)	7.850(−1)		



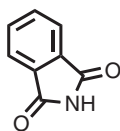
1,10-Phenanthroline

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

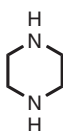
Substance	pK_1	pK_2	pK_3	pK_4
5-Phenylbarbituric acid	2.544(+1)			
2-Phenyl-2-benzylsuccinic acid	3.69	6.47		
1-Phenylbiguanide	2.13(+2)	10.76(+1)		
4-Phenylbutanoic acid	4.757			
Phenylbutazone	4.5(+1)			
2-Phenylenediamine	< 2(+2)	4.47(+1)		
3-Phenylenediamine	2.65(+2)	4.88(+1)		
4-Phenylenediamine	3.29(+2)	6.08(+1)		
2-Phenylethylamine	9.83(+1)			
β -Phenylethylboronic acid	10.0			
D,L- α -Phenylglycine	1.83(+1)	4.39(0)		
Phenylguanidine	10.77(+1)			
Phenylhydrazine	5.20(+1)			
2-Phenyl-3-hydroxypropanoic acid	3.53			
3-Phenyl-3-hydroxypropanoic acid	4.40			
Phenyliminodiacetic acid (20°C)	2.40	4.98		
Phenylmalonic acid	2.58	5.03		
Phenylmethanethiol	10.70			
2-Phenyl-2-phenethylsuccinic acid (20°C)	3.74	6.52		
2-Phenylphenol	9.55			
3-Phenylphenol	9.63			
4-Phenylphenol	9.55			
Phenylphosphinic acid (17°C)	2.1			
Phenylphosphonic acid	1.83	7.07		
O-Phenylphosphorylserine	2.13(+1)	8.79		
O-Phenylphosphorylserylglycine	3.18(+1)	6.95(0)		
O-Phenylphosphoryl-L-seryl-L-leucine	3.16(+1)	7.12(0)		
N-Phenylpiperazine ($\mu = 0.1$)	8.71(+1)			
2-Phenylpropanoic acid	4.38			
3-Phenylpropanoic acid (35°C)	4.664			
3-Phenyl-1-propylamine	10.39(+1)			
Phenylpropynoic acid (35°C)	2.269			
Phenylselenic acid	4.79			
Phenylselenoacetic acid ($\mu = 0.1$)	3.75			
β -Phenylserine ($\mu = 0.16$)	8.79(0)			
Phenylsuccinic acid (20°C)	3.78	5.55		
Phenylsulfenylacetic acid	2.66			
Phenylsulfonylacetic acid	2.44			
5-Phenyl-1,2,3,4-tetrazole	4.38(+1)			
1-Phenyl-1,2,3-triazole-4-carboxylic acid	2.88			
1-Phenyl-1,2,3-triazole-4,5-dicarboxylic acid	2.13	4.93		
Phosphoramidic acid	3.08	8.63		
O-Phosphorylethanolamine	5.838(+1)	10.638(0)		
O-Phosphorylserylglycine	3.13	5.41	8.01	

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

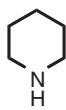
Substance	pK_1	pK_2	pK_3	pK_4
<i>O</i> -Phosphoryl-L-seryl-L-leucine	3.11	5.47	8.26	
Phosphoserine	2.08	5.65	9.74	
Phthalamide	3.79(0)			
Phthalazine	3.47(+1)			
<i>o</i> -Phthalic acid	2.950	5.408		
Phthalimide	9.90(0)			
Physostigmine	1.76(+1)	7.88(0)		
Picric acid (2,4,6-trinitrophenol) (18 °C)	0.419			
Pilocarpine	1.3(+1)	6.85(0)		
Piperazine	5.333(+2)	9.781(+1)		
1,4-Piperazinebis(ethanesulfonic acid) (20 °C)	6.80			
Piperazine-2-carboxylic acid	1.5	5.41	9.53	
Piperidine	11.123(+1)			
2-Piperidinecarboxylic acid	2.12(+1)	10.75(0)		
3-Piperidinecarboxylic acid	3.35(+1)	10.64(0)		
4-Piperidinecarboxylic acid	3.73(+1)	10.72(0)		
1-(2-Piperidinyl)-2-propanone (15 °C)	9.45			
Piperine (15 °C)	1.98(+1)			
Proline	1.952(+1)	10.640(0)		
1,2-Propanediamine	6.607(+2)	9.720(+1)		
1,3-Propanediamine	8.49(+2)	10.47(+1)		
1-Propanethiol	10.86			
1,2,3-Propanetriamine	3.72(+3)	7.95(+2)	9.59(+1)	
1,2,3-Propanetricarboxylic acid	3.67	4.87	6.38	
Propanoic acid	4.874			
Propenoic acid	4.247			
<i>N</i> -Propionylglycine	3.718(0)			
2-Propoxybenzoic acid (20 °C)	4.24			
3-Propoxybenzoic acid (20 °C)	4.20			
4-Propoxybenzoic acid (20 °C)	4.78			
<i>N</i> -Propylalanine	2.21(+1)	10.19(0)		
Propylamine	10.568(+1)			
Propylarsonic acid (18 °C)	4.21	9.09		
Propylenimine	8.18(+1)			
<i>N</i> -Propylglycine ($\mu = 0.1$)	2.38(+1)	10.03(0)		
L-Propylglycine	3.19(+1)	8.97(0)		
Propylmalonic acid	2.97	5.84		
Propylphosphinic acid	3.46			



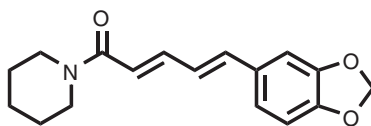
Phthalamide



Piperazine



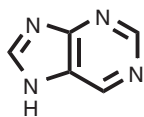
Piperidine



Piperine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Propylphosphonic acid	2.49	8.18		
2-Propylpyridine	6.30(+1)			
N-Propylveratramine	7.20(+1)			
2-Propynoic acid	1.887			
Pseudoecgonine	9.70			
Pseudoisocyanine ($\mu = 0.2$)	4.59(+2)			
Pseudotropine	9.86(+1)			
Pteroylglutamic acid	8.26			
Purine	2.52(+1)	8.92(0)		
Pyrazine	0.6(+1)			
Pyrazinecarboxamide	0.5(+1)			
Pyrazole	2.61(+1)			
Pyridazine	2.33(+1)			
Pyridine	5.17(+1)			
Pyridine- d_5	5.83(+1)			
2-Pyridinealldoxime	3.56(+1)	10.17(0)		
3-Pyridinealldoxime	4.07(+1)	10.39(0)		
4-Pyridinealldoxime	4.73(+1)	10.03(0)		
2-Pyridinecarbaldehyde	3.84(+1)			
3-Pyridinecarbaldehyde	3.80(+1)			
4-Pyridinecarbaldehyde	4.74(+1)			
3-Pyridinecarbamide (nicotinamide)	3.33(+1)			
3-Pyridinecarbonitrile	1.35(+1)			
Pyridine-2-carboxylic acid (picolinic acid)	1.01(+1)	5.29(0)		
Pyridine-3-carboxylic acid (nicotinic acid)	2.07(+1)	4.75(0)		
Pyridine-4-carboxylic acid (isonicotinic acid)	1.84(+1)	4.86(0)		
Pyridine-2,3-dicarboxylic acid	2.36(+1)	7.08(0)		
Pyridine-2,4-dicarboxylic acid	2.23(+1)	7.02(0)		
Pyridine-2,6-dicarboxylic acid	2.16(+1)	6.92(0)		
Pyridine-1-oxide	0.688(+1)			
Pyridoxal	4.20(+1)	8.66(ring OH)		
Pyridoxal-5-phosphate ($\mu = 0.15$)	< 2.5	4.14	6.20	8.69
Pyridoxamine ($\mu = 0.1$)	3.37(+2)	8.01(+1)	10.13(ring OH)	
Pyridoxamine-5-phosphate ($\mu = 0.15$; $pK_5 = 10.92$)	2.5	3.69	5.76	8.61
Pyridoxine (vitamin B ₆) (18°C)	5.00(+1)	8.96(ring OH)		



Purine



Pyrazine



Pyrazole



Pyridazine



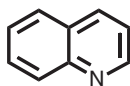
Pyridine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

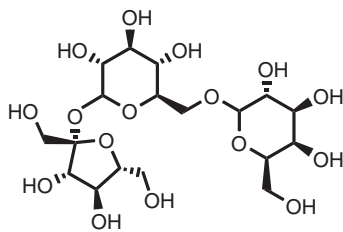
Substance	pK_1	pK_2	pK_3	pK_4
3-(2'-Pyridyl)alanine	1.37(+2)	4.02(+1)	9.22(0)	
3-(3'-Pyridyl)alanine	1.77(+2)	4.64(+1)	9.10(0)	
2-(2'-Pyridyl)benzimidazole ($\mu = 0.16$)	5.58(+1)			
2-(2'-Pyridyl)imidazole ($\mu = 0.005$)	8.98(+1)			
4-(2'-Pyridyl)imidazole ($\mu = 0.1$)	5.49(+1)			
Pyrimidine	1.30(+1)			
2,4(1 <i>H</i> ,3 <i>H</i>)-Pyrimidinedione (uracil)	0.6(+1)	9.46(0)		
2,4,5,6(1 <i>H</i> ,3 <i>H</i>)-Pyrimidinetetrone- 5-oxime	4.57(0)			
Pyrocatecholsulfonephthalein	7.82	9.76	11.73	
Pyroxilidine	11.11(+1)			
Pyrrole-1-carboxylic acid	4.45			
Pyrrole-2-carboxylic acid	4.45			
Pyrrole-3-carboxylic acid	4.453			
Pyrrolidine	11.305(+1)			
Pyrrolidine-2-carboxylic acid (proline)	1.952(+1)	10.640(0)		
2-[2-(<i>N</i> -Pyrrolidinyl)ethyl]pyridine	3.60(+2)	9.39(+1)		
3-[2-(<i>N</i> -Pyrrolidinyl)ethyl]pyridine	4.28(+2)	9.28(+1)		
4-[2(<i>N</i> -Pyrrolidinyl)ethyl]pyridine	4.65(+2)	9.27(+1)		
2-(1-Pyrrolidinylmethyl)pyridine	2.54(+1)	8.56(+1)		
3-(1-Pyrrolidinylmethyl)pyridine	3.14(+2)	8.36(+1)		
4-(1-Pyrrolidinylmethyl)pyridine	3.38(+2)	8.16(+1)		
3-Pyrroline	-0.27(+1)			
Quinidine	4.0(+1)	8.54(0)		
Quinine	4.11(+1)	8.52(0)		
Quinoline	4.80(+1)			
Quinoxaline	0.72(+1)			
D-Raffinose	12.74			
Riboflavin (vitamin B ₂) ($\mu = 0.01$)	ca -0.2	9.69		
α -D-Ribofuranose	12.11			
D-Ribose-5'-phosphonic acid		6.70(-1)	13.05(-2)	



Pyrrolidine



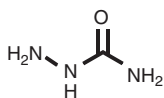
Quinoline



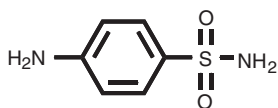
D-Raffinose

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

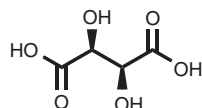
Substance	pK_1	pK_2	pK_3	pK_4
D-Saccharic acid	5.00(0)			
Saccharin (<i>o</i> -benzoic sulfimide)	2.32			
Sarcosine	2.12(+1)	10.20(0)		
Sarcosine amide	8.35(+1)			
Sarcosine dimethylamide	8.86(+1)			
Sarcosine methylamide	8.28(+1)			
Sarcosylglycine ($\mu = 0.16$)	3.15(+1)	8.56(0)		
Sarcosylleucine	3.15(+1)	8.67(0)		
Sarcosylsarcosine	2.92(+1)	9.15(0)		
Sarcosylserine	3.17(+1)	8.63(0)		
3-Selenosemicarbazide ($\mu = 0.1$)	0.8(+1)			
Semicarbazide ($\mu = 0.1$)	3.53(+1)			
L-Serine	2.186(+1)	9.208(0)		
Serine, methyl ester ($\mu = 0.1$)	7.03(+1)			
Serylglycine ($\mu = 0.15$)	2.10(+1)	7.33(0)		
L-Seryl-L-leucine	3.08(+1)	7.45(0)		
Solanine	7.34(+1)			
D-Sorbitol (17.5°C)	13.60			
L-(−)-Sorbose (18°C)	11.55			
Sparteine	4.49(+1)	11.76(0)		
Spinacemine ($\mu = 0.1$)	4.895(+2)	8.90(+1)		
Spinacine	1.649(+2)	4.936(+1)	8.663(0)	
L-Strychnine (15°C)	2.50	8.20		
Succinamic acid (succinic acid monoamide)	4.39(0)			
Succinic acid	4.207	5.635		
DL-Succinimide	9.623			
β -(4'-Sulfaminophenyl)alanine	1.99(+1)	8.64(0)	10.26(−1)	
3-Sulfamylbenzoic acid	3.54			
4-Sulfamylbenzoic acid	3.47			
4-Sulfamylphenylphosphoric acid	1.42	6.38	10.0	
Sulfanilamide	10.43(+1)			
Sulfoacetic acid		4.0		
3-Sulfobenzoic acid		3.78		
4-Sulfobenzoic acid		3.72		
3-Sulfophenol	0.39	9.07		
4-Sulfophenol	0.58	8.70		
2-Sulfopropanoic acid	1.99			
5-Sulfosalicylic acid	2.49	12.00		
Sylvic acid	7.62			
D-Tartaric acid	3.036	4.366		
<i>meso</i> -Tartaric acid	3.22	4.81		



Semicarbazide



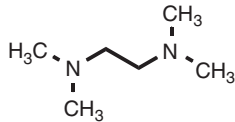
Sulfanilamide



D-Tartaric acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Tetracycline ($\mu = 0.005$)	3.30(+1)	7.68	9.69	
Tetradehydroyohimbine	10.59(+1)			
Tetraethylenepentamine [$\mu = 0.1$; $pK_5 = 9.67(+1)$]	2.98(+5)	4.72(+4)	8.08(+3)	9.10(+2)
1,4,5,6-Tetrahydro- 1,2-dimethylpyridine	11.38(+1)			
1,4,5,6-Tetrahydro-2-methylpyridine	9.53(+1)			
cis-Tetrahydronaphthalene- 2,3-dicarboxylic acid (20 °C)	3.98	6.47		
trans-Tetrahydronaphthalene- 2,3-dicarboxylic acid (20 °C)	4.00	5.70		
5,6,7,8-Tetrahydro-1-naphthol	10.28			
5,6,7,8-Tetrahydro-2-naphthol	10.48			
Tetrahydroserpentine	10.55(+1)			
2,3,5,6-Tetramethylbenzoic acid	3.415			
Tetramethylenebis(thioacetic acid) (18 °C)	3.463	4.423		
Tetramethylenediamine	9.22(+2)	10.75(+1)		
N,N,N',N'- Tetramethylethylenediamine	2.20(+2)	6.35(+1)		
2,3,5,6-Tetramethyl- 4-methylaminopyridine	0.07(+1)			
2,2,6,6-Tetramethylpiperidine ($\mu = 0.5$)	1.24(+1)			
2,3,5,6-Tetramethylpyridine (20 °C)	7.90(+1)			
Tetramethylsuccinic acid	3.50	7.28		
1,2,3,4-Tetrazole	4.90			
Thebaine	7.95(+1)			
2-Thenoyltrifluoroacetone	5.70(0)			
Theobromine	0.68(+1)	7.89		
Theophylline	< 1(+1)	8.80		
Thiazoline	2.53(+1)			
Thioacetic acid	3.33			
o-Thiocresol	6.64			
m-Thiocresol	6.58			
p-Thiocresol	6.52			
Thiocyanatoacetic acid	2.58			
2,2'-Thiodiacetic acid	3.32	4.29		
4,4'-Thiodibutanoic acid (18 °C)	4.351	5.275		



N,N,N',N'-Tetramethylethylenediamine



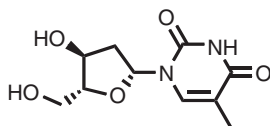
1,2,3,4-Tetrazole



Thiazoline

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
3,3'-Thiodipropionic acid (18°C)	4.085	5.075		
3-Thio- <i>S</i> -methylcarbazine ($\mu = 0.1$)	7.563(+1)			
1-Thionylcarboxylic acid	3.53			
2-Thionylcarboxylic acid	4.10			
2-Thiophenecarboxylic acid (30°C)	3.529			
3-Thiophenecarboxylic acid (3-thenoic acid)	4.10			
Thiophenol	6.50			
3-Thiosemicarbazide ($\mu = 0.1$)	1.5(+1)			
3-Thiosemicarbazide-1,1-diacetic acid (30°C)	2.94	4.07		
Thiourea	2.03(+1)			
Thorin	3.7	8.3	11.8	
Thymidine	9.79	12.85		
<i>p</i> -Toluenesulfonic acid	1.7			
Toluhydroquinone	10.03	11.62		
<i>o</i> -Toluidine	4.45(+1)			
<i>m</i> -Toluidine	4.71(+1)			
<i>p</i> -Toluidine	5.08(+1)			
<i>o</i> -Tolylacetic acid (18°C)	4.36			
<i>p</i> -Tolylacetic acid (18°C)	4.36			
<i>o</i> -Tolylarsonic acid	3.82	8.85		
<i>m</i> -Tolylarsonic acid	3.82	8.60		
<i>p</i> -Tolylarsonic acid	3.70	8.68		
<i>o</i> -Tolylphosphonic acid	2.10	7.68		
<i>m</i> -Tolylphosphonic acid	1.88	7.44		
<i>p</i> -Tolylphosphonic acid	1.84	7.33		
3-Tolylselenic acid	4.80			
4-Tolylselenic acid	4.88			
Triacetylmethane	5.81			
Triallylamine	8.31(+1)			
1,3,5-Triazine-2,4,6-triol	7.20	11.10		
1 <i>H</i> -1,2,3-Triazole		9.26		
1 <i>H</i> 1,2,4-Triazole	2.386(+1)	9.972		
1,2,3-Triazole-4-carboxylic acid	3.22	8.73		
1,2,3-Triazole-4,5-dicarboxylic acid	1.86	5.90	9.30	
1,2,4-Triazolidine-3,5-dione (urazole)	5.80			
Tribromoacetic acid	-0.147			
2,4,6-Tribromobenzoic acid	1.41			
Trichloroacetic acid	0.52			
Trichloroacrylic acid	1.15			



Thymidine

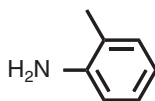
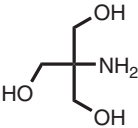
*o*-Toluidine

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

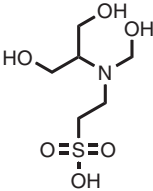
Substance	pK_1	pK_2	pK_3	pK_4
3,3,3-Trichlorolactic acid	2.34			
Trichloromethylphosphonic acid	1.63	4.81		
2,4,5-Trichlorophenol	7.37			
3,4,5-Trichlorophenol	7.839			
Tricine (20 °C)	8.15			
Triethanolamine	7.76(+1)			
Triethylamine	10.72(+1)			
Triethylenediamine	4.18(+2)	8.19(+1)		
Triethylenetetramine (20 °C)	3.32(+4)	6.67(+3)	9.20(+2)	9.92(+1)
Triethylsuccinic acid	2.74			
Trifluoroacetic acid	0.50			
Trifluoroacrylic acid	1.79			
4,4,4-Trifluoro-2-aminobutanoic acid	1.600(+1)	8.169(0)		
4,4,4-Trifluoro-3-aminobutanoic acid	2.756(+1)	5.822(0)		
4,4,4-Trifluorobutanoic acid	4.16			
α,α,α -Trifluoro- <i>m</i> -cresol	8.950			
4,4,4-Trifluorocrotonic acid	3.15			
5,5,5-Trifluoroleucine	2.045(+1)	8.942(0)		
3-(Trifluoromethyl)aniline	3.5(+1)			
4-(Trifluoromethyl)aniline	2.6(+1)			
3-Trifluoromethylphenol	8.950			
5-Trifluoromethyl-1,2,3,4-tetrazole	1.70			
6,6,6-Trifluoronorleucine	2.164(+1)	9.463(0)		
5,5,5-Trifluoronorvaline	2.042(+1)	8.916(0)		
5,5,5-Trifluoropentanoic acid	4.50			
3,3,3-Trifluoropropanoic acid	3.06			
4,4,4-Trifluorothreonine	1.554(+1)	7.822(0)		
4,4,4-Trifluorovaline	1.537(+1)	8.098(0)		
1,2,3-Trihydroxybenzene (pyrogallol)	9.03(0)	11.63(−1)		
1,3,5-Trihydroxybenzene (phloroglucinol)	8.45(0)	8.88(−1)		
2,4,6-Trihydroxybenzoic acid	1.68(0)			
3,4,5-Trihydroxybenzoic acid	4.19(0)	8.85(−1)		
3,4,5-Trihydroxycyclohex-1-ene- 1-carboxylic acid				
[D(−)-shikimic acid]	4.15			
2,4,6-Tri(hydroxymethyl)phenol	9.56			
Triisobutylamine	10.42(+1)			
Trimethylamine	9.80(+1)			
3-(Trimethylamino)phenol	8.06			
4-(Trimethylamino)phenol	8.35			
2,4,6-Trimethylaniline	4.38(+1)			
2,4,6-Trimethylbenzoic acid	3.448			
Trimethylenebis(thioacetic acid) (18 °C)	3.435	5.383		
2,3,4-Trimethylphenol	10.59			
2,4,5-Trimethylphenol	10.57			
2,4,6-Trimethylphenol	10.88			
3,4,5-Trimethylphenol	10.25			
2,3,6-Trimethylpyridine ($\mu = 0.5$)	7.60(+1)			

TABLE 8.1 pK_A Values of Organic Materials in Water at 25°C (*continued*)

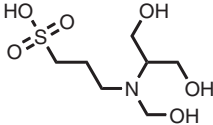
Substance	pK_1	pK_2	pK_3	pK_4
2,4,6-Trimethylpyridine	7.43(+1)			
2,4,6-Trimethylpyridine-1-oxide	1.990(+1)			
3-(Trimethylsilyl)benzoic acid	4.089			
4-(Trimethylsilyl)benzoic acid	4.192			
2,4,5-Trimethylthiazole ($\mu = 0.1$)	4.55			
2,4,6-Trinitroaniline (picramide)	-10.23(+1)			
2,4,6-Trinitrobenzene acid	0.654			
2,2,2-Trinitroethanol	2.36			
Trinitromethane (20°C)	0.17			
Triphenylacetic acid	3.96			
Tripropylamine	10.66(+1)			
Tris(2-hydroxyethyl)amine	7.762(+1)			
Tris(hydroxymethyl)aminomethane (TRIS)	8.08(+1)			
2-[Tris(hydroxymethyl)methyl amino]-1-ethanesulfonic acid (TES)	7.50			
3-[Tris(hydroxymethyl)methyl amino]-1-propanesulfonic acid (TAPS) (20°C)	8.4			
N-[Tris(hydroxymethyl)methyl]-glycine (tricine)	2.023(+1)	8.135		
Tris(trimethylsilyl)amine	4.70(+1)			
Trithiocarbonic acid (20°C)	2.64			
Tropacocaine (15°C)	9.88(+1)			
3-Tropanol (tropine)	10.33(+1)			
Trypsin ($\mu = 0.1$)	6.25			
L-Tryptophan	2.38(+1)	9.39(0)		
DL-Tyrosine	2.18(+1)	9.21(0)	10.47(OH)	
Tyrosine amide	7.48	9.89		



Tris(hydroxymethyl)aminomethane



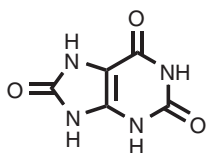
2-[Tris(hydroxymethyl)methylamino]-1-ethanesulfonic acid



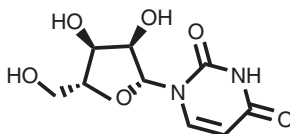
3-[Tris(hydroxymethyl)methylamino]-1-propanesulfonic acid

TABLE 8.1 pK_A Values of Organic Materials in Water at 25 °C (*continued*)

Substance	pK_1	pK_2	pK_3	pK_4
Tyrosine, ethyl ester	7.33	9.80		
Tyrosylarginine ($\mu = 0.01$)	2.65(+1)	7.39(0)	9.36(-1)	11.62(-2)
Tyrosyltyrosine	3.52(+1)	7.68(0)	9.80(-1)	10.26(-2)
α -Ureidobutanoic acid	3.886(0)			
γ -Ureidobutanoic acid	4.683(0)			
β -Ureidopropanoic acid	4.487(0)			
Uric acid	5.40	5.53		
Uridine	9.30			
Uridine-5'-diphosphoric acid	7.16			
Uridine-5'-phosphoric acid (5'-uridylic acid)	6.63			
Uridine-5'-triphosphoric acid	7.58			
DL-Valine	2.286(+1)	9.719(0)		
L-Valine	2.296(+1)	9.79(0)		
Valine amide ($\mu = 0.2$)	8.00			
L-Valine, methyl ester	7.49(+1)			
L-Valylglycine	3.23(+1)	8.00(0)		
Vetramine	7.49(+1)			
Veratrine	8.85(+1)			
Vinylmethylaniline	9.69(+1)			
2-Vinylpyridine	4.98(+1)			
4-Vinylpyridine	5.62(+1)			
Vitamin B ₁₂	7.64(+1)			
Xanthine (40 °C)	0.68(+1)			
Xanthosine	< 2.5(+1)	5.67(0)	12.00(-1)	
Xylenol Orange [$pK_5 = 10.46(-4)$; $pK_6 = 12.28(-5)$]		2.58(-1)	3.23(-2)	6.37(-3)
D-(+)-Xylose	12.15(0)			
Zincon		4	7.85	15



Uric acid



Uridine

Table 8.2 records the acidities of inorganic compounds expressed as their pK_A values (see page 8.2 for a discussion of pK_A). When more than one ionizable proton is present, pK_1 , pK_2 , etc. values are given. Cations formed from the indicated compound by protonation are indicated by “(+1)” or “(+2)” for a dication.

Temperature values different from 25 °C are given in parentheses as are other relevant variations. For example, the dissociation constant for acetic acid- d_1 is reported in D_2O .

TABLE 8.2 Proton-Transfer Reactions of Inorganic Materials in Water at 25 °CThe protonation states of cations are designated by values (+1), (+2), etc. that follow pK_a values.

Substance	Formula	pK_1	pK_2	pK_3	pK_4
Aluminic acid (alumina)	H_3AlO_3	11.2			
Amidophosphoric acid	$H_2NPO(OH)_2$	3.3	8.28		
Aminodisulfonic acid	$HN(SO_3H)_2$			8.50	
Ammonium ion	NH_4^+	9.24			
Arsenic acid	H_3AsO_4	2.25	6.77	11.53	
Arsenous acid	$HAsO_2$ or $HAs(OH)_4$	9.23			
Boric acid, ortho-	H_3BO_3	9.236	12.74		
Boric acid, etra-	$H_2B_4O_7$	4	9		
Carbonic acid	$CO_2 + H_2O$	6.35	10.53		
	(without including dehydration constant)	3.76	10.329		
	$CO_2 + D_2O$ (solvent)	6.77	11.076		
Chloric acid	$HClO_3$	-1.58			
Chlorous acid	$HClO_2$	2.021			
Chlorosulfonic acid	$HOSO_2Cl$	-10.43			
Chromic acid	H_2CrO_4	-0.98	6.50		
Cyanic acid	$HO-CN$	3.47			
Deuterium oxide	D_2O (solvent)	14.87			
Diamidophosphoric acid	$(H_2N)_2PO_2H$	4.83			
Dithionic acid	$H_2S_2O_6$	-3.4	-0.2		
Dithionous acid	$H_2S_2O_4$	0.35	2.45		
Ferricyanic acid	$H_3Fe(CN)_6$	< 1			
Ferrocyanic acid	$H_2(Fe(CN)_6)^{2-}$			2.57	4.35
Fluorophosphoric acid	$FPO(OH)_2$		4.79		
Hexapolyphosphoric acid	$H_8P_6O_{19}$	ca 2.1	2.19	5.98	8.13
Hydrazinium(2+) ion (20 °C)	$^+H_3NNH_3^+$	-0.88 (+2)	7.956 (+1)		
Hydrazinosulfuric acid	H_2NNHSO_3H	3.85			
Hydrazoic acid	HN_3	4.64			
Hydrocyanic acid	HCN	9.21			
Hydrogen bromide	HBr	-20.68			
Hydrogen chloride	HCl	-6.1			
Hydrogen fluoride	HF	3.17			
Hydrogen iodide	HI	-9.5			
Hydrogen peroxide	H_2O_2	11.58			
Hydrogen polysulfide (20 °C)	H_2S_4	3.8	6.3		
Hydrogen selenide	H_2Se	3.89	11.0		
Hydrogen sulfide	H_2S	6.96	12.90		
Hydrogen telluride (20 °C)	H_2Te	2.64	11-12		
Hydroperoxy radical	$HO_2 = H^+ + O_2^-$	4.45			
Hydroxide radical	OH^\cdot	11.9			
Hydroxylamine- <i>N,N</i> -di sulfonic acid	$HON(SO_3H)_2$			11.85	
Hydroxylamine- <i>N</i> -sulfonic acid	$HONH-OSO_2H$		ca 12.5		
Hydroxylammonium ion	$HONH_3^+$	5.98			

TABLE 8.2 Proton-Transfer Reactions of Inorganic Materials in Water at 25 °C (*continued*)

Substance	Formula	pK ₁	pK ₂	pK ₃	pK ₄
Hypobromous acid	HBrO	8.597			
Hypochlorous acid	HCIO	7.54			
Hypoiodous acid	HIO	10.64			
Hyponitrous acid	HON=NOH	7.05	11.54		
Hypophosphoric acid (20 °C)	H ₄ P ₂ O ₆	2	2.19		
Hypophosphorus acid	HPH ₂ O ₂	1.23			
Hyposulfurous acid	H ₂ S ₂ O ₄	0.35	2.45		
Imidodiphosphoric acid	(HO) ₂ PO—NH— PO(OH) ₂	ca 2	2.85	7.08	9.72
Iodic acid (30 °C)	HIO ₃	0.815			
Nitramide	O ₂ NNH ₂	6.48			
Nitric acid	HNO ₃	1.38			
Nitrous acid	HNO ₂	3.14			
Osmic acid	H ₂ OsO ₅ (mainly OsO ₄)	12.0	14.5		
Perchloric acid	HClO ₄ (completely dissociated up to 10M)				
Periodic acid, para-	H ₅ IO ₆	1.55	8.27		
Permanganic acid	HMnO ₄	−2.25			
Peroxide radical	HO ₂	4.90			
Peroxoboric acid	H ₃ BO ₃ + H ₂ O ₂ = (H ₂ BO ₃ ·H ₂ O ₂) [−] + H ⁺	7.91			
Peroxochromic acid	H ₂ CrO ₅	4.30			
Peroxomonosulfuric acid	H ₂ SO ₅	1.0	9.3		
Perxenic acid	H ₄ XeO ₆	ca 2	ca 6	ca 10	
Phosphoric acid, ortho-	H ₃ PO ₄	2.148	7.198	12.38	
Deuterated	D ₃ PO ₃	2.420	7.201		
Phosphoric acid, di-	H ₄ P ₂ O ₇	0.91	2.10	6.70	9.38
Phosphorous acid (20 °C)	H ₂ PHO ₃	1.20	6.70		
Selenic acid	H ₂ SeO ₄	−3	1.74		
Selenous acid	H ₂ SeO ₃	2.27	7.78		
Silicic acid	H ₂ SiO ₃	9.77	11.80		
Sulfamic acid	HOSO ₂ NH ₂	0.988			
Sulfuric acid	H ₂ SO ₄	ca −3	1.987		
Sulfurous acid	SO ₂ + H ₂ O (includes dehydration constant)	1.89	7.20		
Telluric acid	H ₆ TeO ₆	7.70	10.99		
Tellurous acid	H ₂ TeO ₃	2.46	7.7		
Tetraperoxo-chromic acid (30 °C)	H ₃ CrO ₈	7.16			
Tetrapolyphosphoric acid (pK ₅ = 6.63; pK ₆ = 8.34)	H ₆ P ₄ O ₁₃			1.3	2.23
Thiocyanic acid	HSCN	0.95			
Thiosulfuric acid	H ₂ S ₂ O ₃	0.60	1.5–1.7		
Trimetaphosphoric acid	H ₃ P ₃ O ₄			2.0	
Tripolyphosphoric acid (μ > 1)* (pK ₅ = 9.26)	H ₅ P ₃ O ₁₀	−0.51	1.20	2.30	6.61
Trithiocarbonic acid (20 °C)	H ₂ CS ₃	2.68	8.18		

TABLE 8.2 Proton-Transfer Reactions of Inorganic Materials in Water at 25 °C (*continued*)

Substance	Formula	pK ₁	pK ₂	pK ₃	pK ₄
Tungstic acid (20 °C)	H ₂ WO ₄	ca 3.5	ca 4.6		
Vanadic acid	H ₃ VO ₄	3.78	7.8	13.0	
Water	H ₂ O	14.003			
Xenon trioxide	XeO ₃ (aqueous) = HXeO ₄ ⁻ + H ⁺	10.8			

* Ionic strength.

TABLE 8.3 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures*Abbreviations Used in the Table*

(+1), monoprotonated cation

(−1), monoanion

 pK_{auto} , negative logarithm (base 10) of autoprotolysis constant

(0), neutral molecule

(−2), dianion

 pK_{sp} , negative logarithm (base 10) of solubility product

Substance	Temperature, °C									
	0	5	10	15	20	25	30	35	40	50
Acetic acid (0)	4.780	4.770	4.762	4.758	4.757	4.756	4.757	4.762	4.769	4.787
DL- <i>N</i> -Acetylalanine (+1)		3.699	3.699	3.703	3.708	3.715	3.725	3.733	3.745	3.774
β -Acetylaminopropionic (+1)		4.479	4.465	4.465	4.449	4.445	4.444	4.443	4.445	4.457
<i>N</i> -Acetyl glycine (+1)		3.682	3.676	3.673	3.667	3.670	3.673	3.678	3.685	3.706
α -Alanine										
(+1)	2.42		2.39		2.35	2.34	2.33	2.33	2.33	2.33
(0)	10.59		10.29		10.01	9.87	9.74	9.62	9.49	9.26
2-Aminobenzenesulfonic acid (0), pK_2	2.633	2.591	2.556	2.521	2.448	2.459	2.431	2.404	2.380	2.338
3-Aminobenzenesulfonic acid (0), pK_2	4.075	4.002	3.932	3.865	3.799	3.738	3.679	3.622	3.567	3.464
4-Aminobenzenesulfonic acid (0), pK_2	3.521	3.457	3.398	3.338	3.283	3.227	3.176	3.126	3.079	2.989
3-Aminobenzoic acid (0)					4.90	4.79	4.75		4.68	4.60
4-Aminobenzoic acid (0)					4.95	4.85	4.90		4.95	5.10
2-Aminobutyric acid										
(+1)			2.334			2.286		2.289 ^{37.5°C}		2.297
(0)			10.530			9.380		9.518 ^{37.5°C}		9.234
4-Aminobutyric acid										
(+1)			4.057	4.046	4.038	4.031	4.027	4.025	4.027	4.032
(0)			11.026	10.867	10.706	10.556	10.409	10.269	10.114	9.874
2-Aminoethylsulfonic acid (0)			9.452	9.316	9.186	9.061	8.940	8.824	8.712	9.499
2-Amino-3-methylpentanoic acid										
(+1)	2.365 ^{1°C}		2.338 ^{12.5°C}			2.320		2.317 ^{37.5°C}		2.332
(0)	10.460 ^{1°C}		10.100 ^{12.5°C}			9.758		9.439 ^{37.5°C}		9.157

2-Amino-2-methyl- 1,3-propanediol	9.612	9.433	9.266	9.104	8.951	8.801	8.659	8.519	8.385	8.132
2-Amino-2-methylpropionic acid (+1)	2.419 ^{1 °C}		2.380 ^{12.5 °C}			2.357		2.351 ^{37.5 °C}		2.356
(0)	10.960 ^{1 °C}		10.580 ^{12.5 °C}			10.205		9.872 ^{37.5 °C}		9.561
2-Aminopentanoic acid (+1)	2.376 ^{1 °C}		2.347			2.318			2.309	2.313
(0)	10.508 ^{1 °C}			10.154 ^{12.5 °C}		9.808		9.490 ^{37.5 °C}		9.198
3-Aminopropionic acid (+1)	3.656	3.627		3.583		3.551		3.524	3.517	
(0)	11.000	10.830		10.526		10.235		9.963	9.842	
4-Aminopyridine (+1)	9.873	9.704	9.549	9.398	9.252	9.114	8.978	8.846	8.717	8.477
Ammonium ion (+1)	10.081	9.904	9.731	9.564	9.400	9.425	9.093	8.947	8.805	8.539
Arginine (+1)	1.914	1.885	1.870	1.849	1.837	1.823	1.814	1.801	1.800	1.787
(0)	9.718	9.563	9.407	9.270	9.123	8.994	8.859	8.739	8.614	8.385
Barbituric acid (+1)				3.969	3.980	4.02	4.00	4.008	4.017	4.032
(0)				8.493	8.435	8.372	8.302	8.227	8.147	7.974
Benzoic acid (0)		4.231	4.220	4.215	4.206	4.204	4.203	4.207	4.219	4.223
Boric acid (0)	9.508	9.439	9.380	9.327	9.280	9.236	9.197	9.161	9.132	9.080
Bromoacetic acid (0)				2.875	2.887	2.902	2.918	2.936		
3-Bromobenzoic acid (0)				3.818	3.813	3.810	3.808	3.810	3.813	
4-Bromobenzoic acid (0)				4.011	4.005	3.99	4.001	4.001	4.003	
Bromopropynoic acid (0)			1.786	1.814	1.839	1.855	1.879	1.900	1.919	
3- <i>tert</i> -Butylbenzoic acid (0)				4.266	4.231	4.199	4.170	4.143	4.119	
4- <i>tert</i> -Butylbenzoic acid (0)				4.463	4.425	4.389	4.354	4.320	4.287	
2-Butynoic acid (0)			2.618	2.626	2.611	2.620	2.618	2.621	2.631	
Butyric acid (0)	4.806	4.804	4.803	4.805	4.810	4.817	4.827	4.840	4.854	4.885
DL- <i>N</i> -Carbamoylalanine (+1)		3.898	3.894	3.891	3.890	3.892	3.896	3.902	3.908	3.931
<i>N</i> -Carbamoylglycine (+1)		3.911	3.900	3.889	3.879	3.876	3.874	3.873	3.875	3.888

TABLE 8.3 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (*continued*)

Substance	Temperature, °C									
	0	5	10	15	20	25	30	35	40	50
Carbon dioxide + water										
(0)	6.583	6.517	6.465	6.429	6.382	6.365	6.327	6.31	6.296	6.297
(−1)	10.627	10.558	10.499	10.431	10.377	10.33	10.290	10.25	10.220	10.172
Chloroacetic acid (0)				2.845	2.856	2.867	2.883	2.900		
3-Chlorobenzoic acid (0)				3.838	3.831	3.83	3.825	3.826	3.829	
4-Chlorobenzoic acid (0)				4.000	3.991	3.986	3.981	3.980	3.981	
Chloropropynoic acid (0)			1.766	1.796	1.820	1.845	1.864	1.879	1.893	
Citric acid										
(0)	3.220	3.200	3.176	3.160	3.142	3.128	3.116	3.109	3.099	3.095
(−1)	4.837	4.813	4.797	4.782	4.769	4.761	4.755	4.751	4.750	4.757
(−2)	6.393	6.386	6.383	6.384	6.388	6.396	6.406	6.423	6.439	6.484
Cyanoacetic acid (0)		2.445	2.447	2.452	2.460	2.460	2.482	2.496	2.511	
2-Cyano-2-methylpropionic acid										
(0)		2.342	2.360	2.379	2.400	2.422	2.446	2.471	2.498	
5,5-Diethylbarbituric acid (0)	8.40	8.30	8.22	8.169	8.094	8.020	7.948	7.877	7.808	7.673
Diethylmalonic acid										
(0)			2.129	2.136	2.144	2.151	2.160	2.172	2.187	
(−1)			7.400	7.401	7.408	7.417	7.428	7.441	7.457	
2,3-Dimethylbenzoic acid (0)				3.663	3.687	3.771	3.726	3.762	3.788	
2,4-Dimethylbenzoic acid (0)				4.154	4.187	4.217	4.244	4.268	4.290	
2,5-Dimethylbenzoic acid (0)				3.911	3.954	3.990	4.020	4.045	4.065	
2,6-Dimethylbenzoic acid (0)				3.234	3.304	3.362	3.409	3.445	3.472	
3,5-Dimethylbenzoic acid (0)				4.292	4.299	4.302	4.304	4.306	4.306	
<i>N,N'</i> -Dimethylethyleneamine-										
<i>N,N'</i> -diacetic acid										
(0)	6.294		6.169		6.047		5.926		5.803	
(−1)	10.446		10.268		10.068		9.882		9.684	

<i>N,N</i> -Dimethylglycine (0)		10.34		10.14		9.94		9.76		
3,5-Dinitrobenzoic acid (0)			2.60		2.73		2.85		2.96	3.07
2-Ethylbutyric acid (0)	4.623		4.664		4.710	4.751	4.758		4.812	4.869
5-Ethyl-5-phenylbarbituric acid (0)				7.592	7.517	7.445	7.377	7.311	7.248	7.130
Fluoroacetic acid (0)				2.555	2.571	2.586	2.604	2.624		
Formic acid (0)	3.786	3.772	3.762	3.757	3.753	3.751	3.752	3.758	3.766	3.782
2-Furancarboxylic acid (0)						3.164	3.200	3.216	3.239	
Glucose-1-phosphate (0)		6.506	6.500	6.499	6.500	6.504	6.510	6.519	6.531	6.561
Glycerol-1-phosphoric acid (−1)		6.642	6.641	6.643	6.648	6.656	6.666	6.679	6.695	6.733
Glycerol-2-phosphoric acid (0)		1.223	1.245	1.271	1.301	1.335	1.372	1.413	1.457	1.554
(−1)		6.657	6.650	6.646	6.646	6.650	6.657	6.666	6.679	6.712
Glycine (+1)			2.397	2.380	2.36	2.351	2.34	2.33	2.327	2.32
(0)		10.34	10.193	10.044	9.91	9.780	9.65	9.53	9.412	9.19
Glycolic acid (0)	3.875		3.844 ^{12.5°C}			3.831		3.833 ^{37.5°C}		3.849
Glycylasparagine (+1)		2.968	2.958	2.952	2.943	2.942	2.942	2.944	2.947	2.959
<i>N</i> -Glycylglycine (+1)	3.201					3.126				3.159
			8.594 ^{12.5°C}			8.252		7.948 ^{37.5°C}		7.668
Hexanoic acid (0)	4.840		4.839		4.849		4.865		4.890	4.920
Hydrogen cyanide (0)			9.63	9.49	9.36	9.21	9.11	8.99	8.88	
Hydrogen peroxide (0)	12.23			11.86	11.75	11.65	11.55	11.45		11.21
Hydrogen sulfide (0)		7.33	7.24	7.13	7.05	6.97	6.90	6.82	6.79	6.69
(−1)		13.5		13.2		12.90	12.75	12.6		
4-Hydroxybenzoic acid (0)				4.596	4.586	4.582	4.577	4.576	4.578	
Hydroxylamine (0)				6.186	6.063	5.948		5.730		
2-Hydroxy-1-naphthoic acid (0)										
(−1)					3.29		3.24		3.19	3.26
4-Hydroxyproline (+1)	1.900 ^{1°C}		1.850 ^{12.5°C}						9.61	9.58
(0)	10.274 ^{1°C}		9.958 ^{12.5°C}			1.818		1.798 ^{37.5°C}		1.796
						9.662		9.394 ^{37.5°C}		9.138

TABLE 8.3 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (*continued*)

Substance	Temperature, °C									
	0	5	10	15	20	25	30	35	40	50
2-Hydroxypropionic acid (0)	3.880	3.873	3.868	3.861	3.857	3.858	3.861	3.867	3.873	3.895
DL-2-Hydroxysuccinic acid (0)	3.537	3.520	3.494	3.482	3.472	3.458	3.452	3.446	3.444	3.445
(-1)	5.119	5.108	5.098	5.096	5.096	5.097	5.099	5.104	5.117	5.149
Hypobromous acid (0)				8.83		8.60		8.47	8.37 ^{45 °C}	
Hypochlorous acid (0)	7.82	7.75	7.69	7.63	7.58	7.54	7.50	7.46		7.05
Imidazole (+1)	7.581	7.467	7.334	7.216	7.103	6.993	6.887	6.784	6.685	6.497
Iodoacetic acid (0)				3.143	3.158	3.175	3.193	3.213		
DL-Isoleucine (+1)	2.365		2.338 ^{12.5 °C}			2.318		2.317 ^{37.5 °C}		2.332
(0)	10.460		10.100 ^{12.5 °C}			9.758		9.439 ^{37.5 °C}		9.157
Isopropylmalonic acid, mononitrile (0)		2.299	2.320	2.343	2.365	2.401	2.427	2.452	2.481	
Lactic acid (0)	3.880	3.873	3.868	3.862	3.857	3.858	3.861	3.867	3.873	3.895
Lead sulfate, pK _{sp}	8.01			7.87		7.80		7.73		7.63
DL-Leucine (+1)	2.383 ^{1 °C}		2.348 ^{12.5 °C}			2.328		2.327 ^{37.5 °C}		2.333
(0)	10.458 ^{1 °C}		10.095 ^{1.5 °C}			9.744		9.434 ^{37.5 °C}		9.142
Malonic acid (-1)	5.670	5.665	5.667	5.673	5.683	5.696	5.710	5.730	5.753	5.803
Mannose (0)			12.45			12.08			11.81	
Mercury(I) chloride, pK _{sp}			18.65	18.48	18.27	17.88		16.79		
Methanol (solvent), pK _{auto}		17.12		16.84		16.71	16.65	16.53		
Methylamine (+1)	11.496		11.130		10.787	10.62	10.466		10.161	9.876
Methylaminodiacetic acid (0)	2.138		2.142		2.146		2.150		2.154	
(-1)	10.474		10.287		10.088		9.920		9.763	

3-Methylbenzoic acid (0)				4.303	4.285	4.269	4.256	4.244	4.235	
4-Methylbenzoic acid (0)				4.390	4.376	4.362	4.349	4.336	4.322	
3-Methylbutyric acid (0)	4.726		4.742		4.767		4.794		4.831	4.871
4-Methylpentanoic acid (0)	4.827		4.827		4.837		4.853		4.879	4.908
5-Methyl-5-phenylbarbituric acid (0)				8.104	8.057	8.011	7.966	7.922	7.879	7.797
2-Methylpropionic acid (0)	4.825		4.827		4.840	4.853	4.886		4.918	4.955
2-Methyl-2-propylamine (+ 1)		11.439	11.240	11.048	10.862	10.682	10.511	10.341		
Nitric acid (0)	− 1.65					− 1.38				− 1.20
Nitrilotriacetic acid (0)	1.69		1.65		1.65		1.66		1.67	
(− 1)	2.95		2.95		2.94		2.96		2.98	
(− 2)	10.59		10.45		10.33		10.23			
4-Nitrobenzoic acid (0)				3.448	3.444	3.441	3.441	3.442	3.445	
Nitrous acid (0)				3.244	3.177	3.138		3.100		
DL-Norleucine (+ 1)	2.394		2.356 ^{12.5 °C}			2.335		2.324 ^{37.5 °C}		2.328
(0)	10.564		10.190 ^{12.5 °C}			9.834		9.513 ^{37.5 °C}		9.224
Oxalic acid (− 1)	4.210	4.216	4.227	4.240	4.254	4.272	4.295	4.318	4.349	4.409
2,4-Pentanedione (0)	9.07					8.95			8.90	
Pentanoic acid (0)	4.823		4.763		4.835	4.842	4.851		4.861	4.906
Phenylalanine (0)			9.75			9.31			8.96	
Phosphoric acid (0)	2.056	2.073	2.088	2.107	2.127	2.148	2.171	2.196	2.224	2.277
(− 1)	7.313	7.282	7.254	7.231	7.213	7.198	7.189	7.185	7.181	7.183
<i>o</i> -Phthalic acid (0)	2.925	2.927	2.931	2.937	2.943	2.950	2.958	2.967	2.978	3.001
(− 1)	5.432	5.418	5.410	5.405	5.405	5.408	5.416	5.427	5.442	5.485
Piperidine (+ 1)	11.963	11.786	11.613	11.443	11.280	11.123	10.974	10.818	10.670	10.384
Proline (+ 1)	2.011		1.964 ^{12.5 °C}			1.952		1.950 ^{37.5 °C}		1.958
(0)	11.296		10.972 ^{12.5 °C}			10.640		10.342 ^{37.5 °C}	10.064	

TABLE 8.3 Selected Equilibrium Constants in Aqueous Solution at Various Temperatures (*continued*)

Substance	Temperature, °C									
	0	5	10	15	20	25	30	35	40	50
Propenoic acid (0)				4.267	4.250	4.247	4.249	4.267	4.301	
<i>N</i> -Propionylglycine (+1)		3.728	3.723	3.718	3.716	3.718	3.721	3.725	3.731	3.750
Propynoic acid (0)			1.791	1.829	1.867	1.887	1.940	1.932	1.963	
Pyrrolidine (+1)	12.17	11.98	11.81	11.63	11.43	11.30	11.15	10.99	10.84	11.56
Serine										
(+1)	2.296 ^{1°C}		2.232 ^{12.5°C}			2.186		2.154 ^{37.5°C}		2.132
(0)	9.880 ^{1°C}		9.542 ^{12.5°C}			9.208		8.904 ^{37.5°C}		8.628
Silver bromide, pK_{sp}		13.33		12.83	12.57	12.30	12.07	11.83	11.61	11.19
Silver chloride, pK_{sp}		10.595		10.152		9.749		9.381	9.21	8.88
Succinic acid										
(0)	4.285	4.263	4.245	4.232	4.218	4.207	4.198	4.191	4.188	4.186
(−1)	5.674	5.660	5.649	5.642	5.639	5.635	6.541	5.647	5.654	5.680
Sulfuric acid (−1)	1.778	1.812 ^{4.3°C}		1.894		1.987	2.05	2.095	2.17	2.246
Sulfurous acid (0)	1.63		1.74			1.89		1.98		2.12
D-Tartaric acid										
(0)	3.118	3.095	3.075	3.057	3.044	3.036	3.025	3.019	3.018	3.021
(−1)	4.426	4.407	4.391	4.381	4.372	4.366	4.365	4.367	4.372	4.391
2,3,5,6-Tetramethylbenzoic acid (0)				3.310	3.367	3.415	3.453	3.483	3.505	
Threonine										
(+1)	2.200 ^{1°C}		2.132 ^{12.5°C}			2.088		2.070 ^{37.5°C}		2.055
(0)	9.748 ^{1°C}		9.420 ^{12.5°C}			9.100		8.812 ^{37.5°C}		8.548
<i>o</i> -Toluidine (0)				4.58	4.495	4.45	4.345	4.28	4.20	
1,2,4-Triazole										
(+1)				2.451	2.418	2.386	2.327			
(0)				10.205	10.083	9.972	9.768			
3,4,5-Trihydroxybenzoic acid (0)					4.19		4.30		4.38	4.53

Tris(2-hydroxyethyl)amine (+1)	8.290	8.173	8.067	7.963	7.861	7.762	7.666	7.570	7.477	7.299
2,4,6-Trimethylbenzoic acid (0)				3.325	3.391	3.448	3.498	3.541	3.577	
3-Trimethylsilylbenzene acid (0)				4.142	4.116	4.089	4.060	4.029	3.996	
4-Trimethylsilylbenzoic acid (0)				4.270	4.230	4.192	4.155	4.119	4.084	
β -Ureidopropionic acid (0)		4.514	4.505	4.497	4.490	4.487	4.486	4.486	4.488	4.500
DL-Valine										
(+1)	2.320		2.297 ^{12.5°C}			2.296		2.292 ^{37.5°C}		2.310
(0)	10.413		10.064 ^{12.5°C}			9.719		9.405 ^{37.5°C}		9.124

TABLE 8.4 Indicators for Aqueous Acid–Base Titrations

Table 8.4 lists selected common indicators. The table is arranged according to function over increasing pH range or transition interval given (third column). Note that this range may vary appreciably from one observer to another, and that it is also affected by ionic strength, temperature, and illumination. The values given should therefore be considered to be approximate. These values refer to solutions having low ionic strengths and a temperature of about 25 °C. In the fourth column the pK_A ($-\log K_A$) of the indicator as determined spectrophotometrically is listed. In the fifth and sixth columns, the wavelength of maximum absorption is given for the acidic and basic forms of the indicator, respectively. The lower to higher pH color change is given in the last column. The abbreviations used to describe the colors of the two forms of the indicator are as follows:

- B, Blue
- C, Colorless
- G, Green
- O, Orange
- OBr, Orange-brown
- P, Purple
- R, Red
- V, Violet
- Y, Yellow

Indicator	Chemical name	pH range	pK _A	λ _{max} , nm		Color change
				Acid	Base	
Cresol red (acid range)	<i>o</i> -Cresolsulfonephthalein	0.2–18				R–Y
Cresol purple (acid range)	<i>m</i> -Cresolsulfonephthalein	1.2–2.8	1.51	533		R–Y
Thymol blue (acid range)	Thymolsulfonephthalein	1.2–2.8	1.65	544	430	R–Y
Tropeolin OO	Diphenylamino- <i>p</i> -benzene sodium sulfonate	1.3–3.2	2.0	527		R–Y
2,6-Dinitrophenol	2,6-Dinitrophenol	2.4–4.0	3.69			C–Y
2,4-Dinitrophenol	2,4-Dinitrophenol	2.5–4.3	3.90			C–Y
Methyl yellow	Dimethylaminoazobenzene	2.9–4.0	3.3	508		R–Y
Methyl orange	Dimethylaminoazobenzene sodium sulfonate	3.1–4.4	3.40	522	464	R–O
Bromophenol blue	Tetrabromophenolsulfonephthalein	3.0–4.6	3.85	436	592	Y–BV
Bromocresol green	Tetrabromo- <i>m</i> -cresol-sulfonephthalein	4.0–5.6	4.68	444	617	Y–B
Methyl red	<i>o</i> -Carboxybenzeneazo-dimethylaniline	4.4–6.2	4.95	530	427	R–Y
Chlorophenol red	Dichlorophenolsulfonephthalein	5.4–6.8	6.0		573	Y–R
Bromocresol purple	Dibromo- <i>o</i> -cresolsulfonephthalein	5.2–6.8	6.3	433	591	Y–P
Bromophenol red	Dibromophenolsulfonephthalein	5.2–6.8			574	Y–R
<i>p</i> -Nitrophenol	<i>p</i> -Nitrophenol	5.3–7.6	7.15	320	405	C–Y
Bromothymol blue	Dibromothymolsulfonephthalein	6.2–7.6	7.1	433	617	Y–B
Neutral red	Aminodimethylaminotoluphen-azonium chloride	6.8–8.0	7.4			R–Y
Phenol red	Phenolsulfonephthalein	6.4–8.0	7.9	433	558	Y–R

TABLE 8.4 Indicators for Aqueous Acid–base Titrations (*continued*)

Indicator	Chemical name	pH range	pK _A	λ_{\max} , nm		Color change
				Acid	Base	
<i>m</i> -Nitrophenol	<i>m</i> -Nitrophenol	6.4–8.8	8.3		570	C–Y
Cresol red	<i>o</i> -Cresolsulfonephthalein	7.2–8.8	8.2	434	572	Y–R
<i>m</i> -Cresol purple	<i>m</i> -Cresolsulfonephthalein	7.6–9.2	8.32		580	Y–P
Thymol blue	Thymolsulfonephthalein	8.0–9.6	8.9	430	596	Y–B
Phenolphthalein	Phenolphthalein	8.0–10.0	9.4		553	C–R
α -Naphtholbenzein	α -Naphtholbenzein	9.0–11.0				Y–B
Thymolphthalein	Thymolphthalein	9.4–10.6	10.0		598	C–B
Alizarin yellow	5-(<i>p</i> -Nitrophenylazo)salicylic acid, Na salt	10.0–12.0	11.16			Y–V
Tropeolin O	<i>p</i> -Sulfobenzeneazoresorcinol	11.0–13.0				Y–OBr
Nitramine	2,4,6-Trinitrophenyl-methylnitroamine	10.8–13.0				C–OBr

BUFFER SOLUTIONS**TABLE 8.5** National Institute of Standards and Technology (formerly National Bureau of Standards U.S.). Reference PH Buffer Solutions.

Temperature °C	Secondary standard 0.05 M Potassium tetraoxalate	Potassium hydrogen tartrate (saturated at 25 °C)	0.05 M Potassium dihydrogen citrate	0.05 M Potassium hydrogen phthalate	0.025 M KH ₂ PO ₄ , 0.025 M Na ₂ HPO ₄	0.0087 M KH ₂ PO ₄ , 0.0302 M Na ₂ HPO ₄	0.01 M Na ₂ B ₄ O ₇	0.025 M NaHCO ₃ , 0.025 M Na ₂ CO ₃	Secondary standard Ca(OH) ₂ (saturated at 25 °C)
0	1.666		3.860	4.003	6.984	7.534	9.464	10.317	13.423
5	1.668		3.840	3.999	6.951	7.500	9.395	10.245	13.207
10	1.670		3.820	3.998	6.923	7.472	9.332	10.179	13.003
15	1.672		3.802	3.999	6.900	7.448	9.276	10.118	12.810
20	1.675		3.788	4.002	6.881	7.429	9.225	10.062	12.627
25	1.679	3.557	3.776	4.008	6.865	7.413	9.180	10.012	12.454
30	1.683	3.552	3.766	4.015	6.853	7.400	9.139	9.966	12.289
35	1.688	3.549	3.759	4.024	6.844	7.389	9.102	9.925	12.133
38	1.691	3.548		4.030	6.840	7.384	9.081		12.043
40	1.694	3.547	3.753	4.035	6.838	7.380	9.068	9.889	11.984
45	1.700	3.547		4.047	6.834	7.373	9.038		11.841
50	1.707	3.549	3.749	4.060	6.833	7.367	9.011	9.828	11.705
55	1.715	3.554		4.075	6.834		8.985		11.574
60	1.723	3.560		4.091	6.836		8.962		11.449
70	1.743	3.580		4.126	6.845		8.921		
80	1.766	3.609		4.164	6.859		8.885		
90	1.792	3.650		4.205	6.877		8.850		
95	1.806	3.674		4.227	6.886		8.833		
Dilution value $\Delta pH_{1/2}$	+0.186	+0.049	0.024	+0.052	+0.080	+0.070	+0.01	0.079	-0.28

Source: R. G. Bates, *J. Res. Natl. Bur. Stand. (U.S.)*, **66A**:179 (1962) and B. R. Staples and R. G. Bates, *ibid*, **73A**: 37 (1969).

TABLE 8.6 Compositions of National Institute of Standards and Technology. Standard pH Buffer Solutions*Air weight of material per liter of buffer solution*

Standard	Weight, g
$\text{KH}_3(\text{C}_2\text{O}_4)_2 \cdot 2\text{H}_2\text{O}$, 0.05 M	12.61
Potassium hydrogen tartrate, about 0.034 M	Saturated at 25 °C
Potassium hydrogen phthalate, 0.05 M	10.12
Phosphate (solution 1)	
KH_2PO_4 , 0.025 M	3.39
Na_2HPO_4 , 0.025 M	3.53
Phosphate (solution 2)	
KH_2PO_4 , 0.008665 M	1.179
Na_2HPO_4 , 0.03032 M	4.30
$\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$, 0.01 M	3.80
Carbonate	
NaHCO_3 , 0.025 M	2.10
Na_2CO_3 , 0.025 M	2.65
$\text{Ca}(\text{OH})_2$, about 0.0203 M	Saturated at 25 °C

Standard Reference pH Buffer Solutions

The buffer value for the National Institute of Standards and technology (U.S.) reference pH buffer solutions is given below:

Buffer solution	KH tartrate	0.05 M KH_2 citrate	0.05 M KH phthalate	0.025 M KH_2PO_4 , 0.025 M Na_2HPO_4	0.0087 M KH_2PO_4 , 0.0302 M Na_2HPO_4	0.01 M $\text{Na}_2\text{B}_4\text{O}_7$	0.025 M NaHCO_3 , 0.025 M Na_2CO_3
Buffer value β	0.027	0.034	0.016	0.029	0.016	0.020	0.029

For the secondary pH reference standards, the buffer value is 0.070 for potassium tetroxalate and 0.09 for calcium hydroxide.

To prepare the standard pH buffer solutions recommended by the National Bureau of Standards (U.S.), the indicated weights of the pure materials in Table 8.6 should be dissolved in water of specific conductivity not greater than 5 micromhos. The tartrate, phthalate, and phosphates can be dried for 2 h at 110 °C before use. Potassium tetroxalate and calcium hydroxide need not be dried. Fresh-looking crystals of borax should be used. Before use, excess solid potassium hydrogen tartrate and calcium hydroxide must be removed. Buffer solutions pH 6 or above should be stored in plastic containers and should be protected from carbon dioxide with soda-lime traps. The solutions should be replaced

within 2 to 3 weeks, or sooner if formation of mold is noticed. A crystal of thymol may be added as a preservative.

Buffer Solutions other than Standards

The range of the buffering effect of a single weak acid group is approximately one pH unit on either side of the pK_A . The ranges of some useful buffer systems are collected in Table 8.7. After all the components have been brought together, the pH of the resulting solution should be determined at the temperature to be employed with reference to standard reference solutions. Buffer components should be compatible with other components in the system under study; this is particularly significant for buffers employed in biological studies. Check tables of formation constants to ascertain whether metal-binding character exists.

When there are two or more acid groups per molecule, or a mixture is composed of several overlapping acids, the useful range is larger. Universal buffer solutions consist of a mixture of acid groups which overlap such that successive pK_A values differ by 2 pH units or less. The Prideaux–Ward mixture comprises phosphate, phenyl acetate, and borate plus HCl and covers the range from 2 to 12 pH units. The McIlvaine buffer is a mixture of citric acid and Na_2HPO_4 that covers the range from pH 2.2 to 8.0. The Britton–Robinson system consists of acetic acid, phosphoric acid, and boric acid plus NaOH and covers the range from pH 4.0 to 11.5. A mixture composed of Na_2CO_3 , NaH_2PO_4 , citric acid, and 2-amino-2-methyl-1,3-propanediol covers the range from pH 2.2 to 11.0.

TABLE 8.7 pH Values of Buffer Solutions for Control Purposes

Materials*	pH range
Glycine and HCl	1.0–3.7
Citrate and HCl	1.3–4.7
<i>p</i> -Toluenesulfonate and <i>p</i> -toluenesulfonic acid	1.1–3.3
Formate and HCl	2.8–4.6
Succinic acid and borax	3.0–5.8
Phenyl acetate and HCl	3.5–5.0
Acetate and acetic acid	3.7–5.6
Succinate and succinic acid	4.8–6.3
2-(<i>N</i> -Morpholino)ethanesulfonic acid and NaOH	5.2–7.1
2,2-Bis(hydroxymethyl)-2,2',2''-nitrilotriethanol and HCl	5.8–7.2
KH_2PO_4 and borax	5.8–9.2
<i>N</i> -Tris(hydroxymethyl)methyl-2-aminoethanesulfonic acid and NaOH	6.8–8.2
KH_2PO_4 and Na_2HPO_4	6.1–7.5
<i>N</i> -2-Hydroxyethylpiperazine- <i>N'</i> -2-ethanesulfonic acid and NaOH	6.9–8.3
Triethanolamine and HCl	6.9–8.5
Diethylbarbiturate (veronal) and HCl	7.0–8.5
Tris(hydroxymethyl)aminomethane and HCl	7.2–9.0
<i>N</i> -Tris(hydroxymethyl)methylglycine and HCl	
<i>N,N</i> -Bis(2-hydroxyethyl)glycine and HCl	
Borax and HCl	7.6–8.9
Glycine and NaOH	8.2–10.1
Ammonia (aqueous) and NH_4Cl	8.3–9.2
Ethanolamine and HCl	8.6–10.4

Borax and NaOH	9.4–11.1
Carbonate and hydrogen carbonate	9.2–11.0
Na ₂ HPO ₄ and NaOH	11.0–12.0

General directions for the preparation of buffer solutions of varying pH but fixed ionic strength are given by Bates.* Preparation of McIlvaine buffered solutions at ionic strengths of 0.5 and 1.0 and Britton–Robinson solutions of constant ionic strength have been described by Elving et al.† and Frugoni,‡ respectively.

* Bates, *Determination of pH, Theory and Practice*, Wiley, New York, 1964, pp. 121–122.

† Elving, Markowitz, and Rosenthal, *Anal. Chem.*, **28**:1179 (1956).

‡ Frugoni, *Gazz. Chim. Ital.*, **87**:403 (1957).

REFERENCE ELECTRODES

TABLE 8.8 Potentials of Reference Electrodes (in volts) as a Function of Temperature

Liquid-junction potential included

Temp., °C	0.1 M KCl, calomel*	1.0 M KCl, calomel*	3.5 M KCl, calomel*	Saturated KCl, calomel*	1.0 M KCl, Ag/AgCl†	1.0 M KBr, Ag/AgBr‡	1.0 M KI, Ag/AgI§
0	0.3367	0.2883		0.25918	0.23655	0.08128	−0.14637
5					0.23413	0.07961	−0.14719
10	0.3362	0.2868	0.2556	0.25387	0.23142	0.07773	−0.14822
15	0.3361			0.2511	0.22857	0.07572	−0.14942
20	0.3358	0.2844	0.2520	0.24775	0.22557	0.07349	−0.15081
25	0.3356	0.2830	0.2501	0.24453	0.22234	0.07106	−0.15244
30	0.3354	0.2815	0.2481	0.24118	0.21904	0.06856	−0.15405
35	0.3351			0.2376	0.21565	0.06585	−0.15590
38	0.3350		0.2448	0.2355			
40	0.3345	0.2782	0.2439	0.23449	0.21208	0.06310	−0.15788
45					0.20835	0.06012	−0.15998
50	0.3315	0.2745		0.22737	0.20449	0.05704	−0.16219
55					0.20056		
60	0.3248	0.2702		0.2235	0.19649		
70					0.18782		
80				0.2083	0.1787		
90					0.1695	0.0251	

* Bates et al., *J. Res. Natl. Bur. Stand.*, **45**:418 (1950).

† Bates and Bower, *J. Res. Natl. Bur. Stand.*, **53**:283 (1954).

‡ Hetzer, Robinson, and Bates, *J. Phys. Chem.*, **66**:1423 (1962).

§ Hetzer, Robinson, and Bates, *J. Phys. Chem.*, **68**:1929 (1964).

Temp., °C	125	150	175	200	225	250	275
1.0 M KCl, Ag/AgCl*	0.1330	0.1032	0.0708	0.0348	−0.0051	−0.054	−0.090
1.0 M KBr, Ag/AgBr†	−0.0048	−0.0312	−0.0612	−0.0951			

* Greeley et al., *J. Phys. Chem.*, **64**:652 (1960).

† Towns et al., *J. Phys. Chem.*, **64**:1861 (1960).

The values of several additional reference electrodes at 25 °C are listed:

Reference electrode	Potential, V
Ag/AgCl, saturated KCl	0.198
Ag/AgCl, 0.1 M KCl	0.288
Hg/HgO, 1.0 M NaOH	0.140
Hg/HgO, 0.1 M NaOH	0.165
Hg/Hg ₂ SO ₄ , saturated K ₂ SO ₄ (22 °C)	0.658
Hg/HgSO ₄ , saturated KCl	0.655

TABLE 8.9 Potentials of Reference Electrodes (in volts) at 25°C for water–organic solvent mixtures*Electrolyte solution of 1 M HCl*

Solvent, wt %	Methanol, Ag/AgCl	Ethanol, Ag/AgCl	2-Propanol, Ag/AgCl	Acetone, Ag/AgCl	Dioxane, Ag/AgCl	Ethylene glycol, Ag/AgCl	Methanol, calomel	Dioxane, calomel
5			0.2180	0.2190		0.2190		
10	0.2153	0.2146	0.2138	0.2156		0.2160		
20	0.2090	0.2075	0.2063	0.2079	0.2031	0.2101	0.255	0.2501
30		0.2003				0.2036		
40	0.1968	0.1945		0.1859		0.1972	0.243	
45					0.1635			0.2104
50		0.1859		0.158				
60	0.1818	0.173				0.1807		
70		0.158			0.0659		0.216	0.1126
80	0.1492	0.136						
82					−0.0614			−0.0014
90	0.1135	0.196		−0.034				
94.2	0.0841							
98		0.0215						
99							0.103	
100	−0.0099	−0.0081		−0.53				

ELECTRODE POTENTIALS

TABLE 8.10 Potentials of Selected Half-Reactions at 25 °C

This table is a summary of oxidation–reduction half-reactions arranged in order of decreasing oxidation strength and is useful for selecting reagent systems.

Abbreviations Used in the Table
g, gas liq, liquid s, solid

Half-reaction	<i>E</i> °, V
F ₂ (g) + 2H ⁺ + 2e [−]	= 2HF 3.06
O ₃ + 2H ⁺ + 2e [−]	= O ₂ + H ₂ O 2.07
S ₂ O ₈ ^{2−} + 2e [−]	= 2SO ₄ ^{2−} 2.01
Ag ²⁺ + e [−]	= Ag ⁺ 2.00
H ₂ O ₂ + 2H ⁺ + 2e [−]	= 2H ₂ O 1.77
MnO ₄ [−] + 4H ⁺ + 3e [−]	= MnO ₂ (s) + 2H ₂ O 1.70
Ce(IV) + e [−]	= Ce(III) (in 1 M HClO ₄) 1.61
H ₃ IO ₆ + H ⁺ + 2e [−]	= IO ₃ [−] + 3H ₂ O 1.6
Bi ₂ O ₄ (bismuthate) + 4H ⁺ + 2e [−]	= 2BiO ⁺ + 2H ₂ O 1.59
BrO ₃ [−] + 6H ⁺ + 5e [−]	= $\frac{1}{2}$ Br ₂ + 3H ₂ O 1.52
MnO ₄ [−] + 8H ⁺ + 5e [−]	= Mn ²⁺ + 4H ₂ O 1.51
PbO ₂ + 4H ⁺ + 2e [−]	= Pb ²⁺ + 2H ₂ O 1.455
Cl ₂ + 2e [−]	= 2Cl [−] 1.36
Cr ₂ O ₇ ^{2−} + 14H ⁺ + 6e [−]	= 2Cr ³⁺ + 7H ₂ O 1.33
MnO ₂ (s) + 4H ⁺ + 2e [−]	= Mn ²⁺ + 2H ₂ O 1.23
O ₂ (g) + 4H ⁺ + 4e [−]	= 2H ₂ O 1.229
IO ₃ [−] + 6H ⁺ + 5e [−]	= $\frac{1}{2}$ I ₂ + 3H ₂ O 1.20
Br ₂ (liq) + 2e [−]	= 2Br [−] 1.065
ICl ₂ [−] + e [−]	= $\frac{1}{2}$ I ₂ + 2Cl [−] 1.06
VO ₂ ⁺ + 2H ⁺ + e [−]	= VO ²⁺ + H ₂ O 1.00
HNO ₂ + H ⁺ + e [−]	= NO(g) + H ₂ O 1.00
NO ₃ [−] + 3H ⁺ + 2e [−]	= HNO ₂ + H ₂ O 0.94
2Hg ²⁺ + 2e [−]	= Hg ₂ ²⁺ 0.92
Cu ²⁺ + I [−] + e [−]	= CuI 0.86
Ag ⁺ + e [−]	= Ag 0.799
Hg ₂ ²⁺ + 2e [−]	= 2Hg 0.79
Fe(III) + e [−]	= Fe ²⁺ 0.771
O ₂ (g) + 2H ⁺ + 2e [−]	= H ₂ O ₂ 0.682
2HgCl ₂ + 2e [−]	= Hg ₂ Cl ₂ (s) + 2Cl [−] 0.63
Hg ₂ SO ₄ (s) + 2e [−]	= 2Hg + SO ₄ ^{2−} 0.615
H ₃ AsO ₄ + 2H ⁺ + 2e [−]	= HAsO ₂ + 2H ₂ O 0.581
Sb ₂ O ₅ + 6H ⁺ + 4e [−]	= 2SbO ⁺ + 3H ₂ O 0.559
I ₃ [−] + 2e [−]	= 3I [−] 0.545
Cu ⁺ + e [−]	= Cu 0.52
VO ²⁺ + 2H ⁺ + e [−]	= V ³⁺ + H ₂ O 0.337
Fe(CN) ₆ ^{3−} + e [−]	= Fe(CN) ₆ ^{4−} 0.36
Cu ²⁺ + 2e [−]	= Cu 0.337
UO ₂ ²⁺ + 4H ⁺ + 2e [−]	= U ⁴⁺ + 2H ₂ O 0.334
BiO ⁺ + 2H ⁺ + 3e [−]	= Bi + H ₂ O 0.32
Hg ₂ Cl ₂ (s) + 2e [−]	= 2Hg + 2Cl [−] 0.2676
AgCl(s) + e [−]	= Ag + Cl [−] 0.2223

TABLE 8.10 Potentials of Selected Half-Reactions at 25 °C (*continued*)

Half-reaction		E° , V
$\text{SbO}^+ + 2\text{H}^+ + 3e^-$	$= \text{Sb} + \text{H}_2\text{O}$	0.212
$\text{CuCl}_3^{2-} + e^-$	$= \text{Cu} + 3\text{Cl}^-$	0.178
$\text{SO}_4^{2-} + 4\text{H}^+ + 2e^-$	$= \text{SO}_2(\text{aq}) + 2\text{H}_2\text{O}$	0.17
$\text{Sn}^{4+} + 2e^-$	$= \text{Sn}^{2+}$	0.154
$\text{S} + 2\text{H}^+ + 2e^-$	$= \text{H}_2\text{S}(\text{g})$	0.141
$\text{TiO}^{2+} + 2\text{H}^+ + e^-$	$= \text{Ti}^{3+} + \text{H}_2\text{O}$	0.10
$\text{S}_4\text{O}_6^{2-} + 2e^-$	$= 2\text{S}_2\text{O}_3^{2-}$	0.08
$\text{AgBr}(\text{s}) + e^-$	$= \text{Ag} + \text{Br}^-$	0.071
$2\text{H}^+ + 2e^-$	$= \text{H}_2$	0.0000
$\text{Pb}^{2+} + 2e^-$	$= \text{Pb}$	-0.126
$\text{Sn}^{2+} + 2e^-$	$= \text{Sn}$	-0.136
$\text{AgI}(\text{s}) + e^-$	$= \text{Ag} + \text{I}^-$	-0.152
$\text{Mo}^{3+} + 3e^-$	$= \text{Mo}$	ca-0.2
$\text{N}_2 + 5\text{H}^+ + 4e^-$	$= \text{H}_2\text{NNH}_3^+$	-0.23
$\text{Ni}^{2+} + 2e^-$	$= \text{Ni}$	-0.246
$\text{V}^{3+} + e^-$	$= \text{V}^{2+}$	-0.255
$\text{Co}^{2+} + 2e^-$	$= \text{Co}$	-0.277
$\text{Ag}(\text{CN})_2^- + e^-$	$= \text{Ag} + 2\text{CN}^-$	-0.31
$\text{Cd}^{2+} + 2e^-$	$= \text{Cd}$	-0.403
$\text{Cr}^{3+} + e^-$	$= \text{Cr}^{2+}$	-0.41
$\text{Fe}^{2+} + 2e^-$	$= \text{Fe}$	-0.440
$2\text{CO}_2 + 2\text{H}^+ + 2e^-$	$= \text{H}_2\text{C}_2\text{O}_4$	-0.49
$\text{H}_3\text{PO}_3 + 2\text{H}^+ + 2e^-$	$= \text{H}_3\text{PO}_2 + \text{H}_2\text{O}$	-0.50
$\text{U}^{4+} + e^-$	$= \text{U}^{3+}$	-0.61
$\text{Zn}^{2+} + 2e^-$	$= \text{Zn}$	-0.763
$\text{Cr}^{2+} + 2e^-$	$= \text{Cr}$	-0.91
$\text{Mn}^{2+} + 2e^-$	$= \text{Mn}$	-1.18
$\text{Zr}^{4+} + 4e^-$	$= \text{Zr}$	-1.53
$\text{Ti}^{3+} + 3e^-$	$= \text{Ti}$	-1.63
$\text{Al}^{3+} + 3e^-$	$= \text{Al}$	-1.66
$\text{Th}^{4+} + 4e^-$	$= \text{Th}$	-1.90
$\text{Mg}^{2+} + 2e^-$	$= \text{Mg}$	-2.37
$\text{La}^{3+} + 3e^-$	$= \text{La}$	-2.52
$\text{Na}^+ + e^-$	$= \text{Na}$	-2.714
$\text{Ca}^{2+} + 2e^-$	$= \text{Ca}$	-2.870
$\text{Sr}^{2+} + 2e^-$	$= \text{Sr}$	-2.89
$\text{K}^+ + e^-$	$= \text{K}$	-2.925
$\text{Li}^+ + e^-$	$= \text{Li}$	-3.045

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C

The solvent systems in this table are listed below:

A, acetonitrile and a perchlorate salt such as LiClO_4 or a tetraalkyl ammonium salt

B, acetic acid and an alkali acetate, often plus a tetraalkyl ammonium iodide

C, 0.05 to 0.175 M tetraalkyl ammonium halide and 75% 1,4-dioxane

D, buffer plus 50% ethanol (EtOH)

Abbreviations Used in the Table

Bu, butyl

M, molar

MeOH, methanol

Et, ethyl

Me, methyl

PrOH, propanol

EtOH, ethanol

Compound	Solvent system	$E_{1/2}$
Unsaturated aliphatic hydrocarbons		
Acrylonitrile	C but 30% EtOH	-1.94
Allene	C	-2.29
1,3-Butadiene	A	-2.03
	C	-2.59
1,3-Butadiyne	C	-1.89
1-Buten-2-yne	C	-2.40
1,4-Cyclohexadiene	A	-1.6
Cyclohexene	A	-1.89
1,3,5,7-Cyclooctatetraene	B	-1.42
	C	-1.51
Diethyl fumarate	B, pH 4.0	-0.84
Diethyl maleate	B, pH 4.0	-0.95
2,3-Dimethyl-1,3-butadiene	A	-1.83
Dimethylfulvene	C	-1.89
Diphenylacetylene	C	-2.20
1,1-Diphenylethylene	B	-1.52
	C	-2.19
Ethyl methacrylate	0.1 N LiCl + 25% EtOH	-1.9
2-Methyl-1,3-butadiene	A	-1.84
2-Methyl-1-butene	A	-1.97
1-Piperidino-4-cyano-4-phenyl- 1,3-butadiene	LiClO_4 in dimethylformamide	-0.16
<i>trans</i> -Stilbene	B	-1.51
Tetrakis(dimethylamino)ethylene	A	-0.75
Aromatic hydrocarbons		
Acenaphthene	A	-0.95
	B	-1.36
	C	-2.58
Anthracene	A	-0.84
	B	-1.20
	C	-1.94

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25 °C (*continued*)

Compound	Solvent system	$E_{1/2}$
Aromatic hydrocarbons (<i>continued</i>)		
Azulene	A	-0.71
	C	-1.66, -2.26, -2.56
1,2-Benzanthracene	C	-2.03, -2.54
2,3-Benzanthracene	A	-0.54, -1.20
Benzene	A	-2.08
1,2-Benzo[<i>a</i>]pyrene	A	-0.76
Biphenyl	A	-1.48
	B	-1.91
	C	-2.70
Chrysene	A	-1.22
1,2,5,6-Dibenzanthracene	A	-1.00, -1.26
1,2-Dihydronaphthalene	C	-2.57
9,10-Dimethylantracene	A	-0.65
2,3-Dimethylnaphthalene	A	-1.08, -1.34
9,10-Diphenylantracene	A	-0.92
Fluorene	A	-1.25
	B	-1.65
	C	-2.65
Hexamethylbenzene	A	-1.16
	B	-1.52
Indan	A	-1.59, -2.02
Indene	A	-1.23
	C	-2.81
1-Methylnaphthalene	A	-1.24
	B	-1.53
	C	-2.46
2-Methylnaphthalene	A	-1.22
	B	-1.55
	C	-2.46
Naphthalene	A	-1.34
	B	-1.72
Pentamethylbenzene	A	-1.28
	B	-1.62
Phenanthrene	A	-1.23
	B	-1.68
	C	-2.46, -2.71
Phenylacetylene	C	-2.37
Pyrene	A	-1.06, -1.24
<i>trans</i> -Stilbene	B	-1.51
	C	-2.26
Styrene	C	-2.35
1,2,3,5-Tetramethylbenzene	A	-1.50, -1.99
1,2,4,5-Tetramethylbenzene	A	-1.29
Tetraphenylethylene	C	-2.05

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C (*continued*)

Compound	Solvent system	$E_{1/2}$
Aromatic hydrocarbons (<i>continued</i>)		
1,4,5,8-Tetraphenylnaphthalene	A	-1.39
Toluene	A	-1.98
1,2,3-Trimethylbenzene	A	-1.58
1,2,4-Trimethylbenzene	A	-1.41
1,3,5-Trimethylbenzene	A	-1.50
	B	-1.90
Triphenylene	A	-1.46, -1.55
Triphenylmethane	C	-1.01, -1.68, -1.96
<i>o</i> -Xylene	A	-1.58, -2.04
<i>m</i> -Xylene	A	-1.58
<i>p</i> -Xylene	A	-1.56
Aldehydes		
Acetaldehyde	B, pH 6.8-13	-1.89
Benzaldehyde	McIlvaine buffer, pH 2.2	-0.96, -1.32
Bromoacetaldehyde	pH 8.5	-0.40
	pH 9.8	-1.58, -1.82
Chloroacetaldehyde	Ammonia buffer, pH 8.4	-1.06, -1.66
Cinnamaldehyde	Buffer + EtOH, pH 6.0	-0.9, -1.5, -1.7
Crotonaldehyde	B, pH 1.3-2.0	-0.92
	Ammonia buffer, pH 8.0	-1.30
Dichloroacetaldehyde	Ammonia buffer, pH 8.4	-1.03, -1.67
3,7-Dimethyl-2,6-octadienal	0.1 M Et ₄ NI	-1.56, -2.22
Formaldehyde	0.05 M KOH + 0.1 M KCl, pH 12.7	-1.59
2-Furaldehyde	pH 1-8	-0.86, -0.07 pH
	pH 10	-1.43
Glucose	Phosphate buffer, pH 7	-1.55
Glyceraldehyde	Britton-Robinson buffer, pH 5.0	-1.47
	Britton-Robinson buffer, pH 8.0	-1.55
Glycolaldehyde	0.1 M KOH, pH 13	-1.70
Glyoxal	B, pH 3.4	-1.41
4-Hydroxybenzaldehyde	Britton-Robinson buffer, pH 1.8	-1.16
	Britton-Robinson buffer, pH 6.8	-1.45
4-Hydroxy-2-methoxybenzaldehyde	McIlvaine buffer, pH 2.2	-1.05
	McIlvaine buffer, pH 5.0	-1.16, -1.36
	McIlvaine buffer, pH 8.0	-1.47
<i>o</i> -Methoxybenzaldehyde	Britton-Robinson buffer, pH 1.8	-1.02
	Britton-Robinson buffer, pH 6.8	-1.49
<i>p</i> -Methoxybenzaldehyde	Britton-Robinson buffer, pH 1.8	-1.17
	Britton-Robinson buffer, pH 6.8	-1.48
Methyl glyoxal	A, pH 4.5	-0.83

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25 °C (*continued*)

Compound	Solvent system	$E_{1/2}$
<i>Aldehydes (continued)</i>		
<i>m</i> -Nitrobenzaldehyde	Buffer + 10% EtOH, pH 2.0	-0.28, -1.20
Phthalaldehyde	Buffer, pH 3.1	-0.64, -1.07
	Buffer, pH 7.3	-0.89, -1.29
2-Propenal (acrolein)	pH 4.5	-1.36
	pH 9.0	-1.1
Propionaldehyde	0.1 M LiOH, pH 13	-1.93
Pyrrole-2-carbaldehyde	0.1 M HCl + 50% EtOH	-1.25
Salicylaldehyde	McIlvaine buffer, pH 2.2	-0.99, -1.23
	McIlvaine buffer, pH 5.0	-1.20, -1.30
	McIlvaine buffer, pH 8.0	-1.32
Trichloroacetaldehyde	Ammonia buffer, pH 8.4	-1.35, -1.66
	0.1 M KCl + 50% EtOH	-1.55
<i>Ketones</i>		
Acetone	B, pH 9.3	-1.52
	C	-2.46
Acetophenone	D + McIlvaine buffer, pH 4.9	-1.33
	D + McIlvaine buffer, pH 7.2	-1.58
	D + McIlvaine buffer, pH 1.3	-1.08
7 <i>H</i> -Benz[<i>de</i>]anthracen-7-one	0.1 N H ₂ SO ₄ + 75% MeOH	-0.96
Benzil	D + McIlvaine buffer, pH 1.3	-0.27
	D + McIlvaine buffer, pH 4.9	-0.50
Benzoin	D + McIlvaine buffer, pH 1.3	-0.90
	D + McIlvaine buffer, pH 8.6	-1.49
Benzophenone	D + McIlvaine buffer, pH 1.3	-0.94
	D + McIlvaine buffer, pH 8.6	-1.36
Benzoylacetone	Buffer, pH 2.6	-1.60
	Buffer, pH 5.3 and pH 7.6	-1.68
	Buffer, pH 9.7	-1.72
Bromoacetone	0.1 M LiCl	-0.29
2,3-Butanedione	0.1 M HCl	-0.84
3-Buten-2-one	0.1 M KCl	-1.42
Butyrophenone	0.1 M NH ₄ Cl + 50% EtOH	-1.55
D-Carvone	0.1 M Et ₄ Ni + 80% EtOH	-1.71
Chloroacetone	0.1 M LiCl	-1.18
Coumarin	McIlvaine buffer, pH 2.0	-0.95
	McIlvaine buffer, pH 5.0	-1.11, -1.44
Cyclohexanone	C	-2.45
<i>cis</i> -Dibenzoylethylene	D, pH 1	-0.30
	D, pH 11	-0.62, -1.65
<i>trans</i> -Dibenzoylethylene	D, pH 1	-0.12
	D, pH 11	-0.57, -1.52
Dibenzoylmethane	D, pH 1.3	-0.59
	D, pH 11.3	-1.30, -1.62

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C (*continued*)

Compound	Solvent system	$E_{1/2}$
Ketones (<i>continued</i>)		
9,10-Dihydro-9-oxoanthracene	D, pH 2.0	-0.93
1,5-Diphenyl-1,5-pentanedione	A	-2.10
1,5-Diphenylthiocarbazone	D, pH 7.0	-0.6
Flavanone	Acetate buffer + Me ₄ NOH + 50% 2-PrOH, pH 6.1	-1.30
	Acetate buffer + Me ₄ NOH + 50% 2-PrOH, pH 9.6	-1.51
Fluorescein	Acetate buffer, pH 2.0	-0.50
	Phthalate buffer, pH 5.0	-0.65
	Borate buffer, pH 10.1	-1.18, -1.44
Fructose	0.02 M LiCl	-1.76
Girard derivatives of aliphatic ketones	pH 8.2	-1.52
<i>o</i> -Hydroxyacetophenone	D, pH 5	-1.36
<i>p</i> -Hydroxyacetophenone	D, pH 5	-1.46
1,2,3-Indantrione (ninhydrin)	Britton–Robinson buffer, pH 2.5	-0.67, -0.83
	Britton–Robinson buffer, pH 4.5	-0.73, -1.01
	Britton–Robinson buffer, pH 6.8	-0.10, -0.90, -1.20
	Britton–Robinson buffer, pH 9.2	-1.35
α -Ionone	C	-1.59, -2.08
Isatin	Phosphate buffer + citrate buffer, pH 2.9	-0.3, -0.5
	Phosphate buffer + citrate buffer, pH 4.3	-0.3, -0.5, -0.8
	Phosphate buffer + citrate buffer, pH 5.4	-0.8
4-Methyl-3,5-heptadien-2-one	A	-0.64
4-Methyl-2,6-heptanedione	A	-1.28
4-Methyl-3-penten-2-one	D + McIlvaine buffer, pH 1.3	-1.01
	D + McIlvaine buffer, pH 11.3	-1.60
4-Phenyl-3-buten-2-one	D, pH 1.3	-0.72
	D, pH 8.6	-1.27
Phthalide	0.1 M Bu ₄ NI + 50% dioxane	-0.20
Phthalimide	pH 4.2	-1.1, -1.5
	pH 9.7	-1.2, -1.4
Pulegone	C	-1.74
Quinalizarin	Phosphate buffer + 1% EtOH, pH 8.0	-0.56
Testosterone	D + Britton–Robinson buffer, pH 2.6	-1.20
	D + Britton–Robinson buffer, pH 5.8	-1.40
	D + Britton–Robinson buffer, pH 8.8	-1.53, -1.79

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25 °C (*continued*)

Compound	Solvent system	$E_{1/2}$
Quinones		
Anthraquinone	Acetate buffer + 40% dioxane, pH 5.6	-0.51
	Phosphate buffer + 40% dioxane, pH 7.9	-0.71
<i>o</i> -Benzoquinone	Britton–Robinson buffer, pH 7.0	+0.20
	Britton–Robinson buffer, pH 9.0	+0.08
2,3-Dimethylnaphthoquinone	D, pH 5.4	-0.22
1,2-Naphthoquinone	Phosphate buffer, pH 5.0	-0.03
	Phosphate buffer, pH 7.0	-0.13
1,4-Naphthoquinone	Britton–Robinson buffer, pH 7.0	-0.07
	Britton–Robinson buffer, pH 9.0	-0.19
Acids		
Acetic acid	A	-2.3
Acrylic acid	pH 5.6	-0.85
Adenosine-5'-phosphoric acid	HClO ₄ + KClO ₄ , pH 2.2	-1.13
4-Aminobenzenesulfonic acid	0.05 M Me ₄ NI	-1.58
3-Aminobenzoic acid	pH 5.6	-0.67
Anthranilic acid	pH 5.6	-0.67
Ascorbic acid	Britton–Robinson buffer, pH 3.4	+0.17
	Britton–Robinson buffer, pH 7.0	-0.06
Barbituric acid	Borate buffer, pH 9.3	-0.04
Benzoic acid	A	-2.1
Benzoylformic acid	Britton–Robinson buffer, pH 2.2	-0.48
	Britton–Robinson buffer, pH 5.5	-0.85, -1.26
	Britton–Robinson buffer, pH 7.2	-0.98, -1.25
	Britton–Robinson buffer, pH 9.2	-1.25
Bromoacetic acid	pH 1.1	-0.54
2-Bromopropionic acid	pH 2.0	-0.39
Crotonic acid	C	-1.94
Dibromoacetic acid	pH 1.1	-0.03, -0.59
Dichloroacetic acid	pH 8.2	-1.57
5,5-Diethylbarbituric acid	Borate buffer, pH 9.3	0.00
Flavanol	D, pH 5.6	-1.25
	D, pH 7.7	-1.40
Folic acid	Britton–Robinson buffer, pH 4.6	-0.73
Formic acid	0.1 M KCl	-1.66
Fumaric acid	HCl + KCl, pH 2.6	-0.83
	Acetate buffer, pH 4.0	-0.93
	Acetate buffer, pH 5.9	-1.20
2,4-Hexadienedioic acid	Acetate buffer, pH 4.5	-0.97
Iodoacetic acid	pH 1	-0.16
Maleic acid	Britton–Robinson buffer, pH 2.0	-0.70
	Britton–Robinson buffer, pH 4.0	-0.97
	Britton–Robinson buffer, pH 6.0	-1.11, -1.30
	Britton–Robinson buffer, pH 10.0	-1.51

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C (*continued*)

Compound	Solvent system	$E_{1/2}$
<i>Acids (continued)</i>		
Mercaptoacetic acid	B, pH 6.8	-0.38
Methacrylic acid	D + 0.1 M LiCl	-1.69
Nitrobenzoic acids	Buffer + 10% EtOH, pH 2.0	-0.2, -0.7
Oxalic acid	B, pH 5.4-6.1	-1.80
2-Oxo-1,5-pentanedioic acid	HCl + KCl, pH 1.8	-0.59
	Ammonia buffer, pH 8.2	-1.30
2-Oxopropionic acid	Britton-Robinson buffer, pH 5.6	-1.17
	Britton-Robinson buffer, pH 6.8	-1.22, -1.53
	Britton-Robinson buffer, pH 9.7	-1.51
Phenolphthalein	Phthalate buffer, pH 2.5	-0.67
	Phthalate buffer, pH 4.7	-0.80
	D, pH 9.6	-0.98, -1.35
Picric acid	pH 4.2	-0.34
	pH 11.7	-0.36, -0.56, -0.96
1,2,3-Propenetricarboxylic acid	pH 7.0	-2.1
Trichloroacetic acid	Ammonia buffer, pH 8.2	-0.84, -1.57
	Phosphate buffer, pH 10.4	-0.9, -1.6
3,4,5-Trihydroxybenzoic acid	Phosphate buffer, pH 2.9	+0.50
	Phosphate buffer, pH 8.8	+0.1
<i>p</i> -Aminophenol	Britton-Robinson buffer, pH 6.3	+0.14
	Britton-Robinson buffer, pH 8.6	-0.04
	Britton-Robinson buffer, pH 12.0	-0.16
<i>o</i> -Chlorophenol	pH 5.6	-0.63
<i>m</i> -Chlorophenol	pH 5.6	-0.73
<i>p</i> -Chlorophenol	pH 5.6	-0.65
<i>o</i> -Cresol	pH 5.6	-0.56
<i>m</i> -Cresol	pH 5.6	-0.61
<i>p</i> -Cresol	pH 5.6	-0.54
1,2-Dihydroxybenzene	pH 5.6	-0.35
1,3-Dihydroxybenzene	pH 5.6	-0.61
1,4-Dihydroxybenzene	pH 5.6	-0.23
<i>o</i> -Methoxyphenol	pH 5.6	-0.46
<i>m</i> -Methoxyphenol	pH 5.6	-0.62
<i>p</i> -Methoxyphenol	pH 5.6	-0.41
1-Naphthol	A	-0.74
2-Naphthol	A	-0.82
1,2,3-Trihydroxybenzene	Britton-Robinson buffer, pH 3.1	+0.35
	Britton-Robinson buffer, pH 6.5	+0.10
	Britton-Robinson buffer, pH 9.5	-0.10
<i>Halogen compounds</i>		
Bromobenzene	A	-1.98
	C	-2.32
1-Bromobutane	C	-2.27

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25 °C (*continued*)

Compound	Solvent system	$E_{1/2}$
Halogen compounds (<i>continued</i>)		
Bromoethane	C	−2.08
Bromomethane	C	−1.63
1-Bromonaphthalene (also 2-bromonaphthalene)	A	−1.55, −1.60
3-Bromo-1-propene	C	−1.29
<i>p</i> -Bromotoluene	A	−1.72
Carbon tetrachloride	C	−0.78, −1.71
Chlorobenzene	A	−2.07
Chloroform	C	−1.63
Chloromethane	C	−2.23
3-Chloro-1-propene	C	−1.91
α -Chlorotoluene	C	−1.81
<i>p</i> -Chlorotoluene	A	−1.76
<i>N</i> -Chloro- <i>p</i> -toluenesulfonamide	0.5 M K ₂ SO ₄	−0.13
9,10-Dibromoanthracene	A	−1.15, −1.47
<i>p</i> -Dibromobenzene	C	−2.10
1,2-Dibromobutane	D + 1% Na ₂ SO ₃	−1.45
Dibromoethane	C	−1.48
<i>meso</i> -2,3-Dibromosuccinic acid	Acetate buffer, pH 4.0	−0.23, −0.89
Dichlorobenzenes	C	−2.5
Dichloromethane	C	−1.60
Diiodomethane	C	−1.12, −1.53
Hexabromobenzene	C	−0.8, −1.5
Hexachlorobenzene	C	−1.4, −1.7
Iodobenzene	A	−1.72
Iodoethane	C	−1.67
Iodomethane	A	−2.12
	C	−1.63
Tetrabromomethane	C	−0.3, −0.75, −1.49
Tetraiodomethane	C	−0.45, −1.05, −1.46
Tribromomethane	C	−0.64, −1.47
α,α,α -Trichlorotoluene	C	−0.68, −1.65, −2.00
Nitro and nitroso compounds		
1,2-Dinitrobenzene	Phthalate buffer, pH 2.5	−0.12, −0.32, −1.26
	Borate buffer, pH 9.2	−0.38, −0.74
1,3-Dinitrobenzene	Phthalate buffer, pH 2.5	−0.17, −0.29
	Borate buffer, pH 9.2	−0.46, −0.68
1,4-Dinitrobenzene	Phthalate buffer, pH 2.5	−0.12, −0.33
	Borate buffer, pH 9.2	−0.35, −0.80

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C (*continued*)

Compound	Solvent system	$E_{1/2}$
Nitro and nitroso compounds (<i>continued</i>)		
Methyl nitrobenzoates	Buffer + 10% EtOH, pH 2.0	−0.20 to −0.25 −0.68 to −0.74
<i>p</i> -Nitroacetophenone	Britton–Robinson buffer, pH 2.2	−0.16, −0.61, −1.09
	Britton–Robinson buffer, pH 10.0	−0.51, −1.40, −1.73
<i>o</i> -Nitroaniline	0.03 M LiCl + 0.02 M benzoic acid in EtOH	−0.88
<i>m</i> -Nitroaniline	Britton–Robinson buffer, pH 4.3	−0.3, −0.8
	Britton–Robinson buffer, pH 7.2	−0.5
<i>p</i> -Nitroaniline	Britton–Robinson buffer, pH 9.2	−0.7
	pH 2.0	−0.36
	Acetate buffer, pH 4.6	−0.5
<i>o</i> -Nitroanisole	Buffer + 10% EtOH, pH 2.0	−0.29, −0.58
<i>p</i> -Nitroanisole	Buffer + 10% EtOH, pH 2.0	−0.35, −0.64
1-Nitroanthraquinone	Britton–Robinson buffer, pH 7.0	−0.16
Nitrobenzene	HCl + KCl + 8% EtOH, pH 0.5	−0.16, −0.76
	Phthalate buffer, pH 2.5	−0.30
	Borate buffer, pH 9.2	−0.70
Nitrocresols	Britton–Robinson buffer, pH 2.2	−0.2 to −0.3
	Britton–Robinson buffer, pH 4.5	−0.4 to −0.5
	Britton–Robinson buffer, pH 8.0	−0.6
Nitroethane	Britton–Robinson buffer + 30% MeOH, pH 1.8	−0.7
	Britton–Robinson buffer + 30% MeOH, pH 4.6	−0.8
2-Nitrohydroquinone	Phosphate buffer + citrate buffer, pH 2.1	−0.2
	Phosphate buffer + citrate buffer, pH 5.2	−0.4
	Phosphate buffer + citrate buffer, pH 8.0	−0.5
Nitromethane	Britton–Robinson buffer + 30% MeOH, pH 1.8	−0.8
	Britton–Robinson buffer + 30% MeOH, pH 4.6	−0.85
<i>o</i> -Nitrophenol	Britton–Robinson buffer + 10% EtOH, pH 2.0	−0.23
	Britton–Robinson buffer + 10% EtOH, pH 4.0	−0.4
	Britton–Robinson buffer + 10% EtOH, pH 8.0	−0.65
	Britton–Robinson buffer + 10% EtOH, pH 10.0	−0.80

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C (*continued*)

Compound	Solvent system	$E_{1/2}$
Nitro and nitroso compounds (<i>continued</i>)		
<i>m</i> -Nitrophenol	Britton–Robinson buffer + 10% EtOH, pH 2.0	−0.37
	Britton–Robinson buffer + 10% EtOH, pH 4.0	−0.40
	Britton–Robinson buffer + 10% EtOH, pH 8.0	−0.64
	Britton–Robinson buffer + 10% EtOH, pH 10.0	−0.76
<i>p</i> -Nitrophenol	Britton–Robinson buffer + 10% EtOH, pH 2.0	−0.35
	Britton–Robinson buffer + 10% EtOH, pH 4.0	−0.50
	Britton–Robinson buffer + 10% EtOH, pH 8.0	−0.82
1-Nitropropane	Britton–Robinson buffer + 30% MeOH, pH 1.8	−0.73
	Britton–Robinson buffer + 30% MeOH, pH 8.6	−0.88
	Britton–Robinson buffer + 30% MeOH, pH 8.0	−0.95
2-Nitropropane	McIlvaine buffer, pH 2.1	−0.53
	McIlvaine buffer, pH 5.1	−0.81
Nitrosobenzene	McIlvaine buffer, pH 6.0	−0.03
	McIlvaine buffer, pH 8.0	−0.14
1-Nitroso-2-naphthol	D + buffer, pH 4.0	+0.02
	D + buffer, pH 7.0	−0.20
	D + buffer, pH 9.0	−0.31
<i>N</i> -Nitrosophenylhydroxylamine	pH 2.0	−0.84
<i>o</i> -Nitrotoluene	Phthalate buffer, pH 2.5	−0.35, −0.66
	Phthalate buffer, pH 7.4	−0.60, −1.06
<i>m</i> -Nitrotoluene (also <i>p</i> -nitrotoluene)	Phthalate buffer, pH 2.5	−0.30, −0.53
	Phthalate buffer, pH 7.4	−0.58, −1.06
Tetranitromethane	pH 12.0	−0.41
1,3,5-Trinitrobenzene	Phthalate buffer, pH 4.1	−0.20, −0.29, −0.34
	Borate buffer, pH 9.2	−0.34, −0.48, −0.65
Heterocyclic compounds containing nitrogen		
Acridine	D, pH 8.3	−0.80, −1.45
Cinchonine	B, pH 3	−0.90
2-Furanmethanol	Britton–Robinson buffer, pH 2.0	−0.96
	Britton–Robinson buffer, pH 5.8	−1.38, −1.70
2-Hydroxyphenazine	Britton–Robinson buffer, pH 4.0	−0.24

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C (*continued*)

Compound	Solvent system	$E_{1/2}$
Heterocyclic compounds containing nitrogen (<i>continued</i>)		
8-Hydroxyquinoline	B, pH 5.0	-1.12
	Phosphate buffer, pH 8.0	-1.18, -1.71
3-Methylpyridine	D + 0.1 M LiCl	-1.76
4-Methylpyridine	D + 0.1 M LiCl	-1.87
Phenazine	Phosphate buffer + citrate buffer, pH 7.0	-0.36
Pyridine	Phosphate buffer + citrate buffer, pH 7.0	-1.75
Pyridine-2-carboxylic acid	B, pH 4.1	-1.10
	B, pH 9.3	-1.48, -1.94
Pyridine-3-carboxylic acid	0.1 M HCl	-1.08
Pyridine-4-carboxylic acid	Britton–Robinson buffer, pH 6.1	-1.14
	pH 9.0	-1.39, -1.68
Pyrimidine	Citrate buffer, pH 3.6	-0.92, -1.24
	Ammonia buffer, pH 9.2	-1.54
Quinoline-8-carboxylic acid	pH 9	-1.11
Quinoxaline	Phosphate buffer + citrate buffer, pH 7.0	-0.66, -1.52
Azo, hydrazine, hydroxylamine, and oxime compounds		
Azobenzene	D, pH 4.0	-0.20
	D, pH 7.0	-0.50
Azoxybenzene	Buffer + 20% EtOH, pH 6.3	-0.30
Benzoin-1-oxime	Buffer, pH 2.0	-0.88
	Buffer, pH 5.6	-1.08
	Buffer, pH 8.2	-1.67
Benzoylhydrazine	0.13 M NaOH, pH 13.0	-0.30
Dimethylglyoxime	Ammonia buffer, pH 9.6	-1.63
Hydrazine	Britton–Robinson buffer, pH 9.3	-0.09
Hydroxylamine	Britton–Robinson buffer, pH 4.6	-1.42
	Britton–Robinson buffer, pH 9.2	-1.65
Oxamide	Acetate buffer	-1.55
Phenylhydrazine	McIlvaine buffer, pH 2	+0.19
	0.13 M NaOH, pH 13.0	-0.36
Phenylhydroxylamine	McIlvaine buffer + 10% EtOH, pH 2	-0.68
	McIlvaine buffer + 10% EtOH, pH 4–10	-0.33
Salicylaldoxime	Phosphate buffer, pH 5.4	0.061 pH
Thiosemicarbazide	Borate buffer, pH 9.3	-1.02
Thiourea	0.1 M sulfuric acid	-0.26
		+0.02

TABLE 8.11 Half-Wave Potentials (vs. Saturated Calomel Electrode) of Organic Compounds at 25°C (*continued*)

Compound	Solvent system	$E_{1/2}$
Indicators and dyestuffs		
Brilliant Green	HCl + KCl, pH 2.0	-0.2, -0.5
Indigo carmine	pH 2.5	-0.24
Indigo disulfonate	pH 7.0	-0.37
Malachite Green G	HCl + KCl, pH 2.0	-0.2, -0.5
Metanil yellow	Phosphate buffer + 1% EtOH, pH 7.0	-0.51
Methylene blue	Britton–Robinson buffer, pH 4.9	-0.15
	Britton–Robinson buffer, pH 9.2	-0.30
Methylene green	Phosphate buffer + 1% EtOH, pH 7.0	-0.12
Methyl orange	Phosphate buffer + 1% EtOH, pH 7.0	-0.51
Morin	D, pH 7.6	-1.7
Neutral red	Britton–Robinson buffer, pH 2.0	-0.21
	Britton–Robinson buffer, pH 7.0	-0.57
Peroxide		
Ethyl peroxide	0.02 M HCl	-0.2

SECTION 9

DATA USEFUL IN LABORATORY MANIPULATION AND ANALYSIS

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COOLING MIXTURES

Convenient cooling mixtures can be prepared in several ways. First, an inorganic salt may be mixed with finely shaved dry ice. Such a mixture can be used to maintain temperatures as shown in Table 9.1.

TABLE 9.1 Cooling Mixtures Made from Dry Ice and Salts

Salt	Dry ice, g/100 g	Minimum temperature, °C
CaCl ₂ ·6H ₂ O	41	−9.0
	81	−21.5
	123	−40.3
	143	−55
NH ₄ Cl	25	−15.4
NaBr	66	−28
MgCl ₂	85	−34

A more common method for preparing a low temperature bath is to mix an organic substance with either dry ice or liquid nitrogen. Dry ice (CO₂, −78°C) can be added in small lumps to the solvent until a slight excess of dry ice remains. Alternately, liquid nitrogen (N₂, −196°C) can be poured into the solvent until a slush is formed that consists of the solid–liquid mixture at its melting point.

TABLE 9.2 Dry Ice or Liquid Nitrogen Slush Baths

Substance	Temperature, °C	Substance	Temperature, °C
Ethylene glycol	−13	Acetone–CO ₂	−77
1,2-Dichlorobenzene	−17	Ethyl acetate	−84
Carbon tetrachloride	−22.9	2-Butanone	−87
Bromobenzene	−31	Hexane	−95
Methoxybenzene	−37	Methanol	−98
Chlorobenzene	−45	Carbon disulfide	−112
Bis(2-ethoxyethyl) ether	−44	Bromoethane	−119
<i>N</i> -Methylaniline	−57	Pentane	−130
<i>p</i> -Cymene	−68	2-Methylbutane	−160

HUMIDIFICATION AND DRYING

A saturated aqueous solution in contact with an excess of a definite solid phase at a given temperature will maintain constant humidity in an enclosed space. Table 9.3 identifies a number of salts suitable for this purpose. The aqueous tension (in millimeters of Hg) of a solution at a given temperature is found by multiplying the decimal fraction of the humidity by the aqueous tension at 100% humidity for the specific temperature. For example, the aqueous tension of a saturated solution of NaCl at 20°C is $0.757 \times 17.54 = 13.28$ mmHg and at 80°C is $0.764 \times 355.1 = 271.3$ mmHg.

TABLE 9.3 Humidity (%) Maintained by Saturated Solutions of Various Salts at Specified Temperatures

Solid phase	Temperature, °C						
	10	20	25	30	40	60	80
K ₂ Cr ₂ O ₇			98.0				
K ₂ SO ₄	98	97	97	96	96	96	
KNO ₃	95	93	92.5	91	88	82	
KCl	88	85.0	84.3	84	81.7	80.7	79.5
KBr	86	84	80.7		79.6	79.0	79.3
NaCl	76	75.7	75.3	74.9	74.7	74.9	76.4
NaNO ₃	77	75	73.8	72.8	71.5	67.5	65.5
KI					66.8	63.1	60.8
NaNO ₂		66	65	63.0	61.5	59.3	58.9
Na ₂ CrO ₄ ·4H ₂ O				64.6	61.8	55.6	56.2
NaBr·2H ₂ O	58	57.9	57.7		52.4	49.9	50.0
Na ₂ Cr ₂ O ₇ ·2H ₂ O	58	55	54		53.6	55.2	56.0
Mg(NO ₃) ₂ ·6H ₂ O	57	55	52.9	52	49	43	
K ₂ CO ₃ ·2H ₂ O	47	44	42.8	42	40		
NaI·2H ₂ O		47		36.4	32.3	25.3	23.2
MgCl ₂ ·6H ₂ O	34	33	33.0	33	32	30	
CaCl ₂ ·6H ₂ O	38	32.6	29	26			
KF·2H ₂ O				27.4	22.8	21.0	22.8
KC ₂ H ₃ O ₂ ·1.5H ₂ O	24	23	22.5	22	20		
LiCl·H ₂ O	13	12	11.1	12	11	11	
KOH	13	9	8	7	6	5	
Aqueous tension at 100% humidity, mmHg	9.21	17.54	23.76	31.82	55.32	149.4	355.1

TABLE 9.4 Humidity (%) Maintained by Saturated Solutions of Common Salts at Specified Temperatures

Solid phase	Temperature, °C	Humidity, %
KF	100	22.9
KI	100	56.2
(NH ₄) ₂ SO ₄	20–30	81.1
	108	75
BaCl ₂ ·2H ₂ O	25	90.2
NaF	100	96.6

TABLE 9.5 Drying Agents

Drying agent	Most useful for	Residual water, mg H ₂ O per liter of dry air (25°C)	Grams water removed per gram of desiccant	Regeneration, °C
Al ₂ O ₃	Hydrocarbons	0.002–0.005	0.2	175 (24 h)
Ba(ClO ₄) ₂ ^a	Inert gas streams	0.6–0.8	0.17	140
BaO	Basic gases: hydrocarbons, aldehydes, alcohols	0.0007–0.003	0.12	1000
CaC ₂ ^b	Ethers		0.56	Impossible
CaCl ₂ ^c	Inert organics	0.1–0.2	0.15 (1 H ₂ O) 0.30 (2 H ₂ O)	250
CaH ₂ ^d	Hydrocarbons, ethers, amines, esters, higher alcohols	1 × 10 ⁻⁵	0.85	Impossible
CaO	Ethers, esters, alcohols, amines	0.01–0.003	0.31	Difficult, 1000
CaSO ₄	Most organic substances	0.005–0.07	0.07	225
Dow Desiccant 812 ^e	Most materials	(5–200 ppm)		No
K ₂ CO ₃	Most materials except acids and phenols		0.16	158
KOH	Amines	0.01–0.9		Impossible
LiAlH ₄ ^f	Hydrocarbons		1.9	Impossible
Mg(ClO ₄) ₂ ^a	Gas streams	0.0005–0.002	0.24	250 (high vacuum)
MgO	All but acidic compounds	0.008	0.45	800
MgSO ₄	Most organic compounds	1–12	0.15–0.75	Not feasible
Molecular sieves				
4X	Molecules with effective diameter > 4 Å	0.001	0.18	250
5X	Molecules with effective diameter > 5 Å	0.001	0.18	250
9.5% Na–Pb alloy ^d	Hydrocarbons, ethers	(For solvents only)	0.08	Impossible
Na ₂ SO ₄	Ketones, acids, alkyl and aryl halides	12	1.25	150
P ₂ O ₅	Gas streams; not suitable for alcohols, amines, ketones, or amines	2 × 10 ⁻⁵	0.5	Not feasible
Silica gel	Most organic amines	0.002–0.07	0.2	200–350
Sulfuric acid	Air and inert gas streams	0.003–0.008	Indefinite	Not feasible

^aMay form explosive mixtures on contact with organic material.^bExplosive C₂H₂ formed.^cDrying action slow.^dH₂ formed.^eUsed for column drying of organic liquids.^fStrong reductant.

TABLE 9.6 Solvents of Chromatographic Interest (arranged in order of increasing solvent strength)

Solvent	Boiling point, °C	Solvent strength parameter		Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ (20 °C)	Refractive index (20 °C)	UV cutoff, nm
		e° (SiO ₂)	e° (Al ₂ O ₃)			
Fluoroalkanes			−0.25		1.25	
Pentane	36	0.0	0.0	0.24 ¹⁵ °C	1.358	210
Hexane	69	0.0	0.0	0.31	1.375	210
2,2,4-Trimethylpentane	99		0.01	0.50	1.392	215
Decane	174		0.04	0.93	1.412	210
Cyclohexane	81	−0.05	0.04	0.98	1.426	210
Cyclopentane	49		0.05	0.44	1.407	210
Diisobutylene	101		0.06		1.411	
1-Pentene	30		0.08	0.24 ⁰ °C	1.371	
Carbon disulfide	46	0.14	0.15	0.36	1.626	380
Carbon tetrachloride	77	0.14	0.18	0.97	1.466	265
1-Chlorobutane	78		0.26	0.43	1.402	220
1-Chloropentane	98		0.26	0.58	1.412	225
<i>o</i> -Xylene	144		0.26	0.81	1.505	290
Diisopropyl ether	68		0.28	0.38 ²⁵ °C	1.369	220
2-Chloropropane	35		0.29	0.33	1.378	225
Toluene	111		0.29	0.59	1.497	286
1-Chloropropane	47		0.30	0.35	1.389	225
Chlorobenzene	132		0.40	0.80	1.525	
Benzene	80	0.25	0.32	0.65	1.501	280
Bromoethane	38		0.37	0.40	1.424	
Diethyl ether	35	0.38	0.38	0.25	1.353	218
Diethyl sulfide	92		0.38	0.45	1.443	290
Chloroform	62	0.26	0.40	0.57	1.443	245

TABLE 9.6 Solvents of Chromatographic Interest (*continued*)

Solvent	Boiling point, °C	Solvent strength parameter		Viscosity, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2}$ (20 °C)	Refractive index (20 °C)	UV cutoff, nm
		e° (SiO_2)	e° (Al_2O_3)			
Dichloromethane	41		0.42	0.44	1.425	235
4-Methyl-2-pentanone	116		0.43	0.42 ^{15°C}	1.396	335
Tetrahydrofuran	66		0.45	0.55	1.407	220
1,2-Dichloroethane	84		0.49	0.80	1.445	228
2-Butanone	80		0.51	0.42 ^{15°C}	1.379	330
1-Nitropropane	131		0.53	0.80 ^{25°C}	1.402	380
Acetone	56	0.47	0.56	0.32	1.359	330
1,4-Dioxane	101	0.49	0.56	1.44 ^{15°C}	1.420	215
Ethyl acetate	77	0.38	0.58	0.45	1.372	255
Methyl acetate	56		0.60	0.48 ^{15°C}	1.362	260
1-Pentanol	138		0.61	4.1	1.410	210
Dimethyl sulfoxide	189		0.62	2.47	1.478	265
Aniline	184		0.62	4.40	1.586	
Diethylamine	56		0.63	0.33	1.386	275
Nitromethane	101		0.64	0.67	1.394	380
Acetonitrile	82	0.50	0.65	0.37	1.344	190
Pyridine	115		0.71	0.97	1.510	330
2-Butoxyethanol	170		0.74	3.15 ^{25°C}	1.420	220
1-Propanol	97		0.82	2.25	1.386	210
2-Propanol	82		0.82	2.50	1.377	210
Ethanol	78		0.88	1.20	1.361	210
Methanol	65		0.95	0.59	1.328	210
Ethylene glycol	198		1.11	21.8	1.432	210
Acetic acid	118		large	1.23	1.372	260
Water	100		large	1.00	1.333	191

TABLE 9.7 Solvents having the Same Refractive Index and the Same Density at 25°C

Solvent 1	Solvent 2	Refractive index		Density, g/mL	
		1	2	1	2
Acetone	Ethanol	1.357	1.359	0.788	0.786
Ethyl formate	Methyl acetate	1.358	1.360	0.916	0.935
Ethanol	Propionitrile	1.359	1.363	0.786	0.777
2,2-Dimethylbutane	2-Methylpentane	1.366	1.369	0.644	0.649
2-Methylpentane	Hexane	1.369	1.372	0.649	0.655
Isopropyl acetate	2-Chloropropane	1.375	1.376	0.868	0.865
3-Butanone	Butyraldehyde	1.377	1.378	0.801	0.799
Butyraldehyde	Butyronitrile	1.378	1.382	0.799	0.786
Dipropyl ether	Butyl ethyl ether	1.379	1.380	0.753	0.746
Propyl acetate	Ethyl propionate	1.382	1.382	0.883	0.888
Propyl acetate	1-Chloropropane	1.382	1.386	0.883	0.890
Butyronitrile	2-Methyl-2-propanol	1.382	1.385	0.786	0.781
Ethyl propionate	1-Chloropropane	1.382	1.386	0.888	0.890
1-Propanol	2-Pentanone	1.383	1.387	0.806	0.804
Isobutyl formate	1-Chloropropane	1.383	1.386	0.881	0.890
1-Chloropropane	Butyl formate	1.386	1.387	0.890	0.888
Butyl formate	Methyl butyrate	1.387	1.391	0.888	0.875
Methyl butyrate	2-Chlorobutane	1.392	1.395	0.875	0.868
Butyl acetate	2-Chlorobutane	1.392	1.395	0.877	0.868
4-Methyl-2-pentanone	Pentanitrile	1.394	1.395	0.797	0.795
4-Methyl-2-pentanone	1-Butanol	1.394	1.397	0.797	0.812
2-Methyl-1-propanol	Pentanitrile	1.394	1.395	0.798	0.795
2-Methyl-1-propanol	2-Hexanone	1.394	1.395	0.798	0.810
2-Butanol	2,4-Dimethyl-3-pentanone	1.395	1.399	0.803	0.805
2-Hexanone	1-Butanol	1.395	1.397	0.810	0.812
Pentanitrile	2,4-Dimethyl-3-pentanone	1.395	1.399	0.795	0.805
2-Chlorobutane	Isobutyl butyrate	1.395	1.399	0.868	0.860
Butyric acid	2-Methoxyethanol	1.396	1.400	0.955	0.960
1-Butanol	3-Methyl-2-pentanone	1.397	1.398	0.812	0.808
1-Chloro-2-methylpropane	Isobutyl butyrate	1.397	1.399	0.872	0.860
1-Chloro-2-methylpropane	Pentyl acetate	1.397	1.400	0.872	0.871
Methyl methacrylate	3-Methyl-2-pentanone	1.398	1.398	0.795	0.808
Triethylamine	2,2,3-Trimethylpentane	1.399	1.401	0.723	0.712
Butylamine	Dodecane	1.399	1.400	0.736	0.746
Isobutyl butyrate	1-Chlorobutane	1.399	1.401	0.860	0.875
1-Nitropropane	Propionic anhydride	1.399	1.400	0.995	1.007
Pentyl acetate	1-Chlorobutane	1.400	1.400	0.871	0.881
Pentyl acetate	Tetrahydrofuran	1.400	1.404	0.871	0.885
Dodecane	Dipropylamine	1.400	1.400	0.746	0.736
1-Chlorobutane	Tetrahydrofuran	1.401	1.404	0.871	0.885
Isopentanoic acid	2-Ethoxyethanol	1.402	1.405	0.923	0.926
Dipropylamine	Cyclopentane	1.403	1.404	0.736	0.740
2-Pentanol	4-Heptanone	1.404	1.405	0.804	0.813
3-Methyl-1-butanol	Hexanonitrile	1.404	1.405	0.805	0.801
3-Methyl-1-butanol	4-Heptanone	1.404	1.405	0.805	0.813
Hexanonitrile	4-Heptanone	1.405	1.405	0.801	0.813

TABLE 9.7 Solvents having the Same Refractive Index and the Same Density at 25°C (*continued*)

Solvent 1	Solvent 2	Refractive index		Density, g/mL	
		1	2	1	2
Hexanonitrile	1-Pentanol	1.405	1.408	0.801	0.810
Hexanonitrile	2-Methyl-1-butanol	1.405	1.409	0.801	0.815
4-Heptanone	1-Pentanol	1.405	1.408	0.813	0.810
2-Ethoxyethanol	Pentanoic acid	1.405	1.406	0.926	0.936
2-Heptanone	1-Pentanol	1.406	1.408	0.811	0.810
2-Heptanone	2-Methyl-1-butanol	1.406	1.409	0.811	0.815
2-Heptanone	Dipentyl ether	1.406	1.410	0.811	0.799
2-Pentanol	3-Isopropyl-2-pentanone	1.407	1.409	0.804	0.808
1-Pentanol	Dipentyl ether	1.408	1.410	0.810	0.799
2-Methyl-1-butanol	Dipentyl ether	1.409	1.410	0.815	0.799
Isopentyl isopentanoate	Allyl alcohol	1.410	1.411	0.853	0.847
Dipentyl ether	2-Octanone	1.410	1.414	0.799	0.814
2,4-Dimethyldioxane	3-Chloropentene	1.412	1.413	0.935	0.932
2,4-Dimethyldioxane	Hexanoic acid	1.412	1.415	0.935	0.923
Diethyl malonate	Ethyl cyanoacetate	1.412	1.415	1.051	1.056
3-Chloropentene	Octanoic acid	1.413	1.415	0.932	0.923
2-Octanone	1-Hexanol	1.414	1.416	0.814	0.814
2-Octanone	Octanonitrile	1.414	1.418	0.814	0.810
3-Octanone	3-Methyl-2-heptanone	1.414	1.416	0.830	0.818
3-Methyl-2-heptanone	1-Hexanol	1.415	1.416	0.818	0.814
3-Methyl-2-heptanone	Octanonitrile	1.415	1.418	0.818	0.810
1-Hexanol	Octanonitrile	1.416	1.418	0.814	0.810
Dibutylamine	Allylamine	1.416	1.419	0.756	0.758
Allylamine	Methylcyclohexane	1.419	1.421	0.758	0.765
Butyrolactone	1,3-Propanediol	1.434	1.438	1.051	1.049
Butyrolactone	Diethyl maleate	1.434	1.438	1.051	1.064
2-Chloromethyl-2-propanol	Diethyl maleate	1.436	1.438	1.059	1.064
N-Methylmorpholine	Dibutyl decanedioate	1.436	1.440	0.924	0.932
1,3-Propanediol	Diethyl maleate	1.438	1.438	1.049	1.064
Methyl salicylate	Diethyl sulfide	1.438	1.442	0.836	0.831
Methyl salicylate	1-Butanethiol	1.438	1.442	0.836	0.837
1-Chlorodecane	Mesityl oxide	1.441	1.442	0.862	0.850
Diethylene glycol	Formamide	1.445	1.446	1.128	1.129
Diethylene glycol	Ethylene glycol diglycidyl ether	1.445	1.447	1.128	1.134
Formamide	Ethylene glycol diglycidyl ether	1.446	1.447	1.129	1.134
2-Methylmorpholine	Cyclohexanone	1.446	1.448	0.951	0.943
2-Methylmorpholine	1-Amino-2-propanol	1.446	1.448	0.951	0.961
Dipropylene glycol monoethyl ether	Tetrahydrofurfuryl alcohol	1.446	1.450	1.043	1.050
1-Amino-2-methyl-2-pentanol	2-Butylcyclohexanone	1.449	1.453	0.904	0.901
2-Propylcyclohexanone	4-Methylcyclohexanol	1.452	1.454	0.923	0.908

TABLE 9.7 Solvents having the Same Refractive Index and the Same Density at 25 °C (*continued*)

Solvent 1	Solvent 2	Refractive index		Density, g/mL	
		1	2	1	2
Carbon tetrachloride	4,5-Dichloro-1,3-dioxolan-2-one	1.459	1.461	1.584	1.591
<i>N</i> -Butyldiethanolamine	Cyclohexanol	1.461	1.465	0.965	0.968
<i>D</i> - α -Pinene	<i>trans</i> -Decahydro-naphthalene	1.464	1.468	0.855	0.867
Propylbenzene	<i>p</i> -Xylene	1.490	1.493	0.858	0.857
Propylbenzene	Toluene	1.490	1.494	0.858	0.860
Phenyl 1-hydroxyphenyl ether	1,3-Dimorpholyl-2-propanol	1.491	1.493	1.081	1.094
Phenetole	Pyridine	1.505	1.507	0.961	0.978
2-Furanmethanol	Thiophene	1.524	1.526	1.057	1.059
<i>m</i> -Cresol	Benzaldehyde	1.542	1.544	1.037	1.041

McReynolds' Constants

The *Kovats retention indices* (R.I.) indicate where compounds will appear on a chromatogram with respect to unbranched alkanes injected with the sample. By definition, the R.I. for pentane is 500, for hexane is 600, for heptane is 700, and so on, regardless of the column used or the operating conditions, although the exact conditions and column must be specified, such as liquid loading, particular support used, and any pretreatment. For example, suppose that on a 20% squalane column at 100 °C, the retention times for hexane, benzene, and octane are found to be 15, 16, and 25 min, respectively. On a graph of $\ln t'_R$ (napierian logarithm of the adjusted retention time) of the alkanes versus their retention indices, a R.I. of 653 for benzene is read off the graph. The number 653 for benzene (see the last line of Table 9.8 in the column headed "1" under "Reference compounds") means that it elutes halfway between hexane and heptane on a logarithmic time scale. If the experiment is repeated with a dinonyl phthalate column, the R.I. for benzene is found to be 736 (lying between heptane and octane), which implies that dinonyl phthalate will retard benzene slightly more than squalane will; that is, dinonyl phthalate is slightly more polar than squalane by $\Delta I = 83$ units (the entry in Table 9.8 for dinonyl phthalate in the column headed "1" under "Reference compounds"). The difference gives a measure of solute–solvent interaction due to all intermolecular forces other than London dispersion forces. The latter are the principal solute–solvent effects with squalane.

Now the overall effects due to hydrogen bonding, dipole moment, acid–base properties, and molecular configuration can be expressed as

$$\Sigma \Delta I = ax' + by' + cz' + du' + es'$$

where $x' = \Delta I$ for benzene (the column headed "1" in Table 9.8, intermolecular forces typical of aromatics and olefins), $y' = \Delta I$ for 1-butanol (the column headed "2" in Table 9.8, electron attraction typical of alcohols, nitriles, acids, and nitro and alkyl monochlorides, dichlorides and trichlorides), $z' = \Delta I$ for 2-pentanone (the column headed "3" in Table 9.8, electron repulsion typical of ketones, ethers, aldehydes, esters, epoxides, and dimethylamino derivatives), $u' = \Delta I$ for 1-nitropropane (the column headed "4" in Table 9.8, typical of nitro and nitrile derivatives), and $s' = \Delta I$ for pyridine (or dioxane) (the column headed "5" in Table 9.8).

TABLE 9.8 McReynolds' Constants for Stationary Phases in Gas Chromatography

The McReynolds' constants listed are differences in retention index units between the reference compound run on squalane and on the other phases listed. The last entry in the table shows the absolute retention indices for the reference compounds on squalane. Reference compounds are (1) benzene, (2) 1-butanol, (3) 2-pentanone, (4) 1 nitropropane, and (5) pyridine. (Note that Rohrschneider's constants are based on these reference compounds and may differ slightly from the McReynolds' constants. The reference compounds for Rohrschneider's constants are (1) benzene, (2) ethanol, (3) 2-butanone, (4) nitromethane, and (5) pyridine.) The minimum temperature is that at which normal gas-liquid chromatography (GLC) behavior is expected. Below that temperature, the phase will be a solid or an extremely viscous gum. The maximum temperature is that above which the bleed rate will be excessive.

Liquid phase	Chemical type	Similar liquid phases	Temperature, °C		Reference compounds					
			Minimum	Maximum	1	2	3	4	5	Sum
Squalane	(2,6,10,15,19,23-Hexamethyl)tetracosane		20	150	0	0	0	0	0	0
Paraffin oil					9	5	2	6	11	33
Apolane-87	(24,24-Diethyl-19,29-dioctadecyl)hepta-tetracontane		30	280	21	10	3	12	25	71
Apiezon L			50	250	32	22	15	32	42	143
SE 30		SP-2100, SF 96	50	350	15	53	44	64	41	217
OV-101	Poly(dimethylsiloxane)	OV-1, DC 200, DC 410	50	350	17	57	45	67	43	229
OV-73	Poly(diphenyldimethylsiloxane), 5%:95%	SE 52	0	325	32	72	65	98	67	334
SE 54	Poly(diphenylvinyl-dimethylsiloxane), 5%:1%:94%		50	300	33	72	66	99	67	337
OV-3	Poly(diphenyldimethylsiloxane), 10%:90%		0	350	44	86	81	124	88	423
Dexsil 300	Poly(carboranemethylsiloxane)		50	500	47	80	103	148	96	474
Kel F Wax				150	55	67	114	143	116	495
Apiezon H				300	59	86	81	151	129	506

Dexsil 400	Carborane and methylphenyl-silicone		50	500	72	108	118	166	123	587
OV-7	Poly(diphenyldimethylsiloxane), 20%:80%	DC 550	20	350	69	113	111	171	128	592
Di(2-ethylhexyl) sebacate			0	125	72	168	108	180	125	653
Diisodecyl adipate				175	71	171	113	185	128	668
Decyl octyl adipate					79	179	119	193	134	704
Bis(2-ethylhexyl)-tetrachlorophthalate			0	150	112	150	123	168	181	734
Diisodecyl phthalate			0	175	84	173	137	218	155	767
Dinonyl phthalate			20	150	83	183	147	231	159	803
OV-11	Poly(diphenyldimethylsiloxane), 35%:65%	DC 710	0	350	107	149	153	228	190	827
Dioctyl phthalate			20	125	92	186	150	236	167	831
Hallcomid M-18			40	150	79	268	130	222	146	845
OV-17	Poly(diphenyldimethylsiloxane), 50%:50%		0	325	119	158	162	243	202	884
Dexsil 410	Carborane and methylcyanoethylsilicone		50	500	72	286	174	249	171	952
UCON LB-550-X			0	200	118	271	158	243	206	996
Span 80			15	150	97	266	170	216	268	1017
OV-22	Poly(diphenyldimethylsiloxane), 65%:35%		0	350	160	188	191	283	253	1075
Polypropylene glycol			0	150	128	294	173	264	226	1085
Didecyl phthalate			10	175	136	255	213	320	235	1159
OV-25	Poly(diphenyldimethylsiloxane), 75%:25%		0	350	178	204	208	305	280	1175
Polyphenyl ether OS-138 (6 rings)			0	225	182	233	228	313	293	1249
Neopentyl glycol sebacate		HI-EFF-3CP	50	225	172	327	225	344	326	1394
Squalene			0	100	152	341	328	329	344	1404
UCON 50-HB-280X			0	200	177	362	227	351	302	1419
Tricresyl phosphate			20	125	176	321	250	374	299	1420

Liquid phase	Chemical type	Similar liquid phases	Temperature, °C		Reference compounds					
			Minimum	Maximum	1	2	3	4	5	Sum
Sucrose acetate isobutyrate	Poly(trifluoropropylsiloxane)	SP-2401, FS 1265	0	200	172	330	251	378	295	1426
QF-1			0	250	144	233	355	463	305	1500
OV-210			0	275	146	238	358	468	310	1520
OV-215	Poly(trifluoropropylmethyl-siloxane)	XE 60	0	275	149	240	363	478	315	1545
UCON 50-HB-2000	Emulphor ON-870		0	200	202	394	253	392	341	1582
Triton X-100			0	200	203	399	268	402	362	1634
UCON 50-HB-5100			0	200	214	418	278	421	375	1706
Siponate DS-10			0	200	99	569	320	344	388	1720
Tween 80	Poly(cyanoethylphenyl-methylsiloxane)		0	150	227	430	283	438	396	1747
XE-60			0	250	204	381	340	493	367	1785
OV-225			0	265	228	369	338	492	386	1813
			0	265	228	369	338	492	386	1813
Neopentyl glycol adipate	Igepal CO-880	HI-EFF-3AP	50	225	232	421	311	461	424	1849
UCON 75-H-90000			100	200	255	452	299	470	406	1882
Triton X-305			0	200	262	467	314	488	430	1961
Neopentyl glycol succinate	Poly(ethylene glycol)	HI-EFF-3BP	50	230	272	469	366	539	474	2120
Igepal CO 990			100	200	298	508	345	540	475	2166
Carbowax 20M		FFAP, SP-2300	25	275	322	536	368	572	510	2308
Epon 1001			50	225	284	489	406	539	601	2319
Carbowax 4000			60	200	325	551	375	582	520	2353
Ethylene glycol isophthalate		HI-EFF-2EP	100	225	326	508	425	607	561	2427
Ethylene glycol adipate		HI-EFF-2AP	100	225	372	576	453	655	617	2673
Butane-1,4-diol succinate		HI-EFF-4BP	50	225	369	591	457	661	629	2207
Phenyldiethanolamine succinate		HI-EFF-10BP	0	200	386	555	472	674	654	2741

Diethylene glycol adipate		HI-EFF-1AP, LAC- 1-R-296, SP- 2330	25	275	378	603	460	665	658	2764
Carbowax 1540			50	175	371	639	453	666	641	2770
Hyprose SP-80			0	175	336	742	492	639	727	2936
SILAR-7CP			0	250	440	638	605	844	673	3200
ECNSS-M			30	200	421	690	581	803	732	3227
EGSS-X			90	200	484	710	585	831	778	3388
Ethylene glycol phthalate		HI-EFF-2GP	100	200	453	697	602	816	872	3410
SILAR-9CP			0	250	489	725	631	910	778	3536
SILAR-10C		SP-2340	25	275	523	757	659	942	801	3682
Diethylene glycol succinate		HI-EFF-1BP, LAC-3-R-728	20	200	499	751	593	840	860	3543
Tetrahydroxyethylenediamine		THEED	0	150	463	942	626	801	893	3725
Tetracyanoethylated pentaerythritol			30	175	526	782	677	920	837	3742
Ethylene glycol succinate		HI-EFF-2BP	100	200	537	787	643	903	889	3759
1,2,3,4-Tetrakis- (2-cyanoethoxy)butane			110	200	617	860	773	1048	941	4239
1,2,3,4,5,6-Hexakis (2 cyanoethoxy)cyclohexane			125	150	567	825	713	978	901	3984
1,2,3-Tris- (2-cyanoethoxy)propane			0	175	593	857	752	1028	915	4145
<i>N,N</i> -Bis(2-cyanoethyl)- formamide			0	125	690	991	853	1110	1000	4644
OV-275	Dicyanoallylsilicone		25	250	781	1006	885	1177	1089	4938
Absolute retention index values on squalane for reference compounds					653	590	627	652	699	

SECTION 10

POLYMERS, RUBBERS, FATS, OILS, AND WAXES

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POLYMERS

General

Polymers are macromolecules that result from combinations of individual building blocks called monomer molecules. Most polymers are regular structures in which a single unit repeats many times. This produces a range of macromolecules that have similar structures and molecular weights. The ensemble of molecules typically exhibit average molecular weights but have characteristic properties. Polymerization of ethylene, $\text{CH}_2=\text{CH}_2$, results in polyethylene, $(-\text{CH}_2-\text{CH}_2-)_n$ such that “ n ” is a range of values. If the average chain possesses 1000 monomer units, chains having values of n such as 998, 999, 1001, 1002, etc. will be present as well. There will be more such chains near the average value and fewer or none when n is far from the average value.

In some polymers, long segments of linear polymer chains are oriented in a regular manner with respect to one another. Such polymers have many of the physical characteristics of crystals and are said to be *crystalline*. Polymers that have polar functional groups show a greater tendency to be crystalline. Orientation is aided by alignment of dipoles on different chains. Van der Waals’ interactions between long hydrocarbon chains may provide sufficient total attractive energy to account for a high degree of regularity within the polymers.

Irregularities such as branch points, co-monomer units, and cross-links lead to *amorphous* polymers. These have less regular structures and typically do not have true melting points. Instead, they have glass transition temperatures at which the rigid and glass-like material becomes a viscous liquid as the temperature is raised.

Elastomers. Elastomer is a generic name for polymers that exhibit rubber-like elasticity. Elastomers are soft yet sufficiently elastic that they can usually be stretched several hundred percent under tension. When the stretching force is removed, they quickly retract and recover their original dimensions.

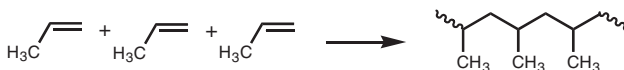
Polymers that soften or melt and then solidify and regain their original properties on cooling are called *thermoplastic*. A thermoplastic polymer is usually a single strand of linear polymer with few if any cross-links.

Thermosetting Polymers. Polymers that soften or melt on warming and then become infusible solids are called *thermosetting*. The term implies that thermal decomposition has not taken place. Thermosetting plastics contain a cross-linked polymer network that extends through the final material, making it stable to heat and insoluble in organic solvents. Many molded plastics are shaped while molten and are then heated further to become rigid solids of desired shapes.

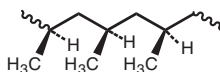
Synthetic Rubbers. Synthetic rubbers are polymers with rubber-like characteristics that are prepared from dienes or olefins. Rubbers with special properties can also be prepared from other polymers, such as polyacrylates, fluorinated hydrocarbons, and polyurethanes.

Structural Differences. Polymers exhibit structural differences resulting from the type of monomer used, the polymerization method employed, and other factors. A *linear* polymer consists of long segments of single strands that are oriented in a regular manner with respect to one another. *Branched* polymers have substituents attached to the repeating units that extend the polymer laterally. When these units participate in chain propagation and link together chains, a *cross-linked* polymer is formed. A *ladder* polymer results when repeating units have a tetravalent structure such that a polymer consists of two backbone chains regularly cross-linked at short intervals.

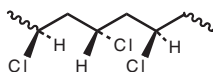
Generally polymers involve bonding of the most substituted carbon of one monomeric unit to the least substituted carbon atom of the adjacent unit in a *head-to-tail* arrangement. An example is the formation of polypropylene from propylene. This is shown for three monomer units. The wavy lines indicate that more monomers would lead to extended chains.



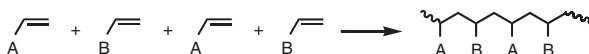
Substituents appear on alternate carbon atoms. *Tacticity* refers to the configuration of substituents relative to the backbone axis. In an *isotactic* arrangement, substituents are on the same plane of the backbone axis; that is, the configuration at each chiral center is identical.



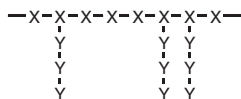
In a *syndiotactic* arrangement, the substituents are in an ordered alternating sequence, appearing alternately on one side and then on the other side of the chain, as shown for a segment of a vinyl chloride polymer. If the sidechains are not in any particular order with respect to each other (random), the polymer is said to be *atactic*.



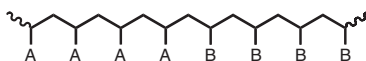
Copolymerization. Copolymerization occurs when a mixture of two or more monomer types polymerizes so that each kind of monomer enters the polymer chain. The fundamental structure resulting from copolymerization depends on the nature of the monomers and the relative rates of monomer reactions with the growing polymer chain. A tendency toward alternation of monomer units is common. Random copolymerization is known but it is rather unusual.



In *graft copolymers* the chain backbone is composed of one kind of monomer and the branches are made up of another kind of monomer. The structure of a *block copolymer* consists of a homopolymer attached to chains of another homopolymer. In either case, *cis* or *trans* (*Z* or *E*) double bond configurations around any double bond not involved in the polymerization will normally be unaltered.



Schematic of a graft copolymer

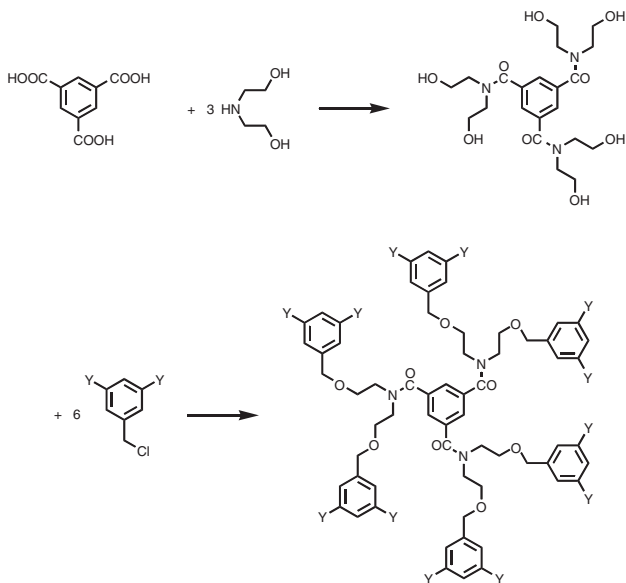


Schematic of a block copolymer

Dendrimers

A relatively recent development in polymer chemistry is the family of compounds known as dendrimers. The term derives from the Greek *dendra* meaning tree. Tree-like structures of this general type have also been referred to as arborols. Dendrimers differ from typical polymers in that they radiate from a central unit or core rather than being either linear or planar. Dendrimers are built up using a “generational” structure in discrete synthetic steps. As a result, the product is nearer to being a single compound than is a typical polymer. A typical dendrimer consists of a multifunctional core unit. Each functional group of the core unit is elaborated by a further molecular unit, often referred to as a “dendritic wedge.” The core unit is usually designated “generation 0” and additional units radiating from it or prior units are designated as higher generations, that is, generation 1, generation 2, etc. When the synthesis begins at the core and radiates outward, it is called a divergent synthesis. Alternately, synthesis may begin at the outside and terminate with a core unit.

The more common divergent method is illustrated in the following scheme. 1,3,5-Tricarboxybenzene (trimesic acid) serves as the core or generation 0. It could be functionalized by converting it into the tris(acid chloride). Reaction with the secondary amine of diethanolamine would give the tris(amide) hexahydroxy compound shown here. This structure represents generations 0 and 1. Treatment with an appropriately substituted benzyl chloride could lead to the hexaether that comprises generations 0, 1, and 2. There are now a dozen “Y” groups that could be further functionalized in going to generation 3. A difficulty is that the functional or protecting groups present at each stage must be compatible with the chemistry used to make the connections.



A second issue is that when subsequent generations involve sterically demanding structural units, incomplete substitution may occur. Thus, in the final structure shown, five

benzyl ethers might form, rather than six, owing to steric crowding. This would introduce a defect in the dendrimer structure. Indeed, some molecules might possess all six benzyl ethers whereas others might lack one or even two. It must be possible to manipulate the substituents designated "Y" in the presence of ether and amide groups to further extend the dendrimer.

Novel dendrimers have novel and unique properties that make them promising candidates for use in the development of nanoscale devices and in drug delivery systems.

Additives to Polymers

Antioxidants. Antioxidants markedly retard the rate of autoxidation throughout the useful life of the polymer. Chain-terminating antioxidants have a reactive —NH or —OH functional group and include compounds such as secondary aryl amines or hindered phenols. They function by transfer of hydrogen to free radicals, principally to peroxy radicals. Butylated hydroxytoluene is a widely used example.

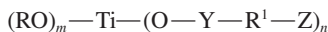
Peroxide-decomposing antioxidants destroy hydroperoxides, the sources of free radicals in polymers. Phosphites and thioesters such as tris(nonylphenyl) phosphite, distearyl pentaerythritol diphosphite, and dialkyl thiodipropionates are examples of peroxide-decomposing antioxidants.

Antistatic Agents. External antistatic agents are usually quaternary ammonium salts of fatty acids and ethoxylated glycerol esters of fatty acids that are applied to the plastic surface. Internal antistatic agents are compounded into plastics during processing. Carbon blacks provide a conductive path through the bulk of the plastic. Other types of internal agents must bloom to the surface after compounding in order to be active. These latter materials are ethoxylated fatty amines and ethoxylated glycerol esters of fatty acids, which often must be individually selected to match chemically each plastic type.

Antistatic agents require ambient moisture to function. Consequently their effectiveness is dependent on the relative humidity. They provide a broad range of protection at 50% relative humidity. Much below 20% relative humidity, only materials that provide a conductive path through the bulk of the plastic to ground (such as carbon black) will reduce electrostatic charging.

Chain-Transfer Agents. Chain-transfer agents are used to regulate the molecular weight of polymers. These agents react with the developing polymer and interrupt the growth of a particular chain. The products, however, are free radicals that are capable of adding to monomers and initiating the formation of new chains. The overall effect is to reduce the average molecular weight of the polymer without reducing the rate of polymerization. Branching may occur as a result of chain transfer between a growing but rather short chain with another and longer polymer chain. Branching may also occur if the radical end of a growing chain abstracts a hydrogen atom from a carbon atom four or five carbons removed from the end. Thiols are commonly used as chain-transfer agents.

Coupling Agents. Coupling agents are molecular bridges between the interface of an inorganic surface (or filler) and an organic polymer matrix. Titanium-derived coupling agents interact with the free protons at the inorganic interface to form organic monomolecular layers on the inorganic surface. The titanate-coupling-agent molecule has six functions:



where

Type	<i>m</i>	<i>n</i>
Monoalkoxy	1	3
Coordinate	4	2
Chelate	1	2

Function 1 is the attachment of the hydrolyzable portion of the molecule to the surface of the inorganic (or proton-bearing) species.

Function 2 is the ability of the titanate molecule to transesterify.

Function 3 affects performance as determined by the chemistry of alkylate, carboxyl, sulfonyl, phenolic, phosphate, pyrophosphate, and phosphite groups.

Function 4 provides van der Waals' entanglement via long carbon chains.

Function 5 provides thermoset reactivity via functional groups such as methacrylates and amines.

Function 6 permits the presence of two or three pendent organic groups. This allows all functionality to be controlled to the first-, second-, or third-degree levels.

Silane coupling agents are represented by the formula



where Y represents a hydrolyzable group (typically alkoxy); Z is a functional organic group, such as amino, methacryloxy, epoxy; and R typically is a short aliphatic linkage that serves to attach the functional organic group to silicon in a stable fashion. Bonding to surface hydroxy groups of inorganic compounds is accomplished by the —SiY₃ portion, either by direct bonding of this group or more commonly via its hydrolysis product —Si(OH)₃. Subsequent reaction of the functional organic group with the organic matrix completes the coupling reaction and establishes a covalent chemical bond from the organic phase through the silane coupling agent to the inorganic phase.

Flame Retardants. Flame retardants are thought to function via several mechanisms, dependent upon the class of flame retardant used. Halogenated flame retardants are thought to function principally in the vapor phase either as a diluent and heat sink or as a free-radical trap that stops or slows flame propagation. Phosphorus compounds are thought to function in the solid phase by forming a glaze or coating over the substrate that prevents the heat and mass transfer necessary for sustained combustion. With some additives, as the temperature is increased, the flame retardant acts as a solvent for the polymer, causing it to melt at lower temperatures and flow away from the ignition source.

Mineral hydrates, such as alumina trihydrate and magnesium sulfate heptahydrate, are used in highly filled thermosetting resins.

Foaming Agents (Chemical Blowing Agents). Foaming agents are added to polymers during processing to form minute gas cells throughout the product. Physical foaming agents include liquids and gases. Compressed nitrogen is often used in injection molding. Common liquid foaming agents are short-chain aliphatic hydrocarbons in the C₅ to C₇ range and their chlorinated or fluorinated analogs.

The chemical foaming agent used varies with the temperature employed during processing. At relatively low temperatures (15–200°C), the foaming agent is often 4,4'-oxybis(benzenesulfonylhydrazide) or *p*-toluenesulfonylhydrazide. In the midrange (160–232°C), either sodium hydrogen carbonate or 1,1'-azobisformamide is used. For the

high range (200–285°C), there are *p*-toluenesulfonylsemicarbazide, 5-phenyltetrazole and analogs, and trihydrazinotriazine.

Inhibitors. Inhibitors slow or stop polymerization by reacting with the initiator or the growing polymer chain. The free radical formed from an inhibitor must be sufficiently unreactive that it does not function as a chain-transfer agent and begin another growing chain. Benzoquinone is a typical free-radical chain inhibitor. The resonance-stabilized free radical usually dimerizes or disproportionates to produce inert products and end the chain process.

Lubricants. Materials such as fatty acids are added to reduce the surface tension and improve the handling qualities of plastic films.

Plasticizers. Plasticizers are relatively nonvolatile liquids which are blended with polymers to alter their properties by intrusion between polymer chains. Diisooctyl phthalate is a common plasticizer. A plasticizer must be compatible with the polymer to avoid bleeding out over long periods of time. Products containing plasticizers tend to be more flexible and workable.

Ultraviolet Stabilizers. 2-Hydroxybenzophenones represent the largest and most versatile class of ultraviolet stabilizers that are used to protect materials from the degradative effects of ultraviolet radiation. They function by absorbing ultraviolet radiation and by quenching electronically excited states.

Hindered amines, such as 4-(2,2,6,6-tetramethylpiperidinyl) decanedioate, serve as radical scavengers and will protect thin films under conditions in which ultraviolet absorbers are ineffective. Metal salts of nickel, such as dibutyldithiocarbamate, are used in polyolefins to quench singlet oxygen or electronically excited states of other species in the polymer. Zinc salts function as peroxide decomposers.

Vulcanization and Curing. Originally, vulcanization implied heating natural rubber with sulfur, but the term is now also employed for curing polymers. When sulfur is employed, sulfide and disulfide cross-links form between polymer chains. This provides sufficient rigidity to prevent *plastic flow*. Plastic flow is a process in which coiled polymers slip past each other under an external deforming force; when the force is released, the polymer chains do not completely return to their original positions.

Organic peroxides are used extensively for the curing of unsaturated polyester resins and the polymerization of monomers having vinyl unsaturation. The —O—O— bond is split into free radicals which can initiate polymerization or cross-linking of various monomers or polymers.

TABLE 10.1 Plastic Families

Acetals	Allyls
Acrylics	Allyl-diglycol-carbonate polymer
Poly(methyl methacrylate) (PMMA)	Diallyl phthalate (DAP) polymer
Poly(acrylonitrile)	Cellulosics
Alkyds	Cellulose acetate resin
Alloys	Cellulose-acetate-propionate resin
Acrylic-poly(vinyl chloride) alloy	Cellulose-acetate-butyrate resin
Acrylonitrile-butadiene-styrene-	Cellulose nitrate resin
poly(vinyl chloride) alloy (ABS-PVC)	Ethyl cellulose resin
Acrylonitrile-butadiene-styrene-	Rayon
polycarbonate alloy (ABS-PC)	Chlorinated polyether
	Epoxy

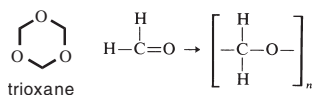
TABLE 10.1 Plastic Families (continued)

Fluorocarbons Poly (tetrafluoroethylene) (PTFE) Poly (chlorotrifluoroethylene) (PCTFE) Perfluoroalkoxy (PFA) resin Fluorinated ethylene–propylene (FEP) resin Poly(vinylidene fluoride) (PVDF) Ethylene–chlorotrifluoroethylene copolymer Ethylene–tetrafluoroethylene copolymer Poly(vinyl fluoride) (PVF)	Polyolefins (PO) Low-density polyethylene (LDPE) High-density polyethylene (HDPE) Ultrahigh-molecular-weight polyethylene (UHMWPE) Polypropylene (PP) Polybutylene (PB) Polyallomers
Melamine formaldehyde	Poly(phenylene oxide)
Melamine phenolic	Poly(phenylene sulfide) (PPS)
Nitrile resins	Polyurethanes
Phenolics	Silicones
Polyamides Nylon 6 Nylon 6/6 Nylon 6/9 Nylon 6/12 Nylon 11 Nylon 12 Aromatic nylons	Styrenics Polystyrene (PS) Acrylonitrile–butadiene–styrene (ABS) copolymer Sytrene–acrylonitrile (SAN) copolymer Styrene–butadiene copolymer
Poly(amide–imide)	Sulfones Polysulfone (PSF) Poly(ether sulfone) Poly(phenyl sulfone)
Poly(aryl ether)	Thermoplastic elastomers Polyolefin Polyester Block copolymers Styrene–butadiene block copolymer Styrene–isoprene block copolymer Styrene–ethylene block copolymer Styrene–butylene block copolymer
Polycarbonate (PC)	Urea formaldehyde
Polyesters Poly(butylene terephthalate) (PBT) [also called polytetramethylene terephthalate (PTMT)] Poly(ethylene terephthalate) (PET) Unsaturated polyesters (SMC, BMC) Butadiene–maleic acid copolymer (BMC) Styrene–maleic acid copolymer (SMC)	Vinyls Poly(vinyl chloride) (PVC) Poly(vinyl acetate) (PVAC) Poly(vinylidene chloride) Poly(vinyl butyrate) (PVB) Poly(vinyl formal) Poly(vinyl alcohol) (PVAL)
Polyimide	
Poly(methylpentene)	

FORMULAS AND KEY PROPERTIES OF PLASTIC MATERIALS

Acetals

Homopolymer. Acetal homopolymers are prepared from formaldehyde and consist of high-molecular-weight linear polymers of formaldehyde. The trimer of formaldehyde is shown to the left and the structure of the polymer is shown at the right, below.



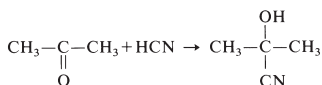
The good mechanical properties of this homopolymer result from the ability of the oxymethylene chains to pack together into a highly ordered crystalline configuration as the polymers change from the molten to the solid state.

Key properties include high melt point, strength and rigidity, good frictional properties, and resistance to fatigue. Higher molecular weight increases toughness but reduces melt flow.

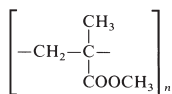
Copolymer. Acetal copolymers are prepared by copolymerization of 1,3,5-trioxane with small amounts of a co-monomer. Carbon-carbon bonds are distributed randomly in the polymer chain. These carbon-carbon bonds help to stabilize the polymer against thermal, oxidative, and acidic attack.

Acrylics

Poly(methyl methacrylate). Acrylic acid is $\text{H}_2\text{C}=\text{CH}-\text{COOH}$ and methacrylic acid is $\text{H}_2\text{C}=\text{C}(\text{CH}_3)\text{COOH}$. These compounds and their methyl esters are both quite reactive and difficult to store and handle. The monomer used to form poly(methyl methacrylate), 2-hydroxy-2-methylpropanenitrile, is prepared by the following reaction:

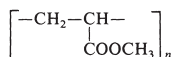


2-Hydroxy-2-methylpropanenitrile is then reacted with methanol (or other alcohol) to yield methacrylate ester. Free-radical polymerization is initiated by peroxide or azo catalysts and produce poly(methyl methacrylate) resins having the following formula:



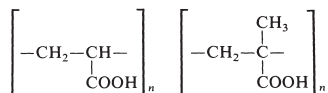
Key properties are good resistance to heat, light, and weathering. This polymer is unaffected by most detergents, cleaning agents, and solutions of inorganic acids, alkalies, and aliphatic hydrocarbons. Poly(methyl methacrylate) has light transmittance of 92% with a haze of 1-3% and its clarity is equal to glass.

Poly(methyl acrylate). The structure of methyl acrylate is $\text{H}_2\text{C}=\text{CH}-\text{COOCH}_3$. The monomer used to prepare poly(methyl acrylate) is produced by the oxidation of propylene. The resin is made by free-radical polymerization initiated by peroxide catalysts and has the following formula:



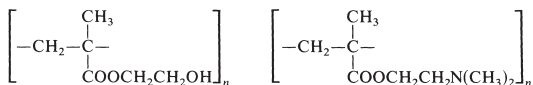
Poly(methyl acrylate) resins vary from soft, elastic, film-forming materials to hard plastics.

Poly(acrylic acid) and Poly(methacrylic acid). Glacial acrylic acid and glacial methacrylic acid can be polymerized to produce water-soluble polymers having the following structures:



These monomers provide a means for introducing carboxyl groups into copolymers. In copolymers these acids can improve adhesion properties, improve freeze-thaw and mechanical stability of polymer dispersions, provide stability in alkalies (including ammonia), increase resistance to attack by oils, and provide reactive centers for cross-linking by divalent metal ions, diamines, or epoxides.

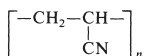
Functional Group Methacrylate Monomers. Hydroxyethyl methacrylate and dimethylaminoethyl methacrylate produce polymers having the following formulas:



The use of hydroxyethyl (also hydroxypropyl) methacrylate as a monomer permits the introduction of reactive hydroxyl groups into the copolymers. This offers the possibility for subsequent cross-linking with an HO-reactive difunctional agent (diisocyanate, diepoxide, or melamineformaldehyde resin). Hydroxyl groups promote adhesion to polar substrates.

Use of dimethylaminoethyl (also *tert*-butylaminoethyl) methacrylate as a monomer permits the introduction of pendent amino groups which can serve as sites for secondary cross-linking, provide a way to make the copolymer acid-soluble, and provide anchoring sites for dyes and pigments.

Poly(acrylonitrile). Acrylonitrile has the formula $\text{H}_2\text{C}=\text{CH}-\text{C}\equiv\text{N}$. Poly(acrylonitrile) polymers have the following formula:



Alkyds

Alkyds are formulated from polyester resins, cross-linking monomers, and fillers of mineral or glass. The unsaturated polyester resins used for thermosetting alkyds are the reaction products of polyfunctional organic alcohols (glycols) and dibasic organic acids. Key properties of alkyds are dimensional stability, colorability, and arc track resistance. Chemical resistance, however, is generally poor.

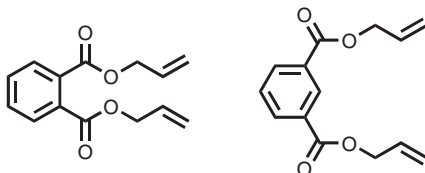
Alloys

Polymer alloys are physical mixtures of structurally different homopolymers or copolymers. The mixture is held together by secondary intermolecular forces such as dipole interaction, hydrogen bonding, or van der Waals' forces.

Homogeneous alloys have a single glass transition temperature which is determined by the ratio of the components. The physical properties of these alloys are averages based on the composition of the alloy. Heterogeneous alloys can be formed when graft or block copolymers are combined with a compatible polymer. Alloys of incompatible polymers can be formed if an interfacial agent can be found.

Allyls

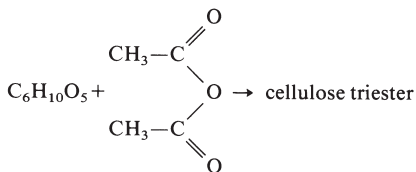
Diallyl Phthalate (and Diallyl 1,3-Phthalate). Phthalic acid is 1,2-dicarboxybenzene. The 1,3-isomer is generally referred to as isophthalic acid. These allyl polymers are prepared from



These resulting polymers are solid, linear, internally cyclized, thermoplastic structures containing unreacted allylic groups spaced at regular intervals along the polymer chain. Compounds derived from these polymers that are molded with mineral, glass, or synthetic fiber filling exhibit good electrical properties under high humidity and high temperature conditions. They also show stable low-loss factors, high surface and volume resistivity, and high arc and track resistance.

Cellulosics

Cellulose Triacetate. Cellulose triacetate is prepared according to the following reaction:



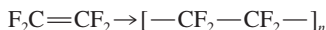
Because cellulose triacetate has a high softening temperature, it must be processed in solution. A mixture of dichloromethane and methanol is a common solvent.

resin and the curing resin (usually an aliphatic polyamine) are packaged separately and mixed together immediately before use.

Epoxy novolac resins are produced by glycidation of the low-molecular-weight reaction products of phenol (or cresol) with formaldehyde. Highly cross-linked systems are formed that have superior performance at elevated temperatures.

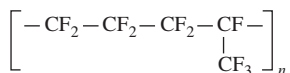
Fluorocarbon

Poly(tetrafluoroethylene). Poly(tetrafluoroethylene) is prepared from tetrafluoroethylene and consists of repeating units in a predominantly linear chain:



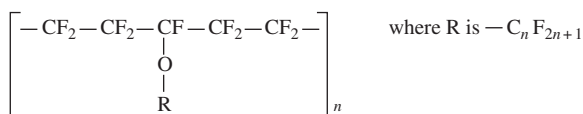
Tetrafluoroethylene polymer has the lowest coefficient of friction of any solid. It has remarkable chemical resistance and a very low brittleness temperature (-100°C). Its dielectric constant and loss factor are low and stable across a broad temperature and frequency range. Its impact strength is high.

Fluorinated Ethylene-Propylene Resin. Polymer molecules of fluorinated ethylene-propylene consist of predominantly linear chains with this structure:



Key properties are its flexibility, translucency, and resistance to all known chemicals except molten alkali metals, elemental fluorine and fluorine precursors at elevated temperatures, and concentrated perchloric acid. It withstands temperatures from -270° to 250°C and may be sterilized repeatedly by all known chemical and thermal methods.

Perfluoroalkoxy Resin. Perfluoroalkoxy resin has the following formula:



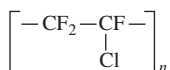
It resembles polytetrafluoroethylene and fluorinated ethylene propylene in its chemical resistance, electrical properties, and coefficient of friction. Its strength, hardness, and wear resistance are about equal to the former plastic and superior to that of the latter at temperatures above 150°C .

Poly(vinylidene fluoride). Poly(vinylidene fluoride) consists of linear chains in which the predominant repeating unit is



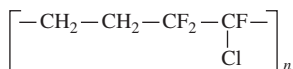
It has good weathering resistance and does not support combustion. It is resistant to most chemicals and solvents and has greater strength, wear resistance, and creep resistance than the preceding three fluorocarbon resins.

Poly(1-chloro-1,2,2-trifluoroethylene). Poly(1-chloro-1,2,2-trifluoroethylene consists of linear chains in which the predominant repeating unit is



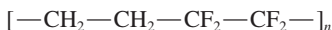
It possesses outstanding barrier properties to gases, especially water vapor. It is surpassed only by the fully fluorinated polymers in chemical resistance. A few solvents dissolve it at temperatures above 100°C, and it is swollen by a number of solvents, especially chlorinated solvents. It is harder and stronger than perfluorinated polymers, and its impact strength is lower.

Ethylene-Chlorotrifluoroethylene Copolymer. Ethylene-chlorotrifluoroethylene copolymer consists of linear chains in which the predominant 1:1 alternating copolymer is



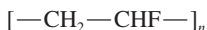
This copolymer has useful properties from cryogenic temperatures to 180°C. Its dielectric constant is low and stable over a broad temperature and frequency range.

Ethylene-Tetrafluoroethylene Copolymer. Ethylene-tetrafluoroethylene copolymer consists of linear chains in which the repeating unit is



Its properties resemble those of ethylene-chlorotrifluoroethylene copolymer.

Poly(vinyl fluoride). Poly(vinyl fluoride) consists of linear chains in which the repeating unit is



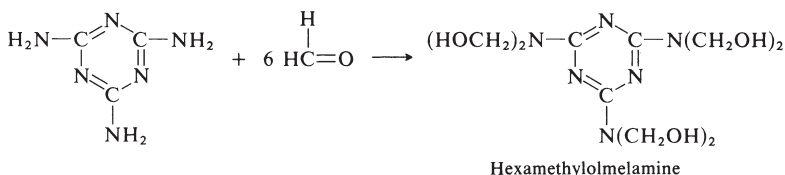
It is used only as a film, and it has good resistance to abrasion and resists staining. It also has outstanding weathering resistance and maintains useful properties from -100 to 150°C.

Nitrile Resins

The principal monomer of nitrile resins is acrylonitrile (see "Polyacrylonitrile"), which constitutes about 70% by weight of the polymer and provides the polymer with good gas barrier and chemical resistance properties. The remainder of the polymer is 20–30% methyl acrylate (or styrene), with 0–10% butadiene to serve as an impact-modifying monomer.

Melamine Formaldehyde

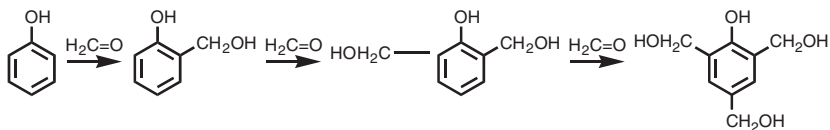
The monomer used for preparing melamine formaldehyde is formed as follows:



Hexamethylolmelamine can further condense in the presence of an acid catalyst; ether linkages can also form (see "Urea Formaldehyde"). A wide variety of resins can be obtained by careful selection of pH, reaction temperature, reactant ratio, amino monomer, and extent of condensation. Liquid coating resins are prepared by reacting methanol or butanol with the initial methylolated products. These can be used to produce hard, solvent-resistant coatings by heating with a variety of hydroxy, carboxyl, and amide functional polymers to produce a cross-linked film.

Phenolics

Phenol-formaldehyde resin. Phenol-formaldehyde resin is prepared from phenol by reaction with formaldehyde. Phenol is an enol, the 2-, 4-, and 6-positions of which are activated for reaction with an electrophile. Phenol is sequentially hydroxymethylated approximately as illustrated below. Dehydration of the phenolic hydroxymethyl groups affords a benzyl cation, a new electrophile that can react with another substituted or unsubstituted molecule of phenol. Both linear polymerization and cross-linking are possible, depending on the ratio of the reactants and the polymerization conditions.

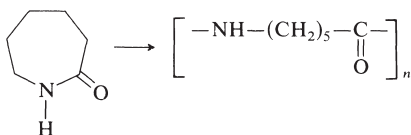


One-Stage Resins. The ratio of formaldehyde to phenol is high enough to allow the thermosetting process to take place without the addition of other sources of cross-links.

Two-Stage Resins The ratio of formaldehyde to phenol is low enough to prevent the thermosetting reaction from occurring during manufacture of the resin. At this point the resin is termed *novolac* resin. Subsequently, hexamethylenetetramine is incorporated into the material to act as a source of chemical cross-links during the molding operation (and conversion to the thermoset or cured state).

Polyamides

Nylon 6, 11, and 12. This class of polymers is polymerized by addition reactions of ring compounds that contain both acid and amine groups on the monomer.



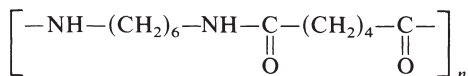
Nylon 6 is polymerized from 2-oxohexamethyleneimine (6 carbons); nylon 11 and 12 are made this way from 11- and 12-carbon rings, respectively.

Nylon 6/6, 6/9, and 6/12. As illustrated below, nylon 6/6 is polymerized from 1,6-hexanedioic acid (six carbons) and 1,6-hexanediamine (six carbons).



1,6-Hexanedioic acid

1,6-Hexanediamine



Poly(hexamethylene 1,6- hexanediamide)

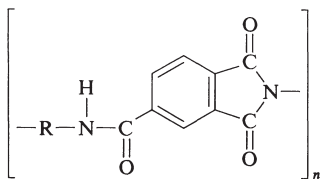
Other nylons are made this way from different combinations of monomers to produce types 6/9, 6/10, and 6/12.

Nylon 6 and 6/6 possess the maximum stiffness, strength, and heat resistance of all the types of nylon. Type 6/6 has a higher melt temperature, whereas type 6 has a higher impact resistance and better processibility. At a sacrifice in stiffness and heat resistance, the higher analogs of nylon are useful primarily for improved chemical resistance in certain environments (acids, bases, and zinc chloride solutions) and for lower moisture absorption.

Aromatic nylons, $[-\text{NH}-\text{C}_6\text{H}_4-\text{CO}-]_n$, (also called aramids) have specialty uses because of their improved clarity.

Poly (amide-imide)

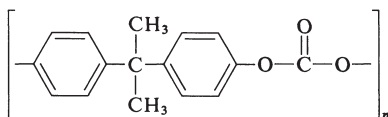
Poly(amide-imide) is the condensation polymer of 1,2,4-benzenetricarboxylic anhydride and various aromatic diamines and has the general structure:



It is characterized by high strength and good impact resistance, and retains its physical properties at temperatures up to to 260°C. Its radiation (gamma) resistance is good.

Polycarbonate

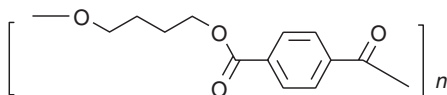
Polycarbonate is a polyester in which dihydric (or polyhydric) phenols are joined through carbonate linkages. The general-purpose type of polycarbonate is based on 2,2-bis(4'-hydroxybenzene) propane (bisphenol A) and has the general structure:



Polycarbonates are the toughest of all thermoplastics. They are window-clear, amazingly strong and rigid, autoclavable, and nontoxic. They have a brittleness temperature of -135°C .

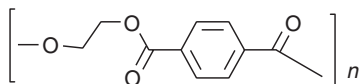
Polyester

Poly(butylene terephthalate). Poly(butylene terephthalate) is prepared in a condensation reaction between dimethyl terephthalate and 1,4-butanediol and its repeating unit has the general structure



This thermoplastic shows good tensile strength, toughness, low water absorption, and good frictional properties, plus good chemical resistance and electrical properties.

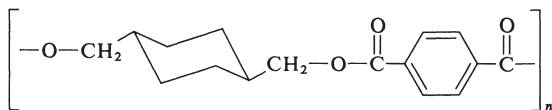
Poly(ethylene terephthalate). Poly(ethylene terephthalate) is prepared by the reaction of either terephthalic acid or dimethyl terephthalate with ethylene glycol, and its repeating unit has the general structure



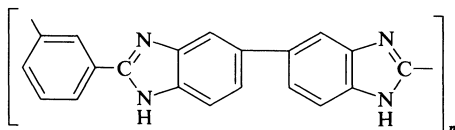
The resin has the ability to be oriented by a drawing process and crystallized to yield a high-strength product.

Unsaturated Polyesters. Unsaturated polyesters are produced by reaction between two types of dibasic acids, one of which is unsaturated, and an alcohol to produce an ester. Double bonds in the body of the unsaturated dibasic acid are obtained by using maleic anhydride or fumaric acid.

PCTA Copolyester. Poly(1,4-cyclohexanedimethylene terephthalic acid) (PCTA) copolyester is a polymer of cyclohexanedimethanol and terephthalic acid, with another acid substituted for a portion of the terephthalic acid otherwise required. It has the following formula:



Polyimides. Polyimides have the following formula:



They are used as high-temperature structural adhesives since they become rubbery rather than melt at about 300°C.

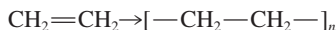
Poly(methylpentene)

Poly(methylpentene) is obtained by a Ziegler-type catalytic polymerization of 4-methyl-1-pentene.

Its key properties are its excellent transparency, rigidity, and chemical resistance, plus its resistance to impact and to high temperatures. It withstands repeated autoclaving, even at 150°C.

Polyolefins

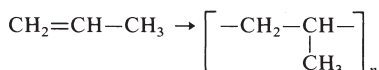
Polyethylene. Polymerization of ethylene results in an essentially straight-chain high-molecular-weight hydrocarbon.



Branching occurs to some extent and can be controlled. Minimum branching results in a “high-density” polyethylene because of its closely packed molecular chains. More branching gives a less compact solid known as “low-density” polyethylene.

A key property is its chemical inertness. Strong oxidizing agents eventually cause some oxidation, and some solvents cause softening or swelling, but there is no known solvent for polyethylene at room temperature. The brittleness temperature is -100°C for both types. Polyethylene has good low-temperature toughness, low water absorption, and good flexibility at subzero temperatures.

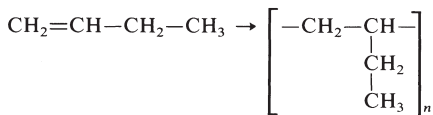
Polypropylene. The polymerization of propylene results in a polymer with the following structure:



The desired form in homopolymers is the isotactic arrangement (at least 93% is required to give the desired properties). Copolymers have a random arrangement. In block copolymers a secondary reactor is used where active polymer chains can further polymerize to produce segments that use ethylene monomer.

Polypropylene is translucent and autoclavable and has no known solvent at room temperature. It is slightly more susceptible to strong oxidizing agents than polyethylene.

Polybutylene. Polybutylene is composed of linear chains having an isotactic arrangement of ethyl side groups along the chain backbone.



It has a helical conformation in the stable crystalline form.

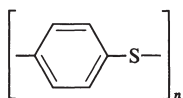
Polybutylene exhibits high tear, impact, and puncture resistance. It also has low creep, excellent chemical resistance, and abrasion resistance with coilability.

Ionomer. Ionomer is the generic name for polymers based on sodium or zinc salts of ethylene-methacrylic acid copolymers in which interchain ionic bonding, occurring randomly between the long-chain polymer molecules, produces solid-state properties.

The abrasion resistance of ionomers is outstanding, and ionomer films exhibit optical clarity. In composite structures ionomers serve as a heat-seal layer.

Poly(phenylene sulfide)

Poly(phenylene sulfide) has the following formula:

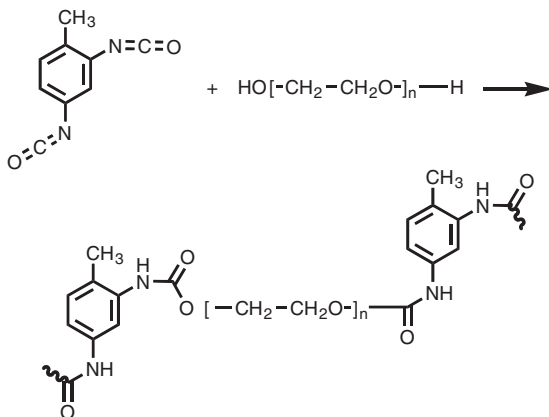


The recurring *para*-substituted benzene rings and sulfur atoms form a symmetrical rigid backbone.

The high degree of crystallization and the thermal stability of the bond between the benzene ring and sulfur are the two properties responsible for the polymer's high melting point, thermal stability, inherent flame retardance, and good chemical resistance. There are no known solvents of poly(phenylene sulfide) that can function below 205°C.

Polyurethane

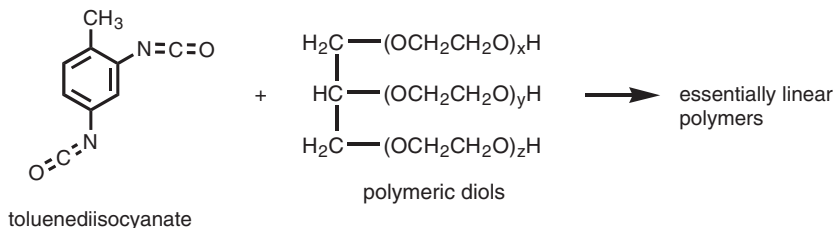
Foams. Polyurethane foams are prepared by the polymerization of polyols with isocyanates. One of the most commonly used reactive isocyanates toluenediisocyanate, TDI. It is made from toluene by nitration and then reduction followed by treatment with phosgene. The isocyanate residue reacts readily with alcohols to give carbamates (urethanes) or amines to give ureas.



Commonly used isocyanates are toluenediisocyanate, methylenediphenylisocyanate, and polymeric isocyanates. Polyols used are macroglycols based on either polyester or polyether. The former [poly(ethylene phthalate) or poly(ethylene 1,6-hexanedioate)] have hydroxyl groups that are free to react with the isocyanate. Most flexible foam is made from 80/20 toluene diisocyanate (which refers to the ratio of 2,4-toluenediisocyanate to 2,6-toluene diisocyanate). High-resilience foam contains about 80% 80/20 toluenediisocyanate and 20% poly(methylene diphenyl isocyanate), while semiflexible foam is almost always 100% poly(methylene diphenyl isocyanate). Much of the latter reacts by trimerization to form isocyanurate rings.

Flexible foams are used in mattresses, cushions, and safety applications. Rigid and semiflexible foams are used in structural applications and to encapsulate sensitive components to protect them against shock, vibration, and moisture. Foam coatings are tough, hard, flexible, and chemically resistant.

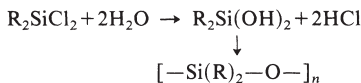
Elastomeric Fiber. Elastomeric fibers are prepared by the polymerization of polymeric polyols with diisocyanates.



The structure of elastomeric fibers is similar to that illustrated for polyurethane foams.

SILICONES

Silicones are formed in the following multistage reaction:



The silanols formed above are unstable and undergo dehydration. On polycondensation, they give polysiloxanes (or silicones) which are characterized by their three-dimensional branched-chain structure. Various organic groups introduced within the polysiloxane chain impart certain characteristics and properties to these resins.

Methyl groups impart water repellency, surface hardness, and noncombustibility.

Phenyl groups impart resistance to temperature variations, flexibility under heat, resistance to abrasion, and compatibility with organic products.

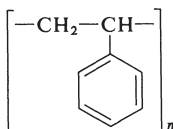
Vinyl groups strengthen the rigidity of the molecular structure by creating easier cross-linkage of molecules.

Methoxy and alkoxy groups facilitate cross-linking at low temperatures.

Oils and gums are nonhighly branched or straight-chain polymers whose viscosity increases with the degree of polycondensation.

Styrenics

Polystyrene. Polystyrene has the following formula:



Polystyrene is rigid with excellent dimensional stability, has good chemical resistance to aqueous solutions, and is an extremely clear material.

Impact polystyrene contains polybutadiene added to reduce brittleness. The polybutadiene is usually dispersed as a discrete phase in a continuous polystyrene matrix. Polystyrene can be grafted onto rubber particles, which assures good adhesion between the phases.

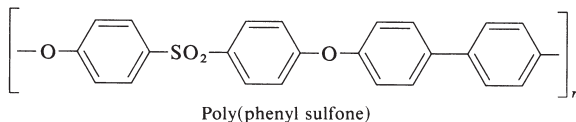
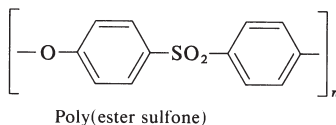
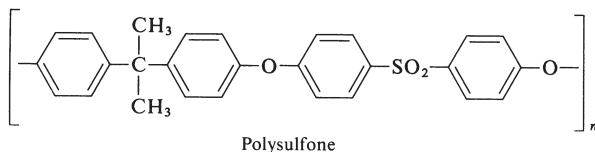
Acrylonitrile–Butadiene–Styrene (ABS) Copolymers. This basic three-monomer system can be tailored to yield resins with a variety of properties. Acrylonitrile contributes heat resistance, high strength, and chemical resistance. Butadiene contributes impact strength, toughness, and retention of low-temperature properties. Styrene contributes gloss, processibility, and rigidity. ABS polymers are composed of discrete polybutadiene particles grafted with the styrene–acrylonitrile copolymer; these are dispersed in the continuous matrix of the copolymer.

Styrene–Acrylonitrile (SAN) Copolymers. SAN resins are random, amorphous copolymers whose properties vary with molecular weight and copolymer composition. An increase in molecular weight or in acrylonitrile content generally enhances the physical properties of the copolymer but at some loss in ease of processing and with a slight increase in polymer color.

SAN resins are rigid, hard, transparent thermoplastics which process easily and have good dimensional stability—a combination of properties unique in transparent polymers.

Sulfones

Below are the formulas for three polysulfones.



The isopropylidene linkage imparts chemical resistance, the ether linkage imparts temperature resistance, and the sulfone linkage imparts impact strength. The brittleness temperature of polysulfones is -100°C . Polysulfones are clear, strong, nontoxic, and virtually unbreakable. They do not hydrolyze during autoclaving and are resistant to acids, bases, aqueous solutions, aliphatic hydrocarbons, and alcohols.

Thermoplastic Elastomers

Polyolefins. In these thermoplastic elastomers the hard component is a crystalline polyolefin, such as polyethylene or polypropylene, and the soft portion is composed of ethylene-propylene rubber. Attractive forces between the rubber and resin phases serve as labile cross-links. Some contain a chemically cross-linked rubber phase that imparts a higher degree of elasticity.

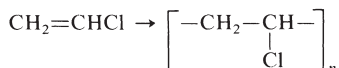
Styrene-Butadiene-Styrene Block Copolymers. Styrene blocks associate into domains that form hard regions. The midblock, which is normally butadiene, ethylene-butene, or isoprene blocks, forms the soft domains. Polystyrene domains serve as cross-links.

Polyurethanes. The hard portion of polyurethane consists of a chain extender and polyisocyanate. The soft component is composed of polyol segments.

Polyesters. The hard portion consists of copolyester, and the soft portion is composed of polyol segments.

Vinyl

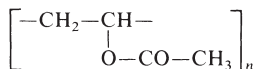
Poly(vinyl chloride) (PVC). Polymerization of vinyl chloride results in the formation of a polymer with the following formula:



When blended with phthalate ester plasticizers, PVC becomes soft and pliable.

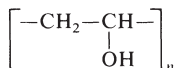
Its key properties are good resistance to oils and a very low permeability to most gases.

Poly(vinyl acetate). Poly(vinyl acetate) has the following formula:



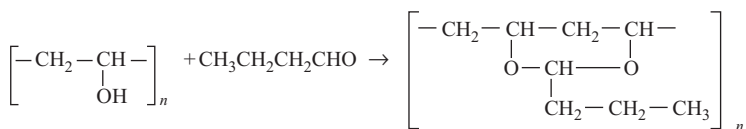
Poly(vinyl acetate) is used in latex water paints because of its weathering, quick-drying, recoatability, and self-priming properties. It is also used in hot-melt and solution adhesives.

Poly(vinyl alcohol). Poly(vinyl alcohol) has the following formula:



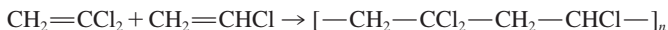
It is used in adhesives, paper coating and sizing, and textile warp size and finishing applications.

Poly(vinyl butyral). Poly(vinyl butyral) is prepared according to the following reaction:



Its key characteristics are its excellent optical and adhesive properties. It is used as the interlayer film for safety glass.

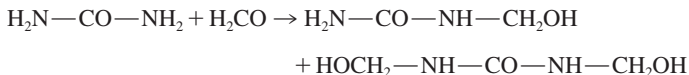
Poly(vinylidene chloride). Poly(vinylidene chloride) is prepared according to the following reaction:



Random copolymer

Urea Formaldehyde

The reaction of urea with formaldehyde yields the following products, which are used as monomers in the preparation of urea formaldehyde resin.



The reaction conditions can be varied so that only one of these monomers is formed. 1-Hydroxymethylurea and 1,3-bis(hydroxymethyl)urea condense in the presence of an acid catalyst to produce urea formaldehyde resins. A wide variety of resins can be obtained by careful selection of the pH, reaction temperature, reactant ratio, amino monomer, and degree of polymerization. If the reaction is carried far enough, an infusible polymer network is produced.

Liquid coating resins are prepared by reacting methanol or butanol with the initial hydroxymethylureas. Ether exchange reactions between the amino resin and the reactive sites on the polymer produce a cross-linked film.

TABLE 10.2 Properties of Commercial Plastics

Properties	Acetal				
	Homopolymer	Copolymer	20% glass-reinforced homopolymer	25% glass-reinforced copolymer	21% poly(tetrafluoroethylene)-filled homopolymer
Physical					
Melting temperature, °C					
Crystalline	175	175	181	175	181
Amorphous					
Specific gravity	1.42	1.41	1.56	1.61	1.54
Water absorption (24 h), %	0.25–0.40	0.22	0.25	0.29	0.20
Dielectric strength, KV · mm ⁻¹	19.7	19.7	19.3	22.8	15.7
Electrical					
Volume (dc) resistivity, ohm-cm	10 ¹⁵	10 ¹⁵	5 × 10 ¹⁴		3 × 10 ¹⁶
Dielectric constant (60 Hz)	3.7	3.7	3.9		3.1
Dielectric constant (10 ⁶ Hz)	3.7	3.7	3.9		3.1
Dissipation (power) factor (60 Hz)					
Dissipation factor (10 ⁶ Hz)	0.005	0.005	0.005		0.005
Mechanical					
Compressive modulus, 10 ³ lb · in ⁻²	670	450			

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	5.29	16 (10% yield)	18 (10% yield)	17 (10% yield)	13 (10% yield)
Elongation at break, %	25–75	40–75	7	3	15–22
Flexural modulus at 23 °C, $10^3 \text{ lb} \cdot \text{in}^2$	380–430	375	730	1 100	340–350
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	14	13	15	28	
Hardness, Rockwell (or Shore)	M94	M78	M90	M79	M78
Impact strength (Izod) at 23 °C, $\text{J} \cdot \text{m}^{-1}$	69–123	53–80	43	96	37–64
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	520	410	1 000	1 250	
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	10	10	8.5	18.5	7.6
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$	9.5–12	8.5			6.9–7.6
Thermal					
Burning rate, $\text{mm} \cdot \text{min}^{-1}$	27.9				
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}$	100	85	36–81		75
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$	124	110	157	163	100
Maximum recommended service temperature, $^\circ\text{C}$	84				
Specific heat, $\text{cal} \cdot \text{g}^{-1}$	0.35				
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.23	0.23			

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Acrylic				Alkyd, molded	Alloy	
						Acrylic poly(vinyl chloride) alloy	Acrylonitrile– butadiene– styrene– poly(vinyl chloride) alloy
	Poly(methyl methacrylate)	Cast sheet	Impact- modified	Heat- resistant			
Physical							
Melting temperature, °C							
Crystalline	90–105	90–105	80–100	100–125		105	
Amorphous							
Specific gravity	1.17–1.20	1.18–1.20	1.11–1.18	1.16–1.19	2.22–2.24		
Water absorption (24h), %	0.1–0.4	0.2–0.4	0.2–0.8	0.2–0.3		0.06	
Dielectric strength, KV·mm ^{−1}	15.7–19.9	17.7–21.7	15.0–19.9	15.7–19.9		> 15.7	19.7
Electrical							
Volume (dc) resistivity, ohm-cm	> 10 ¹⁴	> 10 ¹⁴					
Dielectric constant (60Hz)	3.3–4.5	3.5–4.5			3.8–5.0		
Dielectric constant (10 ⁶ Hz)		3.0–3.5			3.6–4.7		
Dissipation (power) factor (60Hz)		0.04–0.06			0.012–0.026		
Dissipation factor (10 ⁶ Hz)		0.02–0.03			0.01–0.016		
Mechanical							
Compressive modulus, 10 ⁴ lb·in ^{−2}	370–460	390–475	240–370	350–460		330–400	

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	12–18	11–19	4–14	17	16–20	8.4	
Elongation at break, %	2–10	2–7	20–70	3–5		100	
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	420–460	390–475	200–380	460–500		330–400	340
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	13–19	12–17	7–13	12–16		10.7	9.6
Hardness, Rockwell (or Shore)	M85–M105	M80–M100	R105–R120	M95–M105	E76	R99–R105	R100
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	16–27	16–21	43–133	16–21	27–240	800	560
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	380–450	350–450	200–400	350–460		330–335	330
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	7–11	8–11	5–9	10	4.5–6.5	6.5	5.8
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$					10–13		
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$		0.5–2.2			Self-extinguishing		
Coefficient of linear thermal expansion, $10^{-6} \text{ }^\circ\text{C}^{-1}$	50–90	50–90	50–80	50–60	40–55		46
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$	74–99	71–102	74–95	88–104	177–204	71	
Maximum recommended service temperature, $^\circ\text{C}$		60–71			220		
Specific heat, $\text{cal} \cdot \text{g}^{-1}$	0.36	0.35					
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.17–0.25	0.17–0.25	0.17–0.21	0.19			

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Alloy	Allyl			Cellulosic		
	Polycarbonate acrylonitrile– butadiene– styrene alloy	Allyl–diglycol– carbonate polymer	Diallyl phthalate molding		Cellulose acetate		Cellulose– acetate– butyrate resin
			Glass-filled	Mineral-filled	Sheet	Molding	Sheet
Physical							
Melting temperature, °C							
Crystalline		Thermoset	Thermoset	Thermoset	230	230	140
Amorphous	150						
Specific gravity	1.12–1.20	1.3–1.4	1.7–2.0	1.65–1.85	1.27–1.34	1.29–1.34	1.15–1.22
Water absorption (24 h), %	0.21–0.24	0.2	0.12–0.35	0.2–0.5	2–7	1.7–6.5	0.9–2.2
Dielectric strength, $\text{kV} \cdot \text{mm}^{-1}$	17.7	15.0	15.7–17.7	15.7–17.7	11–24	9–24	9–18
Electrical							
Volume (dc) resistivity, ohm-cm					10^{10} – 10^{13}	10^{10} – 10^{13}	10^{10} – 10^{12}
Dielectric constant (60 Hz)					3.4–7.4	3.5–7.5	3.7–4.3
Dielectric constant (10^6 Hz)					3.2–7.0	3.2–7.0	3.3–3.8
Dissipation (power) factor (60 Hz)					0.01–0.06	0.01–0.06	0.01–0.04
Dissipation factor (10^6 Hz)					0.01–0.06	0.01–0.10	0.01–0.04
Mechanical							
Compressive modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$		300					

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	11	21–23	25–35	20–32	22–33	25–36	
Elongation at break, %	10–15		3–5	3–5	17–40	6–40	50–100
Flexural modulus at 23 °C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	300–400	250–330	1 200–1 500	1 000–1 400			740–1 300
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	13.0–13.7	6–13	9–20	8.5–11	6–10	2–16	4–9
Hardness, Rockwell (or Shore)	R117	M95–M100	E80–E87	E61	R85–R120	R100–R123	R50–R95
Impact strength (Izod) at 23 °C, $\text{J} \cdot \text{m}^{-1}$	560	11–21	21–800	16–43	107–454	53–214	133–288
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	370–380	300	1 400–2 200	1 200–2 200			200–250
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	7.0–7.3	5–6	6–11	5–8	4.5–8.0	1.9–9.0	2.6–6.9
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$	8.5				2.2–7.4	4.1–7.6	
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$						1.3–3.8	1.3–3.8
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	63–67	5.4–9.6	0.68–2.4	2.8	100–150	80–180	110–170
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), °C	104–116	60–88	165–288+	160–288	44–91	51–98	49–58
Maximum recommended service temperature, °C							
Specific heat, $\text{cal} \cdot \text{g}^{-1}$					0.3–0.4	0.3–0.42	0.3–0.4
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.25–0.38	0.20–0.21	0.21–0.63	0.30–1.04	0.17–0.34	0.17–0.34	0.17–0.34

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Cellulosic				Chlorinated polyether	Epoxy	
	Cellulose-acetate-butyrate resin, molding	Cellulose-acetate-propionate resin, molding	Ethyl cellulose	Cellulose nitrate		Bisphenol	
						Glass-fiber-reinforced	Mineral-filled
Physical							
Melting temperature, °C							
Crystalline	140	190	135		125	Thermoset	Thermoset
Amorphous							
Specific gravity	1.15–1.22	1.17–1.24	1.09–1.17	1.35–1.40	1.4	1.6–2.0	1.6–2.1
Water absorption (24h), %	0.9–2.2	1.2–2.8	0.8–1.8			0.04–0.20	0.03–0.20
Dielectric strength, kV•mm ^{−1}	9–13	12–17.7	13.8–19.7			9.8–15.7	9.8–15.7
Electrical							
Volume (dc) resistivity, ohm-cm	10 ¹⁰ –10 ¹²			10 ¹⁰			
Dielectric constant (60Hz)	3.5–6.4			7.0–7.5			
Dielectric constant (10 ⁶ Hz)	3.2–6.2		3.01	6.6			
Dissipation (power) factor (60Hz)	0.01–0.04						
Dissipation factor (10 ⁶ Hz)	0.01–0.04						
Mechanical							
Compressive modulus, 10 ³ lb•in ^{−2}						3 000	

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	2.1–7.5	2.4–7.0		2.1–8.0		18 000–40 000	18 000–40 000
Elongation at break, %	40–88	29–100	5–40	40–45	600–800	4	
Flexural modulus at 23 °C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	90–300	120–350				2–4.5	
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	1.8–9.3	2.9–11.4	4–12	9–11	5	8–30	6–18
Hardness, Rockwell (or Shore)	R31–R116	R10–R122	R50–R115	R95–R115	R100	M100–M112	M100–M112
Impact strength (Izod) at 23 °C, $\text{J} \cdot \text{m}^{-1}$	53–582	27 to no break	21	267–374	21	16–533	16–22
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	50–200	60–215		190–220		3	
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	2.6–6.9	2.0–7.8	2–8	7–8	1.5–1.8	5–20	4–10
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$							
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$	1.3–3.8				Self-extinguishing		
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	110–170	110–170	100–200	80–120	6.6	11–50	20–60
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), °C	44–94	44–109	45–88	60–71	185	107–260	107–260
Maximum recommended service temperature, °C					255		
Specific heat, $\text{cal} \cdot \text{g}^{-1}$	0.3–0.4			0.31–0.41			
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.17–0.30	0.17–0.30	0.16–0.30	0.23		0.17–0.42	0.17–1.48

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties Perfluoroalkoxy	Epoxy			Fluorocarbon			
	Casting resin		Novolac resin	Poly(tetrafluoroethylene)		Poly(chloro- trifluoro- ethylene)	
	Unfilled	Flexible	Mineral-filled	Granular	Glass-fiber- reinforced		
Physical							
Melting temperature, °C							
Crystalline	Thermoset	Thermoset	Thermoset	327	327	220	310
Amorphous							
Specific gravity	1.11–1.40	1.05–1.35	1.7–2.1	2.14–2.20	2.2–2.3	2.1–2.2	2.12–2.17
Water absorption (24 h), %	0.08–0.15	0.27–0.50	0.05–0.2	0.01		0.03	
Dielectric strength, kV·mm ⁻¹	11.8–19.7	9.3–15.8	11.8–13.8	18.9	12.6	19.7–23	19.7
Electrical							
Volume (dc) resistivity, ohm-cm	10 ¹² –10 ¹⁷			10 ¹⁸		10 ¹⁸	
Dielectric constant (60 Hz)	3.5–5.0			2.1		2.3–2.7	
Dielectric constant (10 ⁶ Hz)	3.5–5.0			2.1		2.3–2.5	
Dissipation (power) factor (60 Hz)				0.0002		0.001	
Dissipation factor (10 ⁶ Hz)				0.0002		0.005	
Mechanical							
Compressive modulus, 10 ³ lb·in ⁻²				60			

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	15–25	1–14	30	1.7		4.6–7.4	
Elongation at break, %	3–6	20–70	2–4	200–400	200–300	80–250	300
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$			2000	80	235	120	
Flexural strength, rupture or yield, $10^{-3} \text{ lb} \cdot \text{in}^{-2}$	13–21	1–13	16–20		2	7.4–9.3	
Hardness, Rockwell (or Shore)	M80–M110			(D50–D55)	(D60–D70)	R75–R95	(D64)
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	10.7–53	187–267	21	160	144	133–160	No break
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	350	1–350		58–80		150–300	
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	4–13	2–10	6–12	2–5	2–2.7	4.5–6	4–4.3
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$			30				
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$				Self-extinguishing	Self-extinguishing	Self-extinguishing	
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	45–65	20–100	22–30	100	77–100	70	
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$	46–288	23–121	149–260	121 ($66 \text{ lb} \cdot \text{in}^{-2}$)		126 ($66 \text{ lb} \cdot \text{in}^{-2}$)	74 ($66 \text{ lb} \cdot \text{in}^{-2}$)
Maximum recommended service temperature, $^\circ\text{C}$				260		200	
Specific heat, $\text{cal} \cdot \text{g}^{-1}$				0.25		0.22	
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.17–0.21			0.25	0.34–0.40	0.19–0.22	0.25

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Fluorocarbon					Melamine formaldehyde	
	Fluorinated ethylene-propylene resin	Poly(vinylidene fluoride)	Ethylene-tetrafluoroethylene copolymer		Ethylene-chlorotrifluoroethylene copolymer	Cellulose-filled	Glass-fiber-reinforced
			Unfilled	Glass-fiber-reinforced			
Physical							
Melting temperature, °C							
Crystalline	275	156	270	270	245	Thermoset	Thermoset
Amorphous							
Specific gravity	2.14–2.17	1.75–1.78	1.7	1.8	1.68	1.47–1.52	1.5–2.0
Water absorption (24 h), %	< 0.01	0.04–0.06	0.03	0.02	0.01	0.1–0.8	0.09–1.3
Dielectric strength, kV · mm ⁻¹	20–24	10	16	17	19	11–16	5–15
Electrical							
Volume (dc) resistivity, ohm-cm							
Dielectric constant (60 Hz)	2.1	8–9	2.6		2.6		
Dielectric constant (10 ⁶ Hz)	2.1	8–9	2.6		2.6		
Dissipation (power) factor (60 Hz)		High					
Dissipation factor (10 ⁶ Hz)		High					
Mechanical							
Compressive modulus, 10 ³ lb · in ⁻²		120	120	1 200	240		

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	2.2	8.7–10	7.1	10		33–45	20–35
Elongation at break, %	250–330	25–500	100–400	8	200–300	0.6–1.0	0.6
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	80–95	200	200	950	240	1 100	
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$		8.6–11	5.5	10.7	7	9–16	14–23
Hardness, Rockwell (or Shore)	(D60–D65)	(D80)	R50 (D75)	R74	R95	M115–M125	M115
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	No break	192–214	No break	480	No break	11–21	32–961
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	50	120	120	1 200	240	1.1–1.4	1.6–2.4
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	2.7–3.1	5.5–7.4	6.5	12	7	5–13	5–10.5
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$							
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$	Not combustible	Not combustible	Not combustible	Not combustible	Not combustible	Self-extinguishing	Self-extinguishing
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	83–105	85	59	10–32	80	40–45	15–28
Deflection temperature under flexural load (264 $\text{lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$	70 (66 $\text{lb} \cdot \text{in}^{-2}$)	80–90	71	210	77	177–199	190–204
Maximum recommended service temperature, $^\circ\text{C}$	205	150				210	
Specific heat, $\text{cal} \cdot \text{g}^{-1}$	0.28						
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.25	0.19–0.24	0.24		0.16	0.27–0.41	0.41–0.49

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Melamine phenolic, woodflour- and cellulose- filled	Nitrile	Phenolic				
			Unfilled	Woodflour- filled	Glass-fiber- reinforced	Cellulose- filled	Mineral- filled
Physical							
Melting temperature, °C							
Crystalline	Thermoset		Thermoset	Thermoset	Thermoset	Thermoset	Thermoset
Amorphous		95					
Specific gravity	1.5–1.7	1.15	1.24–1.32	1.37–1.46	1.69–2.0	1.38–1.42	1.42–1.84
Water absorption (24 h), %	0.3–0.65	0.28	0.1–0.36	0.3–1.2	0.03–1.2	0.5–0.9	0.1–0.3
Dielectric strength, kV·mm ⁻¹	8.7–12.8	8.7–9.5	9.8–15.8	10.2–15.8	5.5–15.8	11.8–15	7.9–13.8
Electrical							
Volume (dc) resistivity, ohm-cm		1.9 × 10 ¹⁵	1 × 10 ¹² to 7 × 10 ¹²				
Dielectric constant (60 Hz)			6.5–7.5				
Dielectric constant (10 ⁶ Hz)			4.0–5.5				
Dissipation (power) factor (60 Hz)			0.10–0.15				
Dissipation factor (10 ⁶ Hz)			0.04–0.05				
Mechanical							
Compressive modulus, 10 ³ lb·in ⁻²							

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	26–30	12	18–32	25–31	26–70	22–31	22.5–34.6
Elongation at break, %	0.4–0.8	3–4	1.5–2.0	0.4–0.8	0.2	1–2	0.1–0.5
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	1000–1200	500–590	700–1500	1000–1200	2000–33000	900–1300	1000–2000
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	8–10	14	11–17	7–14	15–60	5.5–11	11–14
Hardness, Rockwell (or Shore)	E95–E100	M72–M76	M93–M120	M100–M115	E54–E101	M95–M115	E88
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	11–21	80–256	13–21	11–32	27–960	21–59	14–19
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	800–1700	510–580	700–1500	800–1700	1900–3300		2400
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	6–8	9	6–9	5–9	7–18	3.5–6.5	6–9.7
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$			12–15				
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$			Self-extinguishing				
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	10–40	66	68	30–45	8–21	20–31	19–26
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$	140–154	73	74–80	149–188	177–316	149–177	320–246
Maximum recommended service temperature, $^\circ\text{C}$							
Specific heat, $\text{cal} \cdot \text{g}^{-1}$							
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.17–0.30	0.26	0.15	0.17–0.34	0.34–0.59	0.25–0.38	0.42–0.57

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Polyamide						
	Nylon 6				Nylon 6/6		Nylon 6/6- nylon 6 copolymer
	Molding and extrusion	30–35% glass- fiber- reinforced	High-impact copolymer	Molding	33% glass- fiber- reinforced	Molybdenum disulfide- filled	
Physical							
Melting temperature, °C							
Crystalline	216	216	216	265	265	265	240
Amorphous							
Specific gravity	1.12–1.14	1.35–1.42	1.08–1.17	1.13–1.15	1.38	1.15–1.17	1.08–1.14
Water absorption (24 h), %	2.9	1.2	1.3–1.5	1.0–1.3	1.0	0.8–1.1	1.5–2.0
Dielectric strength, kV • mm ^{−1}	15.8	15.8	22	24		14	15.8
Electrical							
Volume (dc) resistivity, ohm-cm	10 ¹²			10 ¹² –10 ¹⁵			10 ¹⁰
Dielectric constant (60 Hz)	9.8			4.0			16
Dielectric constant (10 ⁶ Hz)	3.7			3.6			4
Dissipation (power) factor (60 Hz)	0.14			0.01–0.02			0.4
Dissipation factor (10 ⁶ Hz)	0.12			0.02–0.03			0.1
Mechanical							
Compressive modulus, 10 ³ lb • in ^{−2}	250						

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	13–16	19		15 (yield)	24.9	12.5	
Elongation at break, %	30–100	3–6	150–270	60	3	15	40
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	390	1500	110–320	420	1300	450	150–410
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	14	33	5–12	17	41	17	
Hardness, Rockwell (or Shore)	R119	M101	R81–R110	R120	M100	R119	R119
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	32–53	160	96 to no break	43–53	117	240	37
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	380	1450				550	150–410
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	11.8	25	7.5–11	12	28	13.7	7.4–12.4
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$	8			8			
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$	Self-extinguishing	Self-extinguishing	Self-extinguishing	Self-extinguishing	Self-extinguishing	Self-extinguishing	Self-extinguishing
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	80–90	20–30	30–40	80	15–20	54	
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$	68–85	210	45–54	75	249	127	77
Maximum recommended service temperature, $^\circ\text{C}$	107			135			
Specific heat, $\text{cal} \cdot \text{g}^{-1}$	0.4			0.4			
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.24	0.24		0.24	0.22		

TABLE 10.2 Properties of Commercial Plastics (continued)

Properties	Polyamide						Poly(amide-imide), unfilled
	Nylon 6/9, molding and extrusion	Nylon 6/12		Nylon 11, molding and extrusion	Nylon 12, molding and extrusion	Aromatic nylon (aramid), molded and unfilled	
		Molding	30–35% glass-fiber-reinforced				
Physical							
Melting temperature, °C							
Crystalline	205	217	217	194	179	275	275
Amorphous							
Specific gravity	1.08–1.10	1.06–1.08	1.31–1.38	1.03–1.05	1.01–1.02	1.30	
Water absorption (24h), %	0.5	0.4	0.2	0.3	0.25	0.6	
Dielectric strength, kV·mm ^{−1}	24	16	21	17	18	31	24
Electrical							
Volume (dc) resistivity, ohm-cm		10 ¹⁵			10 ¹⁴		
Dielectric constant (60Hz)		4.0			3.8		
Dielectric constant (10 ⁶ Hz)		3.5			3.0		
Dissipation (power) factor (60Hz)		0.02			0.07		
Dissipation factor (10 ⁶ Hz)		0.02			0.04		
Mechanical							
Compressive modulus, 10 ³ lb·in ^{−2}				180		290	413

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$		2.4			7.5	30	40
Elongation at break, %	1 125	150	4	300	300	5	12–18
Flexural modulus at 23 °C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	290	290	1 120	150	165	640	664
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$					1.5	25.8	30
Hardness, Rockwell (or Shore)	R111	R114	E40–E50	R108	R106–R109	E90	E78
Impact strength (Izod) at 23 °C, $\text{J} \cdot \text{m}^{-1}$	59	53	139	96	107–300	75	133
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	275	290	1 200	185	180		730
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	8.5	8.8	24	8	8–9	17.5	26.9
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$		8.8					
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$				Self-extinguishing			
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$		90		55–100	67–100	40	36
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), °C	57–60	82	93–218	54	54	260	274
Maximum recommended service temperature, °C				100–120			260
Specific heat, $\text{cal} \cdot \text{g}^{-1}$		0.4		0.58			
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$		0.22		0.34	0.22	0.22	0.25

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Poly(aryl ether), unfilled	Polycarbonate		Thermoplastic polyester			
		Low viscosity	30% glass-fiber- reinforced	Poly(butylene terephthalate)		Poly(ethylene terephthalate)	
				Unfilled	30% glass-fiber- reinforced	Unfilled	30% glass-fiber- reinforced
Physical							
Melting temperature, °C							
Crystalline				232–267	232–267	245	245
Amorphous	160	140	150				
Specific gravity	1.14	1.2	1.4	1.31–1.38	1.52	1.34–1.39	1.27
Water absorption (24 h), %	0.25	0.15	0.14	0.08–0.09	0.06–0.08	0.1–0.2	0.05
Dielectric strength, $\text{kV} \cdot \text{mm}^{-1}$	17	15	19	16–22	18–22		22
Electrical							
Volume (dc) resistivity, ohm-cm		2×10^{16}	$> 10^{16}$		10^{16}	10^{16}	
Dielectric constant (60 Hz)		3.17	3.35				
Dielectric constant (10^6 Hz)		2.96	3.31			3.25	
Dissipation (power) factor (60 Hz)		0.0009	0.011				
Dissipation factor (10^6 Hz)		0.010	0.007				
Mechanical							
Compressive modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$		350	1300				

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$		12.5	18	8.6–14.5	18–23.5	11–15	25
Elongation at break, %	80	110	3–5	50–300	2–4	50–300	3
Flexural modulus at 23 °C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	300	340	1 100	330–400	1 100–1 200	35–450	1 440
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	11	13.5	23	12–16.7	26–29	14–18	33.5
Hardness, Rockwell (or Shore)	R117	M70	M92	M68–M78	M90	M94–M101	M100
Impact strength (Izod) at 23 °C, $\text{J} \cdot \text{m}^{-1}$	427	14	107	43–53	69–85	13–32	101
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	320	345	1 250	280	1 300	400–600	1 440
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	7.5	9.5	19	8.2	17–19	8.5–10.5	23
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$		9.0					
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$		Self-extinguishing	Self-extinguishing				
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	65	68	22	60–95	25	65	29
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), °C	149	138–145	146	50–85	220	38–41	224
Maximum recommended service temperature, °C		143					
Specific heat, $\text{cal} \cdot \text{g}^{-1}$		0.3				0.27	
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.30	0.20	0.22	0.18–0.30	0.30	0.15	

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Thermoplastic polyester		Thermosetting and alkyd polyester				Polyimide, unfilled
	Aromatic polyester		Unsaturated polyester		Alkyd molding compounds		
	Extrusion-transparent	Injection molding	Styrene–maleic acid copolymer, low-shrink	Butadiene–maleic acid copolymer	Putty, mineral-filled	Glass-fiber-reinforced	
Physical	81	1.39 0.01 14	Thermoset	Thermoset	Thermoset	Thermoset	310–365 1.36–1.43 0.24 22
Melting temperature, °C							
Crystalline							
Amorphous							
Specific gravity							
Water absorption (24 h), %							
Dielectric strength, kV·mm ^{−1}							
Electrical							
Volume (dc) resistivity, ohm-cm							> 10 ¹⁶
Dielectric constant (60 Hz)							3–4
Dielectric constant (10 ⁶ Hz)							
Dissipation (power) factor (60 Hz)							
Dissipation factor (10 ⁶ Hz)							
Mechanical							
Compressive modulus, 10 ³ lb·in ^{−2}					2000–3 000		
Compressive strength, rupture or 1% yield, 10 ³ lb·in ^{−2}		10	15–30	14–30	12–38	15–36	30–40

Elongation at break, %	225	7–10	3–5				8–10
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	290	700	1 000–2 500		2 000	2 000	450–500
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	10.6	12	9–35	16–24	6–17	8.5–26	19–28.8
Hardness, Rockwell (or Shore)	R105		40–70 (Barcol)	50–60 (Barcol)	E98	E95	E52–E99
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	101		133–800	214–694	16–27	27–854	80
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$		300	1 000–2 500	1 500–2 500	500–3 000		300
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	6	11	4.5–20	5–10	3–9	4–9.5	10.5–17.1
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$	7						12.5
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$							
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$		29	6–30		20–50	15–33	45–56
Deflection temperature under flexural load (264 $\text{lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$	63	282	190–260	160–177	177–260	204–260	277–360
Maximum recommended service temperature, $^\circ\text{C}$							
Specific heat, $\text{cal} \cdot \text{g}^{-1}$							0.27
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$		0.29		0.76–0.93	0.51–0.89	0.6–0.89	0.10–0.11

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Poly(methyl pentene), unfilled	Polyolefin					
		Polyethylene					
		Low-density	Medium-density	High-density	Ultra high- molecular- weight	Glass-fiber- reinforced, high-density	Ethylene- vinyl acetate copolymer
Physical							
Melting temperature, °C							
Crystalline	230–240						65–90
Amorphous		95–130	120–140	120–140	125–135	120–140	
Specific gravity	0.84	0.910–0.925	0.926–0.94	0.941–0.965	0.94	1.28	0.92–0.95
Water absorption (24 h), %	0.01	< 0.01	< 0.01	< 0.01	< 0.01	0.02	0.05–0.13
Dielectric strength, kV • mm ⁻¹		18–39	18–39	18–39	28	20	24–30
Electrical							
Volume (dc) resistivity, ohm-cm		> 10 ¹⁵	> 10 ¹⁵	< 10 ¹⁵			
Dielectric constant (60 Hz)		2.3	2.3	2.3			
Dielectric constant (10 ⁶ Hz)		2.3	2.3	2.3			
Dissipation (power) factor (60 Hz)		< 0.0005	< 0.0005	< 0.0005			
Dissipation factor (10 ⁶ Hz)		< 0.0005	< 0.0005	< 0.0005			
Mechanical							
Compressive modulus, 10 ³ lb • in ⁻²	114–171						

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	5–6.6			2.7–3.6		7	
Elongation at break, %	10–50	90–800	50–600	20–130	450–525	1.5	550–900
Flexural modulus at 23 °C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	110–260	8–60	60–115	100–260	130–140	800	1–20
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	4–6.5					11	
Hardness, Rockwell (or Shore)	L67–L74	(D40–D51)	(D50–D60)	R30–R50	R50	R75	
Impact strength (Izod) at 23 °C, $\text{J} \cdot \text{m}^{-1}$	16–64	No break	27–854	27–1 068	No break	59	No break
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	160–280	14–38	25–55	60–180			20–120
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	3.5–4	0.6–2.3	1.2–3.5	3.1–5.5	5.6	9	1.4–2.8
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$		0.8–1.2	1.0–2.2	3–4	3.1–4.0		
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$		1.0	1.0	1.0			
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	117	100–220	140–160	110–130	130	48	160–200
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), °C	41	32–41	41–49	43–54	43–49	121	34
Maximum recommended service temperature, °C	175	70	93	200			
Specific heat, $\text{cal} \cdot \text{g}^{-1}$		0.55	0.55	0.46–0.55			
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.17	0.34	0.34–0.42	0.46–0.51		0.46	

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties		Polyolefin				Poly(phenylene sulfide)	
		Polypropylene				Injection molding	40% glass-fiber-reinforced
		Homopolymer	Copolymer	Impact copolymer	Polyallomer		
Physical							
Melting temperature, °C							
Crystalline	126	168	160–168		120–135	290	290
Amorphous							
Specific gravity	0.91–0.925	0.90–0.91	0.89–0.905	0.90	0.90	1.3	1.6
Water absorption (24h), %	0.01–0.02	0.01–0.03	0.03	< 0.03	< 0.01	< 0.02	0.05
Dielectric strength, kV·mm ⁻¹	18	24	24	24	31	15	18
Electrical							
Volume (dc) resistivity, ohm-cm		10 ¹⁷	10 ¹⁷	10 ¹⁷			
Dielectric constant (60 Hz)		2.2–2.6	2.3				
Dielectric constant (10 ⁶ Hz)		2.2–2.6	2.3	2.3			
Dissipation (power) factor (60 Hz)		< 0.0005	0.0001–0.0005				
Dissipation factor (10 ⁶ Hz)		0.0005–0.002	0.0001–0.002	0.0003			
Mechanical							
Compressive modulus, 10 ³ lb·in ⁻²	31	150–300					

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$		5.5–8.0	3.5–8.0			16	21
Elongation at break, %	300–380	100–600	200–700	8–20	400–500	1–2	1
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	45–50	170–250	130–200	130–190	70–110	550	1700
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	2–2.3	6–8	5–7			14	29
Hardness, Rockwell (or Shore)		R80–R102	R50–R96	R40–R90	R50–R85	R123	R123
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	No break	21–53	53–1068	80–900	91–203	< 27	75
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	30–40	165–225	100–170			480	1100
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	3.8–4.4	4.5–6	4–5.5		3–3.8	9.5	19.5
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$	1.7–2.5	4.5–5.4	3.5–4.3	2.5–3.1	3–3.4		
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$							
Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$	128–150	81–100	68–95	60–90	83–100	49	22
Deflection temperature under flexural load (264 $\text{lb} \cdot \text{in}^{-2}$), °C	54–60	48–57	45–57	90–105 (66 $\text{lb} \cdot \text{in}^{-2}$)	51–56	135	249
Maximum recommended service temperature, °C		160	240	140–160			
Specific heat, $\text{cal} \cdot \text{g}^{-1}$		0.44–0.46	0.45–0.50	0.45–0.50			
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.22	0.12	0.15–0.17	0.12–0.17	0.09–0.17	0.29	0.29

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Polyurethane			Silicone			Styrenic
	Casting resin		Thermoplastic elastomer	Cast resin, flexible	Mineral- and/or glass-filled	Epoxy molding and encapsulating compound	Polystyrene
	Liquid	Unsaturated					Crystal
Physical							
Melting temperature, °C							
Crystalline	Thermoset	Thermoset	120–160	Thermoset	Thermoset	Thermoset	85–105
Amorphous							
Specific gravity	1.1–1.5	1.05	1.05–1.25	0.99–1.5	1.8–1.94	1.84	1.04–1.05
Water absorption (24h), %	0.02–1.5	0.1–0.2	0.7–0.9				0.03–0.10
Dielectric strength, $\text{kV} \cdot \text{mm}^{-1}$	12–20		13–25	22	8–15	10	24
Electrical							
Volume (dc) resistivity, ohm-cm	10 ¹¹ –10 ¹⁵		10 ¹¹ –10 ¹³	10 ¹⁴ –10 ¹⁵			> 10 ¹⁶
Dielectric constant (60Hz)							
Dielectric constant (10 ⁶ Hz)							
Dissipation (power) factor (60Hz)							
Dissipation factor (10 ⁶ Hz)							
Mechanical							
Compressive modulus, 10 ³ lb·in ⁻²	10–100		4–9				

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	20		20		10–16	28	11.5–16
Elongation at break, %	100–1 000	3–6	100–1 100	100–700			1–2
Flexural modulus at 23 °C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	10–100	610	10–350		1 000–2 500		380–450
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	0.7–4.5	19	0.7–9 (A65–D80)	(A15–A65)	9–14 M80–M90	17	8–14 M60–M75
Hardness, Rockwell (or Shore) Impact strength (Izod) at 23 °C, $\text{J} \cdot \text{m}^{-1}$	1 334 to flexible	21	No break		13–427	16	13–21
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	10–100		10–350				350–485
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	0.175–10	10–11	1.5–8.4	0.35–1.0	4–6.5	6–8	5.3–7.9
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$							
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$					0–78		
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	100–200		100–200	300–800	20–50	30	70–80
Deflection temperature under flexural load (264 $\text{lb} \cdot \text{in}^{-2}$), °C	Varies over wide range	87–93	Varies over wide range		260	74–100	
Maximum recommended service temperature, °C					371		93
Specific heat, $\text{cal} \cdot \text{g}^{-1}$	0.43		0.43				0.3
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.21		0.07–0.31	0.15–0.31	0.30	0.68	0.09–0.13

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Styrenic						
	Polystyrene		Acrylonitrile-butadiene-styrene copolymer				
	Heat-resistant	Extrusion	Molding				
			Heat-resistant	High-impact	Flame-retarded	Platable	20% glass-reinforced
Physical							
Melting temperature, °C							
Crystalline							
Amorphous	110–125	88–120	110–125	100–110	110–125	100–110	
Specific gravity	1.05–1.09	1.02–1.06	1.05–1.08	1.01–1.04	1.16–1.21	1.06–1.07	1.22
Water absorption (24h), %	0.03–0.12	0.20–0.45	0.20–0.45	0.20–0.45	0.2–0.6		
Dielectric strength, kV · mm ⁻¹	20	14–20	14–20	14–20	14–20	16–22	18
Electrical							
Volume (dc) resistivity, ohm-cm							
Dielectric constant (60Hz)				2.4–5.0			
Dielectric constant (10 ⁶ Hz)				2.4–3.8			
Dissipation (power) factor (60Hz)				0.003–0.008			
Dissipation factor (10 ⁶ Hz)				0.007–0.015			
Mechanical							
Compressive modulus, 10 ³ lb · in ⁻²		150–390	190–440	140–300	130–310		

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	11.5–16	5.2–10	7.2–10	4.5–8	6.5–7.5		14
Elongation at break, %	2–60	20–100	3–20	5–70	5–25		
Flexural modulus at 23 °C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	340–470	130–420	300–400	250–350	300–400	340–390	710
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	8.9–14	4–14	10–13	8–11	9–14	10.5–11.5	15.5
Hardness, Rockwell (or Shore)	L80–L108	R75–R115	R100–R115	R85–R105	R100–R120	R103–R109	M85
Impact strength (Izod) at 23 °C, $\text{J} \cdot \text{m}^{-1}$	21–181	133–640	107–347	347–400	160–640	267–283	64
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	320–460	130–380	300–350	230–330	320–400	330–380	740
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	5–7.8	2.5–8.0	6–7.5	4.8–6.3	5–8	6–6.4	11
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$			5.5–7	4–5.5	4–6		
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$		1.3		1.3			
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	60–70	60–130	60–93	95–110	65–95	47–53	21
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), °C	93–120	77–104 annealed	104–116 annealed	96–102 annealed	90–107 annealed	96–102 annealed	99
Maximum recommended service temperature, °C				110			
Specific heat, $\text{cal} \cdot \text{g}^{-1}$				0.3–0.4			
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$			0.19–0.34				

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Styrenic			Sulfone			
	Styrene-acrylonitrile copolymer		Styrene–butadiene copolymer, high-impact	Polysulfone			
	Unfilled	20% glass-fiber-reinforced		Unfilled	20% glass-fiber-reinforced	Poly(ether sulfone)	Poly(phenyl sulfone)
Physical							
Melting temperature, °C							
Crystalline							
Amorphous	115–125	115–125	90–110	200	200	230	220
Specific gravity	1.07–1.08	1.22	1.03–1.06	1.24	1.46	1.37	1.29
Water absorption (24 h), %	0.2–0.3	0.15–0.20	0.05–0.10	0.22	0.23	0.43	1.1–1.3 (saturated)
Dielectric strength, $\text{kV} \cdot \text{mm}^{-1}$	16–20	20	18	17	17	17	16
Electrical							
Volume (dc) resistivity, ohm-cm				10^{15}			
Dielectric constant (60 Hz)				3.14	3.7		
Dielectric constant (10^6 Hz)				3.26	3.7		
Dissipation (power) factor (60 Hz)				0.004	0.002		
Dissipation factor (10^6 Hz)				0.008	0.009		
Mechanical							
Compressive modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	530			370			

Compressive strength, rupture of 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	14–17	19	4–9	13.9	22		
Elongation at break, %	1–4	1–2	13–50	50–100	2	30–80	60
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	550	100–1 100	280–450	390	1 000	375	330
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	14–17	20	5.3–9.4	15.4	23	18.7	12.4
Hardness, Rockwell (or Shore)	M80–M90	R 122	M10–M68	M69, R 120	R 123	M88	
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	19–27	53	32–192	64	59	85	640
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$	400–560	1 150–1 200	280–465	360	1 200	350	310
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	9–12	15.8–18	3.2–4.9		17		
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$			2.9–4.9	10.2		12.2	10.4
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$							
Coefficient of linear thermal expansion, $10^{-6} \text{ }^\circ\text{C}^{-1}$	36–38	38–40	70–101	52–56	25	55	31
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$	88–104	99	74–93	174	182	203	204
Maximum recommended service temperature, $^\circ\text{C}$				149			
Specific heat, $\text{cal} \cdot \text{g}^{-1}$							
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.12	0.26–0.28	0.12–0.21	0.12	0.38	0.14–0.19	

TABLE 10.2 Properties of Commercial Plastics (*continued*)

Properties	Thermoplastic elastomers				Urea formaldehyde, alpha-cellulose filled	Vinyl	
	Polyolefin	Polyester	Block copolymers of styrene and butadiene or styrene and isoprene	Block copolymers of styrene and ethylene or styrene and butylene		Poly(vinyl chloride) and poly(vinyl acetate)	
						Rigid	Flexible and unfilled
Physical							
Melting temperature, °C							
Crystalline		168–206			Thermoset		
Amorphous						75–105	75–105
Specific gravity	0.88–0.90	1.17–1.25	0.9–1.2	0.9–1.2	1.47–1.52	1.30–1.58	1.16–1.35
Water absorption (24 h), %	0.01		0.19–0.39		0.4–0.8	0.04–0.4	0.15–0.75
Dielectric strength, kV•mm ^{−1}	24–26		16–21		12–16	14–20	12–16
Electrical							
Volume (dc) resistivity, ohm-cm					0.5–5.0	10 ¹² –10 ¹⁵	10 ¹¹ –10 ¹⁴
Dielectric constant (60 Hz)					7.7–9.5	3.2–4.0	5.0–9.0
Dielectric constant (10 ⁶ Hz)					6.7–8.0	3.0–4.0	3.0–4.0
Dissipation (power) factor (60 Hz)					0.036–0.043	0.01–0.02	0.03–0.05
Dissipation factor (10 ⁶ Hz)					0.025–0.035	0.006–0.02	0.06–0.1
Mechanical							
Compressive modulus, 10 ³ lb•in ^{−2}			3.6–120				

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$					25–45	8–13	0.9–1.7
Elongation at break, %	150–300	350–450	500–1 350	600–800	< 1	40–80	200–450
Flexural modulus at 23°C, $10^3 \text{ lb} \cdot \text{in}^{-2}$	1.5–2.0	7–75	4–150	4–100	1 300–1 600	300–500	
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$					10–18	10–16	
Hardness, Rockwell (or Shore)	(A65–A92)	(D40–D72)	(A40–A90)	(A50–A90)	M110–M120	(D65–D95)	(A50–A100)
Impact strength (Izod) at 23°C, $\text{J} \cdot \text{m}^{-1}$	No break	208 to no break	No break	No break	13–21	21–1068	Varies over wide range
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$		1.1–2.5	0.8–50		1 000–1 500	350–600	
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	0.65–2.0	3.7–5.7	0.6–3.0	1–3	5.5–13	6–75	1.5–3.5
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$							
Thermal							
Burning rate, $\text{mm} \cdot \text{min}^{-1}$					Self-extinguishing	Self-extinguishing	Slow to self-extinguishing
Coefficient of linear thermal expansion, $10^{-6} \text{ } ^\circ\text{C}^{-1}$	130–170		130–137		22–36	50–100	70–250
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$			< 0–49		127–143	60–77	
Maximum recommended service temperature, $^\circ\text{C}$					77	70–74	80–105
Specific heat, $\text{cal} \cdot \text{g}^{-1}$					0.6	0.2–0.28	0.36–0.5
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.19–0.21		0.15		0.30–0.42	0.15–0.21	0.13–0.17

TABLE 10.2 Properties of Commercial Plastics (*continued*)

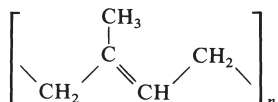
Properties	Poly(vinyl chloride) and poly(vinyl acetate)	Vinyl					
		Poly(vinyl chloride), 15% glass-fiber-reinforced	Poly(vinylidene chloride)	Poly(vinyl formal)	Chlorinated poly(vinyl chloride)	Poly(vinyl butyral), flexible	
	Flexible and filled						
Physical							
Melting temperature, °C							
Crystalline			210				
Amorphous	75–105	75–105		105	110	49	
Specific gravity	1.3–1.7	1.54	1.65–1.72	1.2–1.4	1.49–1.56	1.05	
Water absorption (24 h), %	0.5–1.0	0.01	0.1	0.5–3.0	0.02–0.15	1.0–2.0	
Dielectric strength, kV·mm ⁻¹	9.8–12	24–31	16–24	19		14	
Electrical							
Volume (dc) resistivity, ohm-cm			10 ¹⁴ –10 ¹⁶				
Dielectric constant (60 Hz)			4.5–6.0				
Dielectric constant (10 ⁶ Hz)							
Dissipation (power) factor (60 Hz)							
Dissipation factor (10 ⁶ Hz)							
Mechanical							
Compressive modulus, 10 ³ lb·in ⁻²					335–600		

Compressive strength, rupture or 1% yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$	1.0–1.8	9	2–2.7		9–22	
Elongation at break, %	200–400	2–3	50–250	5–20	4–65	150–450
Flexural modulus at 23°C , $10^3 \text{ lb} \cdot \text{in}^{-2}$		750			380–450	
Flexural strength, rupture or yield, $10^3 \text{ lb} \cdot \text{in}^{-2}$		13.5	4.2–6.2	17–18	14.5–17	
Hardness, Rockwell (or Shore)	(A50–A100)	R118	M50–M65	M85	R117–R122	A10–A100
Impact strength (Izod) at 23°C , $\text{J} \cdot \text{m}^{-1}$	Varies over wide range	53	16–53	43–75	53–299	Varies over wide range
Tensile modulus, $10^3 \text{ lb} \cdot \text{in}^{-2}$		870	50–80	350–600	360–475	
Tensile strength at break, $10^3 \text{ lb} \cdot \text{in}^{-2}$	1–3.5	9.5	3–5	10–12	7.5–9	0.5–3.0
Tensile yield strength, $10^3 \text{ lb} \cdot \text{in}^{-2}$						
Thermal						
Burning rate, $\text{mm} \cdot \text{min}^{-1}$			Self-extinguishing			Slow
Coefficient of linear thermal expansion, $10^{-6}/^\circ\text{C}$			190	64	68–78	
Deflection temperature under flexural load ($264 \text{ lb} \cdot \text{in}^{-2}$), $^\circ\text{C}$		68	54–71	71–77	94–112	
Maximum recommended service temperature, $^\circ\text{C}$			100			
Specific heat, $\text{cal} \cdot \text{g}^{-1}$			0.32			
Thermal conductivity, $\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	0.13–0.17		0.13	0.16	0.14	

FORMULAS AND ADVANTAGES OF RUBBERS

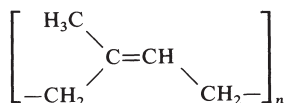
Gutta Percha

Gutta percha is a natural polymer of isoprene (3-methyl-1,3-butadiene) in which the configuration around each double bond is *trans*. It is hard and horny and has the following formula:



Natural Rubber

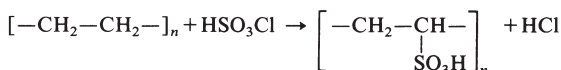
Natural rubber is a polymer of isoprene in which the configuration around each double bond is *cis* (or *Z*):



Its principal advantages are high resilience and good abrasion resistance.

Chlorosulfonated Polyethylene

Chlorosulfonated polyethylene is prepared as follows:



Cross-linking, which can occur as a result of side reactions, causes an appreciable gel content in the final product.

The polymer can be vulcanized to give a rubber with very good chemical (solvent) resistance, excellent resistance to aging and weathering, and good color retention in sunlight.

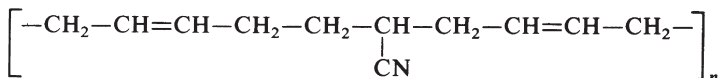
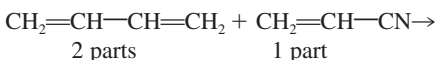
Epichlorohydrin

Epichlorohydrin is a product of covulcanization of epichlorohydrin (epoxy) polymers with rubbers, especially *cis*-polybutadiene.

Its advantages include impermeability to air, excellent adhesion to metal, and good resistance to oils, weathering, and low temperature.

Nitrile Rubber (NBR, GRN, Buna N)

Nitrile rubber can be prepared as follows:

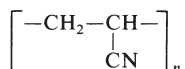


Nitrile rubber is also known as nitrile–butadiene rubber (NBR), government rubber nitrile (GRN), and Buna N.

It possesses resistance to oils up to 120°C and excellent abrasion resistance and adhesion to metal.

Polyacrylate

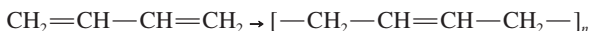
Polyacrylate has the following formula:



It possesses oil and heat resistance to 175°C and excellent resistance to ozone.

cis-Polybutadiene Rubber (BR)

cis-Polybutadiene is prepared by polymerization of butadiene by mostly 1,4-addition.

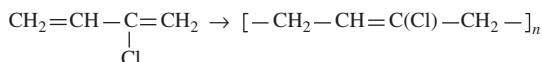


The polybutadiene produced is in the *Z* (or *cis*) configuration.

cis-Polybutadiene has good abrasion resistance, is useful at low temperature, and has excellent adhesion to metal.

Polychloroprene (Neoprene)

Polychloroprene is prepared as follows:



It has very good weathering characteristics, is resistant to ozone and to oil, and is heat-resistant to 100°C.

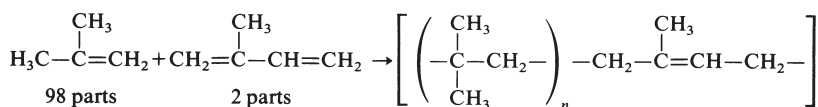
Ethylene–Propylene–Diene Rubber (EPDM)

Ethylene–propylene–diene rubber is polymerized from 60 parts ethylene, 40 parts propylene, and a small amount of nonconjugated diene. The nonconjugated diene permits sulfur vulcanization of the polymer instead of using peroxide.

It is a very lightweight rubber and has very good weathering and electrical properties, excellent adhesion, and excellent ozone resistance.

Polyisobutylene (Butyl Rubber)

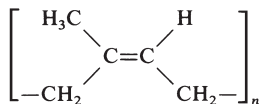
Polyisobutylene is prepared as follows:



It possesses excellent ozone resistance, very good weathering and electrical properties, and good heat resistance.

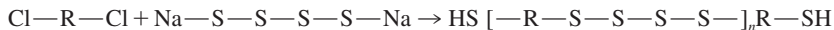
(Z)-Polyisoprene (Synthetic Natural Rubber)

Polymerization of isoprene by 1,4-addition produces polyisoprene that has a *cis* (or *Z*) configuration.



Polysulfide Rubbers

Polysulfide rubbers are prepared as follows:



where R can be



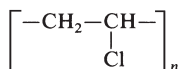
or



Polysulfide rubbers possess excellent resistance to weathering and oils and have very good electrical properties.

Poly(vinyl chloride) (PVC)

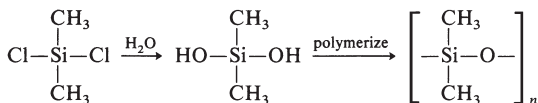
Poly(vinyl chloride) as previously discussed under “Formulas and Key Properties of Plastic Materials” has the following structures:



PVC polymer plus special plasticizers are used to produce flexible tubing which has good chemical resistance.

Silicone Rubbers

Silicone rubbers are prepared as follows:

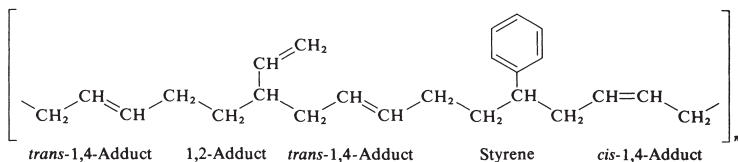


Other groups may replace the methyl groups.

Silicone rubbers have excellent ozone and weathering resistance, good electrical properties, and good adhesion to metal.

Styrene–Butadiene Rubber (GRS, SBR, Buna S)

Styrene–butadiene rubber is prepared from the free-radical copolymerization of one part by weight of styrene and three parts by weight of 1,3-butadiene. The butadiene is incorporated by both 1,4-addition (80%) and 1,2-addition (20%). The configuration around the double bond of the 1,4-adduct is about 80% *trans*. The product is a random copolymer with these general features:



Styrene–butadiene rubber (SBR) is also known as government rubber styrene (GRS) and Buna S.

Urethane

See Table 10.3.

TABLE 10.3 Properties of Natural and Synthetic Rubbers

Rubber	Specific gravity	Durometer hardness (or Shore)	Ultimate elongation % (23 °C)	Tensile strength, lb·in ⁻² (23 °C)	Service temperature, °C	
					Minimum	Maximum
Gutta percha (hard rubber)	1.2–1.95	(65–95)	3–8	4000–1 0,000		104
Natural rubber (NR)	0.93	20–100	750–850	3000–4500	–56	82
Chlorosulfonated polyethylene	1.10	50–95	100–500	500–3000	–54	121
Epichlorohydrin	1.27	60–90	100–400	1000–2500	–46	121
Fluoroelastomers	1.4–1.95	60–90	100–350	2000–3000	–40	232
Isobutene–isoprene rubber (IIR) [also known as government rubber I (GR-I)]	0.91	(40–70)	750–950	2300–3000		121
Nitrile rubber (butadiene–acrylonitrile rubber) (also known as Buna N and NBR)	1.00	30–100	100–600	500–4000	–54	121
Polyacrylate	1.10	40–100	100–400	1000–2200	–18	149
Polybutadiene rubber (BR)	0.93	30–100	100–700	2500–3000	–62	79–100
Polychloroprene (neoprene)	1.23	20–90	800–1000	2000–3500	–54	121
Poly(ethylene–propylene–diene) (EPDM)	0.85	30–100	100–300	1000–3000	–40	149
Polyisobutylene (butyl rubber)	0.92	30–100	100–700	1000–3000	–54	100
Polyisoprene	0.94	20–100	100–750	2000–3000	–54	79–82
Polysulfide (Thiokol ST)	1.34	20–80	100–400	700–1250	–54	82–100
Poly(vinyl chloride) (Koroseal)	1.32	(80–90)		2400–3000		71
Silicone, high-temperature				700–800		316
Silicone	0.98	20–95	50–800	500–1500	–84	232
Styrene–butadiene rubber (SBR) (also known as Buna S)	0.94	40–100	400–600	1600–3700	–60	107
Urethane	0.85	62–95	100–700	1000–8000	–54	100

CHEMICAL RESISTANCE

TABLE 10.4 Resistance of Selected Polymers and Rubbers to Various Chemicals at 20°C

The information in this table is intended to be used only as a general guide. The chemical resistance classifications are E = excellent (30 days of exposure causes no damage), G = good (some damage after 30 days), F = fair (exposure may cause crazing, softening, swelling, or loss of strength), N = not recommended (immediate damage may occur).

	Chemical												
	Acids, dilute or weak	Acids, strong and concentrated	Alcohols, aliphatic	Aldehydes	Alkalies, concentrated	Esters	Ethers	Glycols	Hydrocarbons, aliphatic	Hydrocarbons, aromatic	Hydrocarbons, halogenated	Ketones	Oxidizing agents, strong
Polymers													
Acetals	F	N	F	N	N	N	N	G	N	N	N	N	N
Acrylics: poly(methyl methacrylate)	G	N	E		N	N	E	E	G	N	N	N	N
Allyls: diallyl phthalate	G				N				E	G	G	N	
Cellulosics: cellulose-acetate–butyrate and cellulose–acetate–propionate polymers	F	N	N	N	N	N	N	G	F	N	N	N	
Fluorocarbons	E	E	E	E	E	E	E	E	E	E	E	E	E
Polyamides	N	N	G	E	E	G		G	G	F	F	G	N
Polycarbonates	G	N	G	F	N	N	N	G	N	N	N	N	N
Polyesters	G	G	N		N	N	F	G	G	F	F	N	F
Poly(methyl pentene)	E	E	G	G	E	G	N	E	F	G	N	F	F
Low-density polyethylene	E	E	E	G	E	G	N	E	F	F	N	G	F
High-density polyethylene	E	E	E	E	E	G	N	E	G	G	N	G	F
Polybutadiene	G	F	E							E	E	E	

TABLE 10.4 Resistance of Selected Polymers and Rubbers to Various Chemicals at 20°C (*continued*)

	Chemical												
	Acids, dilute or weak	Acids, strong and concentrated	Alcohols, aliphatic	Aldehydes	Alkalies, concentrated	Esters	Ethers	Glycols	Hydrocarbons, aliphatic	Hydrocarbons, aromatic	Hydrocarbons, halogenated	Ketones	Oxidizing agents, strong
Polymers (<i>continued</i>)													
APolypropylene and polyallomer	E	E	E	E	E	G	N	E	G	F	N	G	F
Polystyrene	N	N	E		N	N		E	N	N	N	N	N
Styrene–acrylonitrile copolymers			N		N			F	N				
Styrene–acrylonitrile–butadiene copolymers		N	G		G	N			F	N	N	N	
Sulfones: polysulfone	G	N	F	F	E	N	F	G	F	N	N	N	G
Vinyls: poly(vinyl chloride)	E	G	E	G	G	N	F	F	G	N	N	N	G
Rubbers													
Natural rubber			E			N	N	E	N	N	N	N	
Nitrile rubber			E			N	G	E	E	N	N	N	
Polychloroprene			E			N	F	E	F	N	N	N	
Polyisobutylene			E			F	F	E	N	N	N	N	
Polysulfide rubbers: Thiokol			E			E	E	E	E	F	N	N	
Styrene–butadiene rubber			E			N	N	E	N	N	N	N	

TABLE 10.5 Common Abbreviations Used in Polymer Chemistry

Acronym	Expansion
ABA	Acrylonitrile–butadiene–acrylate
ABS	Acrylonitrile–butadiene–styrene copolymer
ABS–PC	Acrylonitrile–butadiene–styrene–polycarbonate alloy
ABS–PVC	Acrylonitrile–butadiene–styrene–poly(vinyl chloride) alloy
ACM	Acrylic acid ester rubber
ACS	Acrylonitrile–chlorinated pe–styrene
AES	Acrylonitrile–ethylene–propylene–styrene
AMMA	Acrylonitrile–methyl methacrylate
AN	Acrylonitrile
APET	Amorphous polyethylene terephthalate
APP	Atactic polypropylene
ASA	Acrylic–styrene–acrylonitrile
BR	Butadiene rubber
BS	Butadiene styrene rubber
CA	Cellulose acetate
CAB	Cellulose acetate–butyrate
CAP	Cellulose acetate–propionate
CN	Cellulose nitrate
CP	Cellulose propionate
CPE	Chlorinated polyethylene
CPET	Crystalline polyethylene terephthalate
CPP	Cast polypropylene
CPVC	Chlorinated polyvinyl chloride
CR	Chloroprene rubber
CTA	Cellulose triacetate
DAM	Diallyl maleate
DAP	Diallyl phthalate
DMT	Terephthalic acid, dimethyl ester
ECTFE	Ethylene–chlorotrifluoroethylene copolymer
EEA	Ethylene–ethyl acrylate
EMA	Ethylene–methyl acrylate
EMAA	Ethylene methacrylic acid
EMAC	Ethylene–methyl acrylate copolymer
EMPP	Elastomer modified polypropylene
EnBA	Ethylene normal butyl acrylate
EP	Epoxy resin, also ethylene–propylene
EPM	Ethylene–propylene rubber
ESI	Ethylene–styrene copolymers
EVA(C)	Polyethylene–vinyl acetate
EVOH	Polyethylene–vinyl alcohol copolymers
FEP	Fluorinated ethylene–propylene copolymers
HDI	Hexamethylene diisocyanate
HDPE	High-density polyethylene
HIPS	High-impact polystyrene
HMDI	Diisocyanato dicyclohexylmethane
IPI	Isophorone diisocyanate
LDPE	Low-density polyethylene
LLDPE	Linear low-density polyethylene
MBS	Methacrylate–butadiene–styrene

TABLE 10.5 Common Abbreviations Used in Polymer Chemistry (*continued*)

Acronym	Expansion
MC	Methyl cellulose
MDI	Methylene diphenylene diisocyanate
MEKP	Methyl ethyl ketone peroxide
MF	Melamine formaldehyde
MMA	Methyl methacrylate
MPEG	Polyethylene glycol monomethyl ether
MPF	Melamine–phenol–formaldehyde
NBR	Nitrile butyl rubber
NDI	Naphthalene diisocyanate
NR	Natural rubber
OPET	Oriented polyethylene terephthalate
OPP	Oriented polypropylene
OSA	Olefin–modified styrene–acrylonitrile
PA	Polyamide
PAEK	Poly(aryl ether–ketone)
PAI	Poly(amide–imide)
PAN	Polyacrylonitrile
PB	Polybutylene
PBAN	Poly(butadiene–acrylonitrile)
PBI	Polybenzimidazole
PBN	Polybutylene naphthalate
PBS	Poly(butadiene–styrene)
PBT	Poly(butylene terephthalate)
PC	Polycarbonate
PCD	Polycarbodiimide
PCT	Poly(cyclohexylene–dimethylene terephthalate)
PCTFE	Polychlorotrifluoroethylene
PE	Polyethylene
PEC	Chlorinated polyethylene
PEG	Poly(ethylene glycol)
PEI	Poly(ether–imide)
PEK	Poly(ether–ketone)
PEN	Polyethylene naphthalate
PES	Polyether sulfone
PET	Polyethylene terephthalate
PF	Phenol–formaldehyde copolymer
PFA	Perfluoroalkoxy resin
PI	Polyimide
PIBI	Poly(isobutylene), Butyl rubber
PMDI	Polymeric methylene diphenylene diisocyanate
PMMA	Poly(methyl methacrylate)
PMP	Poly(methylpentene)
PO	Polyolefins
PP	Polypropylene
PPA	Polyphthalamide
PPC	Chlorinated polypropylene
PPO	Poly(phenylene oxide)
PPS	Poly(phenylene sulfide)
PPSU	Poly(phenylene sulfone)

TABLE 10.5 Common Abbreviations Used in Polymer Chemistry (*continued*)

Acronym	Expansion
PS	Polystyrene
PSF	Polysulfone (also PSU)
PSU	Polysulfone (also PSF)
PTFE	Polytetrafluoroethylene
PU	Polyurethane
PUR	Polyurethane
PVA	Poly(vinyl acetate)
PVAL	Poly(vinyl alcohol)
PVB	poly(vinyl butyrate)
PVC	Poly(vinyl chloride)
PVCA	Poly(vinyl chloride–acetate)
PVDA	Poly(vinylidene acetate)
PVDC	Poly(vinylidene chloride)
PVDF	Poly(vinylidene fluoride)
PVF	Poly(vinyl fluoride)
PVOH	Poly(vinyl alcohol)
SAN	Styrene–acrylonitrile copolymer
SB	Styrene–butadiene copolymer
SBC	Styrene block copolymer
SBR	Styrene butadiene rubber
SMA	Styrene–maleic anhydride (also SMC)
SMC	Styrene–maleic anhydride (also SMA)
TA	Terephthalic acid (also TPA)
TDI	Toluene diisocyanate
TEFE	Ethylene–tetrafluoroethylene copolymer
TPA	Terephthalic acid (also TA)
UF	Urea formaldehyde
ULDPE	Ultralow-density polyethylene
UP	Unsaturated polyester resin
UR	Urethane
VLDPE	Very low-density polyethylene
ZNC	Ziegler-Natta catalyst

GAS PERMEABILITY

TABLE 10.6 Gas Permeability Constants ($10^{10}P$) at 25°C for Polymers and Rubbers

The gas permeability constant P is defined as

$$P = \frac{\text{amount of permeant}}{(\text{area}) \times (\text{time}) \times (\text{driving forced across the film})}$$

The gas permeability constant is the amount of gas expressed in cubic centimeters passed in 1 s through a 1-cm² area of film when the pressure across a film thickness of 1 cm is 1 cmHg and the temperature is 25°C. All tabulated values are multiplied by 10^{10} and are in units of seconds⁻¹ (centimeters of Hg)⁻¹. Other temperatures are indicated by exponents and are expressed in degrees Celsius.

Polymer or rubber	Gas						
	He	N ₂	H ₂	O ₂	CO ₂	H ₂ O	Other
Cellulose (cellophane)	0.005 ²⁰	0.003 2	0.006 5	0.002 1	0.004 7	1 900	0.006 ⁴⁵ (H ₂ S); 0.001 7 (SO ₂)
Cellulose acetate	13.6 ²⁰	0.28 ³⁰	3.5 ²⁰	0.78 ³⁰	22.7 ³⁰	5 500	3.5 ³⁰ (H ₂ S); 17 ⁰ (ethylene oxide); 6.8 ⁶⁰ (bromomethane)
Cellulose nitrate	6.9	0.12	2.0 ²⁰	1.95	2.12	6 290	57.1 (NH ₃); 1.76 (SO ₂)
Ethyl cellulose	400 ³⁰	8.4 ³⁰	87 ²⁰	26.5 ³⁰	41.0 ³⁰	12 000 ²⁰	705 (NH ₃); 204 (SO ₂); 420 ⁰ (ethylene oxide)
Gutta percha		2.17	14.4	6.16	35.4	510	
Natural rubber		9.43	52.0	23.3	15.3	2 290	15.7 (CO); 30.1 (CH ₄); 1.68 (C ₃ H ₈); 98.9 (C ₂ H ₂); 550 (CH ₃ C≡CH); 3.59 (SF ₆)
Nylon 6	0.53 ²⁰	0.009 5 ³⁰		0.038 ³⁰	0.10 ³⁰	177	0.33 ³⁰ (H ₂ S); 1.2 ²⁰ (NH ₃); 0.84 ⁶⁰ (CH ₃ Br)
Nylon 11	1.95 ³⁰		1.78 ³⁰		1.00 ⁴⁰		0.344 ³⁰ (Ne); 0.189 ⁴⁰ (Ar); 13.6 ⁵⁰ (propyne)
Poly(acrylonitrile)				0.000 2	0.000 8	300	

Acrylonitrile–styrene copolymer (66:34)				0.048	0.21	2000	
Poly(1,3-butadiene)		6.42	41.9	19.0	138.0	5070	
Poly(<i>cis</i> -1,4-butadiene)	32.6	19.2					19.2 (Ne); 41.0 (Ar)
Butadiene–acrylonitrile copolymer (80:20)	12.2	1.06	15.9	3.85	30.8		24.8 (C ₂ H ₂); 7.7 (propyne)
Butadiene–styrene copolymer (80:20)	13.4	1.71					5.01 (Ne); 4.49 (Ar)
Butadiene–styrene copolymer (92:8)	22.9	5.11					9.70 (Ne); 12.7 (Ar)
Polychloroprene		1.2	13.6	4.0	25.8		3.79 (Ar); 3.27 (CH ₄)
Polyethylene, low-density	4.9	0.969	12.0 ³⁰	2.88	12.6	90	2.88 (CH ₄); 6.81 (C ₂ H ₆); 9.43 (C ₃ H ₈); 1.48 (CO); 49 ⁰ (ethylene oxide); 14.4 (propene); 42.2 (propyne); 0.170 (SF ₆); 472 ⁶⁰ (CH ₃ Br)
Polyethylene, high-density	1.14	0.143	3.0 ²⁰	0.403	0.36	12.0	0.388 (CH ₄); 0.590 (C ₂ H ₆); 0.537 (C ₃ H ₈); 0.008 3 (SF ₆); 1.69 (Ar); 4.01 (propene)
Poly(ethylene terephthalate)							
Crystalline	1.32	0.006 5	3.70 ²⁰	0.035	0.17	130	0.003 2 (CH ₄); 0.08 ⁶⁰ (CH ₃ Br)
Amorphous	3.28	0.013		0.059	0.30		0.009 (CH ₄)
Poly(ethyl methacrylate)	6.82	0.220		1.15	5.00	3200	2.98 (Ne); 0.565 (Ar); 0.370 (Kr); 3.83 (H ₂ S); 0.000 001 65 (SF ₆)
Isobutene–isoprene copolymer (98:2)	8.38	0.324	7.20	1.30	5.16	110 ³⁸	13.6 ⁵⁰ (C ₃ H ₈)
Isoprene–acrylonitrile copolymer (76:24)	7.77	0.181	7.41	0.852	4.32		

TABLE 10.6 Gas Permeability Constants ($10^{10}P$) at 25°C for Polymers and Rubbers (*continued*)

Polymer or rubber	Gas						
	He	N ₂	H ₂	O ₂	CO ₂	H ₂ O	Other
Isoprene-methacrylonitrile copolymer (76:24)		0.596	13.6	2.34	14.1		
Methacrylonitrile-styrene-butadiene copolymer (88:7:5)				0.0048	0.014	600	
Poly(methylpentene)	101	7.83	136	32.0	92.6		
Polypropylene	38 ²⁰	0.44 ³⁰	41 ²⁰	2.3 ³⁰	9.2 ³⁰	51	0.33 ³⁰ (H ₂ S); 9.2 ²⁰ (NH ₃)
Silicone rubber, 10% filler	233 ⁰	227 ⁰	464 ⁰	489 ⁰	3 240	43 000 ³⁵	191 ⁰ (Ne); 550 ⁰ (Ar); 1 020 ⁰ (Kr); 2 550 ⁰ (Xe); 19 000 ⁰ (butane)
Polystyrene	18.7	0.788	23.3	2.63	10.5	1 200	
Poly(tetrafluoroethylene)		1.4	9.8	4.2	11.7		15.7 (NO ₂); 37.5 (N ₂ O ₄)
Poly(trifluoroethylene)	6.8 ²⁰	0.003	0.94 ²⁰	0.025 ⁴⁰	0.048 ⁴⁰	0.29	1.2 ⁰ (ethylene oxide); 4.6 ⁶⁰ (CH ₃ Br)
Poly(vinyl acetate)	12.6 ³⁰		89 ³⁰	0.50 ³⁰			2.64 ³⁰ (Ne); 0.19 ³⁰ (Ar); 0.078 ³⁰ (Kr); 0.050 ³⁰ (CH ₄)
Poly(vinyl alcohol)	0.001 ³⁰	< 0.001 ¹⁴	0.009	0.0089	0.001 ²³		0.007 (H ₂ S); 0.002 ⁰ (ethylene oxide)
Poly(vinyl chloride)	2.05	0.0118	1.70	0.0453	0.157	275	3.92 (Ne); 0.0115 (Ar); 0.0286 (CH ₄)
Poly(vinylidene chloride)	0.31 ³⁴	0.00094 ³⁰		0.0053 ³⁰	0.03 ³⁰	0.5	0.03 ³⁰ (H ₂ S); 0.008 ⁶⁰ (CH ₃ Br)

TABLE 10.7 Vapor Permeability Constants ($10^{10}P$) at 35°C for Polymers

All tabulated values are multiplied by 10^{10} and are in units of seconds⁻¹ (centimeters of Hg)⁻¹.

Polymer	Vapor				
	Benzene	Hexane	Carbon tetrachloride	Ethanol	Ethyl acetate
Cellulose	1.4	0.912	0.836	85.8	13.4
Cellulose acetate	512	2.80	3.74	2980	3595
Poly(acrylonitrile)	2.61	1.59	1.47	0	1.34
Polyethylene, low-density	5300	2910	3810	55.9	513
Polystyrene	10600		6820	0	soluble
Poly(vinyl alcohol)	3.58	2.34	1.61	32.7	2.53

FATS, OILS, AND WAXES

TABLE 10.8 Constants of Fats and Oils

Fat or oil	Solidification point, °C	Specific gravity (15°C/15°C)	Refractive index	Acid value	Saponification value	Iodine value
Animal origin						
Butterfat	20–23	0.91 ^{40°C} _{15°C}	1.455	0.5–35	210–230	26–38
Chicken fat	21–27	0.924		1.2	193–205	66–72
Cod-liver oil	–3	0.92–0.93	0.925 ^{25°C}	5.6	171–189	137–166
Deer fat		0.96–0.97		0.8–5.3	195–200	26–36

TABLE 10.8 Constants of Fats and Oils (*continued*)

Fat or oil	Solidification point, °C	Specific gravity (15°C/15°C)	Refractive index	Acid value	Saponification value	Iodine value
<i>Animal origin (continued)</i>						
Dolphin	−3 to +5	0.91–0.93		2–12	203 (body); 290 (jaw)	127 (body); 33 (jaw)
Goat butter		0.91 – 0.94 ^{38°C} _{38°C}			233–236	25–37
Goose fat	22–24	0.92–0.93		0.6	191–193	58–67
Herring oil		0.92–0.94	0.900 ^{60°C}	1.8–44	170–194	102–149
Horse fat	20–45	0.92–0.93		0–2.4	195–200	75–86
Human fat	15	0.903	1.460		193–200	57–73
Lard oil	−2 to +4	0.913–0.915	1.462	0.1–2.5	193–198	63–79
Lard oil, fatty tissue	27–30	0.93–0.94	1.462	0.5–0.8	195–203	47–67
Menhaden oil	−5	0.92–0.93	1.465 ^{60°C}	3–12	189–193	148–185
Neat's-foot oil	−2 to +10	0.91–0.92	1.464 ^{25°C}	0.1–0.6	193–199	58–75
Porpoise, body oil	−16	0.926		1.2	203	127
Rabbit fat	17–23	0.93–0.94		1.4–7.2	199–203	70–100
Sardine oil	20–22	0.92–0.93	1.466 ^{60°C}	4–25	188–196	130–152
Seal	3	0.915–0.926		1.9–40	188–196	130–152
Shark		0.916–0.919			157–164	115–139
Sperm oil	15.5	0.878–0.884		13	120–137	80–84
Tallow, beef	31–38	0.895		0.25	196–200	35–42
Tallow, mutton	32–41	0.937–0.953	1.457 ^{40°C}	2–14	195–196	48–61
Whale oil	−2 to 0	0.917–0.924	1.460 ^{60°C}	1.9	160–202	90–146
<i>Plant origin</i>						
Acorn	−10	0.916			199	100
Almond	−20 to −15	0.914–0.921		0.5–3.5	183–208	93–103

Babassu oil	22–26	0.893 ^{60 °C}	1.443 ^{60 °C}		247	16
Beechnut oil	–17	0.922			191–196	97–111
Castor oil	–18 to –17	0.960–0.967	1.477	0.1–0.8	175–183	84
Chaulmoogra oil, USP	< –25	0.950 ^{25 °C}			196–213	98–110
Chinese vegetable tallow	24–34	0.918–0.922		2.4	179–206	23–41
Cocoa butter	21.5–23	0.964–0.974	1.457 ^{40 °C}	1.1–1.9	193–195	33–42
Coconut oil	14–22	0.926	1.449 ^{40 °C}	2.5–10	153–262	6–10
Corn (maize) oil	–20 to –10	0.921–0.928	1.473 ^{40 °C}	1.4–2.0	187–193	111–128
Cottonseed oil	–13 to +12	0.918 ^{25 °C} 0.925 ^{25 °C}	1.474 ^{40 °C}	0.6–0.9	194–196	103–111
Hazelnut oil	–18 to –17	0.917			191–197	87
Hemp-seed oil	–28 to –15	0.928–0.934		0.45	190–195	145–162
Linseed oil	–27 to –19	0.930–0.938	1.478 ^{25 °C}	1–3.5	188–195	175–202
Mustard oil, black	16	0.918–0.921	1.475 ^{40 °C}	5.7–7.3	173–175	99–110
Neem oil	–3	0.917	1.462 ^{40 °C}		195	71
Niger-seed oil		0.925	1.471 ^{40 °C}		190	129
Oiticica oil		0.974 ^{25 °C}				140–180
Olive oil	–6	0.914–0.918	1.468 ^{40 °C}	0.3–1.0	185–196	79–88
Palm oil	35–42	0.915	1.458 ^{40 °C}	10	200–205	49–59
Palm kernel oil	24	0.918–0.925	1.457 ^{40 °C}	0.3–0.6	220–231	26–32
Peanut oil	3	0.917–0.926	1.469 ^{40 °C}	0.8	186–194	88–98
Perilla oil		0.930–0.937	1.481 ^{25 °C}		188–194	185–206
Pistachio-nut oil	–10 to –5	0.913–0.919			191	83–87
Poppy-seed oil	–18 to –16	0.924–0.926	1.469 ^{40 °C}	2.5	193–195	128–141
Pumpkin-seed oil	–15	0.923–0.925			188–193	121–130
Rapeseed oil	–10	0.913–0.917	1.471 ^{40 °C}	0.36–1.0	168–179	94–105
Safflower oil	–18 to –13	0.925–0.928	1.462 ^{60 °C}	0.6	188–203	122–141
Sesame oil	–6 to –4	0.919 ^{25 °C} 0.925 ^{25 °C}	1.465 ^{40 °C}	9.8	188–193	103–117
Soybean oil	–16 to –10	0.924–0.927	1.473 ^{40 °C}	0.3–1.8	189–194	122–134
Sunflower-seed oil	–17	0.924–0.926	1.469 ^{40 °C}	11.2	188–193	129–136
Tung oil	–2.5	0.94–0.95	1.517 ^{25 °C}	2	190–197	163–171
White-mustard-seed oil	–16 to –8	0.912–0.916		5.4	171–174	94–98
Wheat-germ oil						125

TABLE 10.9 Constants of Waxes

Wax	Melting point, °C	Specific gravity (15°C/15°C)	Refractive index	Acid value	Saponification value	Iodine value
Bamboo leaf	79–80	0.961 ^{25°C}		14–15	43–44	7.8
Bayberry (myrtle)	47–49	0.99	1.436 ^{80°C}	3–4	205–212	4–9.5
Beeswax, ordinary	62–66	0.95–0.97	1.44–1.48 ^{40°C}	17–21	88–100	8–11
Beeswax, East Indian	61–67	0.95–0.97	1.44 ^{40°C}	5–10.5	87–117	4–10.5
Beeswax, white, USP	61–69	0.95–0.98	1.45–1.47 ^{65°C}	17–24	90–96	7–11
Candelilla	73–77	0.98–0.99	1.45–1.46 ^{85°C}	19–24	55–64	14–20
Cape berry	40–45	1.01	1.45 ^{45°C}	2.5–4.0	211–215	0.5–2.5
Caranda	80–85	0.99–1.00		5.0–9.5	64–79	8–9
Carnauba, No. 1 yellow	86–88	0.99–1.00		1.5–2.5	75–86	
Carnauba, No. 3, crude	86–90	0.99–1.01		3.0–8.5	75–89	
Carnauba, No. 3, refined	86–89	0.96–0.97	1.47 ^{40°C}	3.0–5.0	76–85	7–13.5
Castor oil, hydrogenated	83–88	0.98–0.99 ^{20°C}		1.0–5.0	177–181	2.5–8.5
Chinese insect	80–85	0.95–0.97	1.46 ^{40°C}	2–9	78–93	1.0–2.5
Cotton	68–71	0.96		32	71	25
Cranberry	207–218	0.97–0.98		42–59	131–134	44–53
Esparto	75–79	0.985–0.995		22–27	58–73	7–15

Flax	61–70	0.91–0.99		17–48	37–102	22–29
Japan	49–56	0.97–1.00		4–15	210–235	4–15
Jojoba	11–12	0.86–0.90 ^{25°C}	1.465 ^{25°C}	0.2–0.6	92–95	82–88
Microcrystalline, amber	64–91	0.91–0.94	1.42–1.45 ^{80°C}	0	0	0
Microcrystalline, white	71–89	0.93–0.94	1.441 ^{80°C}	0	0	0
Montan, crude	76–86	1.01–1.02 ^{25°C}		22–31	59–92	14–18
Montan, refined	77–84	1.02–1.04		23–45	72–115	10–14
Ouricury	86–89	0.99–1.01		12–19	88–96	6.9–7.8
Ozokerite	56–82	0.90–1.00		0	0	4–8
Palm	74–86	0.99–1.05		5–11	64–104	9–17
Paraffin, American	49–63	0.896–0.925	1.44–1.48 ^{80°C}	0	0	0
Shellac	79–82	0.97–0.98		12–24	64–83	6–9
Sisal hemp	74–81	1.007–1.010		16–19	56–58	28–29
Spermaceti	41–49	0.905–0.960		0.5–3.0	121–135	2.5–8.5
Sugarcane, refined	76–82	0.96–0.98	1.51 ^{25°C}	8–23	55–70	13–29
Wool	38–40	0.97	1.48 ^{40°C}	6–22	82–130	15–47

SECTION 11

ABBREVIATIONS, CONSTANTS, AND CONVERSION FACTORS

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PHYSICAL CONSTANTS

TABLE 11.1 Fundamental Physical Constants

A. Defined values

Name of unit	Symbol	Definition
SI base units		
Meter (metre) (preferred spelling in U.S. is meter)	m	1 650 763.73 wavelengths in vacuum of the orange-red line of the spectrum of krypton-86
Kilogram	kg	Mass of a cylinder of platinum–iridium alloy kept at Paris
Second	s	Duration of 9 192 631 770 cycles of the radiation associated with a specified transition of the cesium atom
Ampere	A	Magnitude of the current that, when flowing through each of two long parallel wires separated by one meter in free space, results in a force between the two wires 2×10^{-7} newton for each meter of length
Kelvin (degree Kelvin)	K	Defined in the thermodynamic scale by assigning 273.16 K to the triple point of water (freezing point, $273.15\text{ K} = 0^{\circ}\text{C}$)
Candela	cd	Luminous intensity of 1/600 000 of a square meter of a radiating cavity at the temperature of freezing platinum (2042 K)
Mole	mol	Amount of substance which contains as many specified entities (molecules, atoms, ions, electrons, photons, etc.) as there are atoms of carbon-12 in exactly 0.012 kg of that nuclide
Supplementary SI units		
Radian	rad	The plane angle between two radii of a circle which cut off on the circumference an arc equal in length to the radius
Steradian	sr	The solid angle which, having its vertex in the center of a sphere, cuts off an area of the surface of the sphere equal to that of a square with sides of length equal to the radius of the sphere

B. Derived SI units

Quantity and symbol	Name of SI unit	Symbol and definition
Capacitance (electric), C	farad	$F = C \cdot V^{-1}$
Charge (electric), quantity of electricity, Q	coulomb	$C = A \cdot s$
Conductance (electric), $G (= 1/R)$	siemens	$S = \Omega^{-1}$
Energy, work, quantity of heat, H	joule	$J = \text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2}$

TABLE 11.1 Fundamental Physical Constants (*continued*)

Quantity and symbol	Name of SI unit	Symbol and definition
Force	newton	$N = \text{kg} \cdot \text{m} \cdot \text{s}^{-2}$
Frequency	hertz	$\text{Hz} = \text{s}^{-1}$
Illuminance, illumination	lux	$\text{lx} = \text{lm} \cdot \text{m}^{-2}$
Inductance, L	henry	$H = \Omega \cdot \text{s}$
Luminous flux	lumen	$\text{lm} = \text{cd} \cdot \text{sr}$
Magnetic flux	weber	$\text{Wb} = \text{V} \cdot \text{s}$
Magnetic flux density	tesla	$T = \text{Wb} \cdot \text{m}^{-2}$
Potential difference, E	volt	$V = \text{kg} \cdot \text{m}^2 \cdot \text{s}^{-3} \cdot \text{A}^{-1} = \text{J} \cdot \text{A}^{-1} \cdot \text{s}^{-1}$
Power, radiant flux	watt	$W = \text{kg} \cdot \text{m}^2 \cdot \text{s}^{-3} = \text{J} \cdot \text{s}^{-1}$
Pressure, stress	pascal	$\text{Pa} = \text{N} \cdot \text{m}^{-2} = \text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-2}$
Resistance (electric), R	ohm	$\Omega = \text{V} \cdot \text{A}^{-1} = \text{kg} \cdot \text{m}^2 \cdot \text{s}^{-3} \cdot \text{A}^{-2}$

C. Recommended Consistent Values of Constants

The digits in parentheses following a numerical value represent the standard deviation of that value in terms of the final listed digits.

Constant	Symbol and value
Anomalous electron moment correction	$(\mu_e/\mu_0) - 1 = 1.159615(15) \times 10^{-3}$
Atomic mass unit	$u = (10^{-3} \text{ kg} \cdot \text{mol}^{-1})/N_A = 1.660566(9) \times 10^{-27} \text{ kg}$
Avogadro constant	$N_A = 6.022045(31) \times 10^{23} \text{ mol}^{-1}$
Bohr magneton	$\mu_B = e\hbar/2m_e c = 9.274078(36) \times 10^{-24} \text{ J} \cdot \text{T}^{-1}$
Bohr radius	$a_0 = \alpha^2/4\pi R_\infty = 0.52917706(44) \times 10^{-10} \text{ m}$
Boltzmann constant	$k = R/N_A = 1.380662(44) \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$
Charge-to-mass ratio for electron	$e/m_e = 1.758805(5) \times 10^{11} \text{ C} \cdot \text{kg}^{-1}$
Compton wavelength of electron	$\lambda_c = \alpha^2/2R_\infty = 2.426309(4) \times 10^{-12} \text{ m}$
Compton wavelength of neutron	$\lambda_{c,n} = h/m_n c = 1.319591(2) \times 10^{-15} \text{ m}$
Compton wavelength of proton	$\lambda_{c,p} = h/m_p c = 1.321410(2) \times 10^{-15} \text{ m}$
Diamagnetic shielding factor, spherical H_2O molecule	$1 + \sigma(\text{H}_2\text{O}) = 1.00002564(7)$
Electron g -factor	$g_e/2 = \mu_e/\mu_B = 1.001159657(4)$
Electron magnetic moment	$\mu_e = 9.284832(36) \times 10^{-24} \text{ J} \cdot \text{T}^{-1}$
Electron radius (classical)	$\alpha\lambda_c = \mu_0 e^2/4\pi m_e = r_e = 2.817938(7) \times 10^{-15} \text{ m}$
Electron rest mass	$m_e = 0.910953(5) \times 10^{-30} \text{ kg}$ $= 5.485803(2) \times 10^{-4} u$
Elementary charge	$e = 1.602189(5) \times 10^{-19} \text{ C}$
Faraday constant	$N_A e = F = 9.648456(27) \times 10^4 \text{ C} \cdot \text{mol}^{-1}$
Fine structure constant	$\mu_0 c e^2/2\hbar = \alpha = 0.007297351(6)$ $1/\alpha = 1.370360(1)$
First radiation constant	$2\pi\hbar c^2 = c_1 = 3.74183(2) \times 10^{-16} \text{ W} \cdot \text{m}^2$
Gas constant (molar)	$R = P_0 V_m/T_0 = 8.31441(26) \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ $= 82.0568(26) \text{ cm}^3 \cdot \text{atm} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ $= 1.98719(6) \text{ cal} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$
Gravitational constant	$G = 6.672(4) \times 10^{-11} \text{ N} \cdot \text{m}^2 \cdot \text{kg}^{-2}$

TABLE 11.1 Fundamental Physical Constants (*continued*)

Constant	Symbol and value
Gyromagnetic ratio of proton (uncorrected for diamagnetism of H ₂ O)	$\gamma_p = 2.675\,199(8) \times 10^8 \text{ s}^{-1} \cdot \text{T}^{-1}$ $\gamma'_p = 675\,130(8) \times 10^8 \text{ s}^{-1} \cdot \text{T}^{-1}$
Josephson frequency–voltage ratio	$2e/h = 4.835\,939(13) \times 10^{14} \text{ Hz} \cdot \text{V}^{-1}$
Magnetic flux quantum	$\Phi_0 = h/2e = 2.067\,851(5) \times 10^{-15} \text{ Wb}$
Molar standard volume, ideal gas	$V_m = RT_0/P_0 = 0.022\,413\,8(7) \text{ m}^3 \cdot \text{mol}^{-1}$
Muon <i>g</i> -factor	$e\hbar/2m_\mu c = g_\mu/2 = 1.001\,166\,16(31)$
Muon magnetic moment	$\mu_\mu = 4.490\,474(18) \times 10^{-26} \text{ J} \cdot \text{T}^{-1}$
Muon rest mass	$m_\mu = 1.883\,566(11) \times 10^{-27} \text{ kg}$
Neutron rest mass	$m_n = 1.674\,954(9) \times 10^{-27} \text{ kg}$
Normal volume, perfect gas	$V_0 = 2.241\,36(30) \times 10^4 \text{ cm}^3 \cdot \text{mol}^{-1}$
Nuclear magneton	$\mu_N = e\hbar/2m_p c = 5.050\,824(20) \times 10^{-27} \text{ J} \cdot \text{T}^{-1}$
Permeability of vacuum	$\mu_0 = 4\pi \times 10^{-7} \text{ H} \cdot \text{m}^{-1}$
Permittivity of vacuum	$\epsilon_0 = (\mu_0 c^2)^{-1} = 8.854\,187\,82(7) \times 10^{-12} \text{ F} \cdot \text{m}^{-1}$
Planck constant	$h = 6.626\,176(36) \times 10^{-34} \text{ J} \cdot \text{s}$ $\hbar = h/2\pi = 1.054\,589(6) \times 10^{-34} \text{ J} \cdot \text{s}$
Proton magnetic moment:	$\mu_p = 1.410\,617(5) \times 10^{-26} \text{ J} \cdot \text{T}^{-1}$
In Bohr magnetons	$\mu_p/\mu_B = 1.521\,032\,209(16) \times 10^{-3}$
In nuclear magnetons	$\mu_p/\mu_N = 2.792\,845\,6(11)$
Proton rest mass	$m_p = 1.672\,649(9) \times 10^{-27} \text{ kg}$
Quantum–charge ratio	$h/e = 4.135\,701(11) \times 10^{-15} \text{ J} \cdot \text{Hz}^{-1} \cdot \text{C}^{-1}$
Quantum of circulation	$h/m_e = 7.273\,89(1) \times 10^{-4} \text{ J} \cdot \text{s} \cdot \text{kg}^{-1}$
Ratio, electron to proton magnetic moments	$\mu_e/\mu_p = 6.582\,106\,88(7) \times 10^2$
Ratio, <i>kx</i> u (Siegbahn) to angstrom	$= 1.000\,020\,5(56)$
Ratio, muon moment to proton moment	$\mu_\mu/\mu_p = 3.183\,340(7)$
Rydberg constant	$R_\infty = 1.097\,373\,18(8) \times 10^7 \text{ m}^{-1}$
Second radiation constant	$c_2 = hc/k = 1.438\,786(45) \times 10^{-2} \text{ m} \cdot \text{K}$
Speed of light in vacuum	$c = 2.997\,924\,58(12) \times 10^8 \text{ m} \cdot \text{s}^{-1}$
Stefan–Boltzmann constant	$\sigma = (\pi^2/60)k^4/\hbar^3 c^2 = 5.670\,3(7) \times 10^{-8} \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$
Thomson cross section	$\sigma_e = 8\pi r_e^2/3 = 6.652\,448(33) \times 10^{-28} \text{ m}^2$
Voltage–wavelength product	$V\lambda = 1.239\,852(3) \times 10^{-6} \text{ eV} \cdot \text{m}$
Wien displacement constant	$b = 0.289\,78(4) \text{ cm} \cdot \text{K}$
Zeeman splitting constant	$\mu_B/hc = 4.668\,58(4) \times 10^{-5} \text{ cm}^{-1} \cdot \text{G}^{-1}$
Energy equivalents:	
1 atomic mass unit	$u = 931.501\,6(26) \text{ MeV}$
1 proton mass	$m_p = 938.279\,6(27) \text{ MeV}$
1 neutron mass	$m_n = 939.573\,1(27) \text{ MeV}$
1 muon mass	$m_\mu = 105.659\,48(35) \text{ MeV}$
1 electron mass	$m_e = 0.511\,003\,4(14) \text{ MeV}$
1 electronvolt	$1 \text{ eV}/k = 1.160\,450(36) \times 10^4 \text{ K}$ $1 \text{ eV}/hc = 8.065\,479(21) \times 10^3 \text{ cm}^{-1}$ $1 \text{ eV}/h = 2.417\,970(6) \times 10^{14} \text{ Hz}$

Source: E.R. Cohen and B.N. Taylor, *J. Phys. Chem. Ref. Data*, **2**(4): 663 (1973)

GREEK ALPHABET

TABLE 11.2 Greek Alphabet

Capital letter	Lowercase letter	Letter name	Capital letter	Lowercase letter	Letter name
A	α	Alpha	N	ν	Nu
B	β	Beta	Ξ	ξ	Xi
Γ	γ	Gamma	O	o	Omicron
Δ	δ	Delta	Π	π	Pi
E	ε	Epsilon	P	ρ	Rho
Z	ζ	Zeta	Σ	σ	Sigma
H	η	Eta	T	τ	Tau
Θ	θ	Theta	Y	υ	Upsilon
I	ι	Iota	Φ	ϕ	Phi
K	κ	Kappa	X	χ	Chi
Λ	λ	Lambda	Ψ	ψ	Psi
M	μ	Mu	Ω	ω	Omega

PREFIXES

TABLE 11.3 Prefixes for Naming Multiples and Submultiples of Units

For example: 10^{-9} gram is one nanogram, or 1 ng.

Factor	Prefix	Symbol	Factor	Prefix	Symbol
10^{12}	tera	T	10^{-2}	centi	c
10^9	giga	G	10^{-3}	milli	m
10^6	mega	M	10^{-6}	micro	μ
10^3	kilo	k	10^{-9}	nano	n
10^2	hecto	h	10^{-12}	pico	p
10	deka	da	10^{-15}	femto	f
10^{-1}	deci	d	10^{-18}	atto	a

TABLE 11.4 Numerical Prefixes

Number	Prefix	Number	Prefix	Number	Prefix
$\frac{1}{2}$	hemi	6	hexa	13	trideca
1	mono	7	hepta	14	tetradeca
$1\frac{1}{2}$	sesqui	8	octa	15	pentadeca
2	di or bi	9	nona	16	hexadeca
3	tri	10	deca	17	heptadeca
4	tetra	11	undeca	18	octadeca
5	penta	12	dodeca	19	nonadeca

TABLE 11.4 Numerical Prefixes (continued)

Number	Prefix	Number	Prefix	Number	Prefix
20	icosa	34	tetratriaconta	48	octatetraconta
21	henicosa	35	pentatriaconta	49	nonatetraconta
22	docosa	36	hexatriaconta	50	pentaconta
23	tricos	37	heptatriaconta	51	henpentaconta
24	tetracosa	38	octatriaconta	52	dopentaconta
25	pentacosa	39	nonatriaconta	53	tripentaconta
26	hexacosa	40	tetraconta	54	tetrapentaconta
27	heptacosa	41	hentetraconta	55	pentapentaconta
28	octacosa	42	dotetraconta	56	hexapentaconta
29	nonacosa	43	tritetraconta	57	heptapentaconta
30	triaconta	44	tetratetraconta	58	octapentaconta
31	hentriaconta	45	pentatetraconta	59	monapentaconta
32	dotriaconta	46	hexatetraconta	60	hexaconta
33	tritriaconta	47	heptatetraconta		

TRANSFORMATIONS

TABLE 11.5 Conversion Formulas for Solutions Having concentrations expressed in Various Ways

Abbreviations Used in the Table		
wt %, weight percent of solute	<i>m</i> , molality	
MW ₁ , molecular weight of solute	<i>M</i> , molarity	
MW ₂ , molecular weight of solvent	<i>n</i> , mole fraction	
<i>d</i> , density of solution (g · mL ⁻¹)	<i>G</i> , grams of solute per liter of solution	

To obtain	From	Compute
molarity	weight per cent of solute	$M = \frac{10 \, d(\text{wt } \%) }{MW_1}$
molarity	molality	$M = \frac{1000 \, dm}{1000 + (MW_1)m}$
molarity	grams of solute per liter of solution	$M = \frac{G}{MW_1}$
molarity	mole fraction	$M = \frac{1000 \, dn}{n(NW_1) + MW_2(1 - n)}$
mole fraction	weight per cent of solute	$n = \frac{(\text{wt } \%)/MW_1}{(\text{wt } \%)/MW_1 + (100 - \text{wt } \%)/MW_2}$
mole fraction	molality	$n = \frac{(MW_2)m}{(MW_2)m + 1000}$
mole fraction	molarity	$n = \frac{M(MW_2)}{M(MW_2 - MW_1) + 1000 \, d}$

TABLE 11.5 Conversion Formulas for Solutions Having concentrations expressed in Various Ways (continued)

To obtain	From	Compute
mole fraction	grams of solute per liter of solution	$n = \frac{G(MW_2)}{G(MW_2 - MW_1) + 1000 d(MW_1)}$
weight percent of solute	mole fraction	$\text{wt \%} = \frac{100 n(MW_1)}{n(MW_1) + MW_2(1 - n)}$
weight percent of solute	grams of solute per liter of solution	$\text{wt \%} = \frac{G}{10 d}$
weight percent of solute	molarity	$\text{wt \%} = \frac{M(MW_1)}{10 d}$
weight percent of solute	molality	$\text{wt \%} = \frac{100 m(MW_1)}{1000 + m(MW_1)}$
molality	molarity	$m = \frac{1000 M}{1000 d - M(MW_1)}$
molality	grams of solute per liter of solution	$m = \frac{1000 G}{MW_1(1000 d - G)}$
molality	weight percent of solute	$m = \frac{1000(\text{wt \%})}{MW_1(100 - \text{wt \%})}$
molality	mole fraction	$m = \frac{1000 n}{MW_2 - n(MW_2)}$

TABLE 11.6 Conversion Factors

The data have been compared with the *International Standard ISO 31* (1979–80) and the *American Society for Testing and Materials Standard for Metric Practice E 380-79*. Relations which are exact are indicated by an asterisk (*). Factors in parentheses are also exact.

To convert	Into	Multiply by
ampere per square centimeter	ampere per square inch*	6.451 6
ampere-hour	coulomb*	3 600
ampere-turn	gilbert	1.256 637
angstrom	meter*	1×10^{-10}
	nanometer*	0.1
apostib	candela per square meter	0.318 309 9(1 π)
	lambert*	1×10^{-4}
atmosphere	bar*	1.013 25
	inch of mercury	29.921 26
	millimeters of mercury*	760
	millimeter of water	$1.033\,227 \times 10^4$
	newton per square meter*	$1.013\,25 \times 10^5$
	pascal*	$1.013\,25 \times 10^5$
	torr*	760

TABLE 11.6 Conversion Factors (continued)

To convert	Into	Multiply by
bar	atmosphere	0.986923
	dyne per square centimeter*	1×10^6
	millimeter of mercury	750.062
	pascal	1×10^5
barn	square meter*	1×10^{-28}
barrel (petroleum)	gallon (British)	34.9723
	gallon (U.S.)*	42
	liter	158.987
barrel (U.S., dry)	bushel (U.S.)	3.28122
	liter	115.6271
barrel (U.S., liquid)	gallon (U.S.)	31.5
	liter	119.2405
becquerel	curie*	2.7×10^{-11}
British thermal unit (Btu)	calorie	251.996
	joule	1055.056
	kilowatt-hour	2.93071×10^{-4}
	liter-atmosphere	10.4126
bushel (U.S.)	barrel (U.S., dry)	0.304765
	cubic foot	1.244456
	cubic inch*	2150.42
	gallon (U.S.)	9.30918
	liter	3.523907
	pint (U.S., dry)	64
	quart (U.S., dry)	32
calorie	Btu	0.003968320
	joule*	4.1868
	liter-atmosphere	0.0413205
calorie (thermochemical)	joule*	4.184
calorie per minute	watt*	0.06978
calorie per second	watt*	4.1868
candela	Hefner unit	1.11
	lumen per steradian*	1
candela per square centimeter	candela per square foot*	929.3034
	lambert	$3.141593(\pi)$
carat (metric)	gram*	0.2
Celsius (Centigrade) temperature scale, °C	Fahrenheit temperature scale, °F	$\frac{9}{5}(^{\circ}\text{C} + 32) = ^{\circ}\text{F}$
centimeter	foot	0.0328084
	inch	0.3937008
	mil	393.7008
centimeter of mercury	pascal	1333.22
centimeter per second	foot per second	0.0328084

TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by
centimeter-dyne	erg*	1
	joule*	1×10^{-7}
centipoise	pascal-second*	0.001
centistokes	square meter per second*	1×10^{-6}
coulomb	ampere-second*	1
cubic centimeter	cubic foot	3.53147×10^{-5}
	liter*	0.001
	ounce (U.S., fluid)	0.03381402
	quart (U.S., dry)	9.08083×10^{-4}
	quart (U.S., liquid)	0.001056688
cubic centimeter per second	liter per hour*	3.6
curie	becquerel*	3.7×10^{10}
cycle per second	hertz*	1
day (mean solar)	hour*	24
	minute*	1440
	second	8.64×10^4
Debye unit	coulomb-meter	3.33564×10^{-30}
decibel	neper	0.115129255
degree (angle)	circumference	0.00277778(1/360)
	minute (angle)*	60
	quadrant	0.0111111(1/90)
	radian	0.01745329($\pi/180$)
degree Celcius (Centigrade) (temperature difference), °C	degree Fahrenheit, °F*	1.8
	degree Rankine*	1.8
	kelvin*	1
dram (apothecaries or troy)	dram (avoirdupois)	2.1942857
dram (avoirdupois)	grain*	27.34375
	gram	1.7718452
	ounce (avoirdupois)	0.0625(1/16)
dram (U.S., fluid)	cubic centimeter	3.6966912
	ounce (U.S., fluid)*	0.125(1/8)
	pint (U.S., liquid)*	0.0078125(1/128)
dyne	kilogram-force	1.019716×10^{-6}
	newton*	1×10^{-5}
dyne per square centimeter	bar*	1×10^{-6}
	millimeter of mercury	7.500617×10^{-4}
	pascal	0.1
dyne-centimeter	erg*	1
	joule*	1×10^{-7}
	newton-meter*	1×10^{-7}

TABLE 11.6 Conversion Factors (continued)

To convert	Into	Multiply by
dyne-second per square centimeter	poise* pascal-second	1 0.1
electronvolt	erg joule	$1.602\,19 \times 10^{-12}$ $1.602\,19 \times 10^{-19}$
em	millimeter	4.217 52
erg	dyne-centimeter* joule* watt-hour	1 1×10^{-7} $2.777\,78 \times 10^{-11}$
Fahrenheit temperature, °F	Celsius temperature, °C	$\frac{5}{9}({}^{\circ}\text{F} - 32) = {}^{\circ}\text{C}$
fathom	foot*	6
fermi	meter*	1×10^{-15}
foot	centimeter* inch	30.48 12
foot-candle	lumen per square foot* lumen per square meter	1 10.763 9
foot-lambert	candela per square centimeter candela per square foot lambert	$3.426\,26 \times 10^{-4}$ 0.318 309 9 0.001 076 39
gallon (British, imperial)	gallon (U.S.) liter*	1.200 95 4.546 09
gallon (U.S.)	liter ounce (U.S., fluid)* pint (U.S., liquid)*	3.785 412 128 8
gauss	tesla* weber per square meter	1×10^{-4} 1×10^{-4}
gilbert	ampere-turn	0.795 775
grain	milligram*	64.798 91
gram	carat (metric)* grain ounce (avoirdupois) ounce (troy) pound ton (metric)	5 15.432 358 0.035 273 962 0.032 150 747 0.002 204 622 6 1×10^{-6}
gram-force	dyne* newton*	980.665 0.009 806 65
gram-force per square centimeter	pascal*	98.066 5
gram-force-centimeter	joule*	$9.806\,65 \times 10^{-5}$
Hefner unit	candela	0.9
hertz	cycles per second*	1

TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by
hour (mean solar)	minute*	60
	second	3 600
inch	centimeter*	2.54
	foot	0.083 333 3(1/12)
	mil*	1 000
	millimeter*	25.4
joule	Btu	$9.478\,170 \times 10^{-4}$
	calorie	0.238 845 9
	erg*	1×10^7
	liter-atmosphere	0.009 869 233
	newton-meter*	1
	watt-hour	$2.777\,78 \times 10^{-4}$ (1/3600)
kelvin temperature scale, K	Celsius scale, °C	°C + 273.1 = K
kilocalorie per second	kilowatt*	4.186 8
kilogram	ounce (avoirdupois)	35.273 963
	ounce (troy)	32.150 747
	pound	2.204 622 6
	ton (long)	$9.842\,065\,3 \times 10^{-4}$
	ton (metric)	0.001
	ton (short)	0.001 102 311 3
kilometer	foot	3 280.840
	light-year	$1.057\,02 \times 10^{-13}$
	mile (statute)	0.621 371 192
kilowatt	Btu per hour	3 412.14
	horsepower (metric)	1.359 62
	joule per hour*	3.6×10^{-6}
	kilocalorie per hour	859.845
knot	foot per minute	101.268 6
	meter per minute	30.866 7
	mile (nautical) per hour*	1
	mile (statute) per hour	1.150 78
lambert	candela per square centimeter	0.318 310
liter	cubic centimeter*	1 000
	cubic decimeter*	1
	cubic inch	61.023 74
	gallon (U.S.)	0.264 172 1
	ounce (U.S., fluid)	33.814 02
	pint (U.S., liquid)	2.113 376
	quart (U.S., liquid)	1.056 688
liter per minute	gallon (U.S.) per hour	15.850 3
liter-atmosphere	Btu	0.096 037 6
	calorie	24.201 1
	joule*	101.325

TABLE 11.6 Conversion Factors (continued)

To convert	Into	Multiply by
lumen per square centimeter	lux*	1×10^4
lux	lumen per square meter*	1
maxwell	weber*	1×10^{-8}
megaohm	ohm*	1×10^6
meter	angstrom*	1×10^{10}
	foot	3.280 839 895
mho (ohm^{-1})	siemens*	1
micrometer (micron)	angstrom	1×10^4
	millimeter*	0.001
mil	inch*	0.001
	millimeter*	0.025 4
mile (statute)	foot*	5.280
	furlong*	8
	kilometer*	1.609 344
	mile (nautical)	0.868 976
milligram per assay ton	milligram per kilogram	34.285 714
	ounce (troy) per ton (short)*	1
milliliter	cubic centimeter*	1
millimeter	inch	0.039 370 8
millimeter of mercury	atmosphere	0.001 315 789(1/760)
	dyne per square centimeter	1333.224
	pascal	133.322 4
	torr*	1
minute (angle)	circumference	$4.629\,63 \times 10^{-5}$
	degree (angle)	0.016 666 7(1/60)
	radian	$2.908\,88 \times 10^{-4}$
	second (angle)*	60
minute	day	$6.944\,444 \times 10^{-4}$
	hour	0.016 666 7(1/60)
	second*	60
newton	dyne*	1×10^5
newton per square centimeter	pascal*	1×10^4
oersted	ampere per meter	79.577 5
ounce (avoirdupois)	dram*	16
	grain*	437.5
	gram*	28.349 523 125
	ounce (troy)	0.911 458 33
	pound*	0.062 5(1/16)
ounce (U.S., fluid)	cubic centimeter	29.573 530
	gallon (U.S.)*	0.007 812 5(1/128)
	milliliter	29.573 530

TABLE 11.6 Conversion Factors (*continued*)

To convert	Into	Multiply by
	pint (U.S., liquid)*	0.0625(1/16)
	quart (U.S., liquid)*	0.03125(1/32)
parsec	kilometer	3.08568×10^{13}
part per million	gram per ton (metric)*	1
	milligram per kilogram*	1
pascal	bar*	1×10^{-5}
	dyne per square centimeter*	10
	inch of mercury	2.95300×10^{-4}
	millimeter of mercury	7.50062×10^{-3}
	newton per square meter*	1
pascal-second	poise*	10
pica (printer's)	point*	12
pint (U.S., liquid)	cubic centimeter	473.1765
point (printer's, U.S.)	millimeter*	0.3514598
poise	pascal-second*	0.1
pound	dram*	256
	grain*	7000
	gram*	453.59237
	ounce (avoirdupois)*	16
	ton (long)	4.4622857×10^{-4}
	ton (metric)*	4.5359237×10^{-4}
	ton (short)*	$5 \times 10^{-4}(1/2000)$
poundal	gram-force	14.0981
	newton	0.138255
proof (U.S.)	percent alcohol by volume*	0.5
quart (U.S., dry)	cubic centimeter	1101.221
	cubic foot	0.03888925
	pint (U.S., dry)	2
quart (U.S., liquid)	gallon (U.S.)*	0.25
	liter	0.946353
	ounce (U.S., fluid)*	32
	pint (U.S., liquid)*	2
radian	degree (angle)	57.295780
	minute (angle)	3.437.75
	revolution	0.159155
ream	quire*	20
	sheet	480 or 500
revolution	degree (angle)*	360
revolution per minute	radian per second	0.140720
roentgen	coulomb per kilogram*	2.58×10^{-4}
second (angle)	degree	2.77778×10^{-4}
	radian	4.848137×10^{-6}

TABLE 11.6 Conversion Factors (continued)

To convert	Into	Multiply by
siemens	mho (ohm ⁻¹)*	1
steradian	sphere	0.079 577 5
	spherical right angle	0.636 620
stokes	square meter per second*	1 × 10 ⁻⁴
tablespoon (metric)	cubic centimeter*	15
teaspoon (metric)	cubic centimeter*	5
tesla	weber per square meter*	1
ton (long)	kilogram*	1 016.046 908 8
	pound*	2 240
	ton (metric)	1.016 046 9
	ton (short)*	1.12
torr	millimeter of mercury	1
	pascal	133.322 4
volt-second	weber*	1
watt	Btu per hour	3.412 14
	calorie per second	0.238 846
	erg per second*	1 × 10 ⁷
	joule per second*	1
weber	maxwell*	1 × 10 ⁸
X unit	meter	1.002 02 × 10 ⁻¹³

STATISTICS

TABLE 11.7 Values of *t*

df	<i>t</i> _{.60}	<i>t</i> _{.70}	<i>t</i> _{.80}	<i>t</i> _{.90}	<i>t</i> _{.95}	<i>t</i> _{.975}	<i>t</i> _{.99}	<i>t</i> _{.995}
1	0.325	0.727	1.376	3.078	6.314	12.706	31.821	63.657
2	0.289	0.617	1.061	1.886	2.920	4.303	6.965	9.925
3	0.277	0.584	0.978	1.638	2.353	3.182	4.541	5.841
4	0.271	0.569	0.941	1.533	2.132	2.776	3.747	4.604
5	0.267	0.559	0.920	1.476	2.015	2.571	3.365	4.032
6	0.265	0.553	0.906	1.440	1.943	2.447	3.143	3.707
7	0.263	0.549	0.896	1.415	1.895	2.365	2.998	3.499
8	0.262	0.546	0.889	1.397	1.860	2.306	2.896	3.355
9	0.261	0.543	0.883	1.383	1.833	2.262	2.821	3.250
10	0.260	0.542	0.879	1.372	1.812	2.228	2.764	3.169

TABLE 11.7 Values of t (continued)

df	$t_{.60}$	$t_{.70}$	$t_{.80}$	$t_{.90}$	$t_{.95}$	$t_{.975}$	$t_{.99}$	$t_{.995}$
11	0.260	0.540	0.876	1.363	1.796	2.201	2.718	3.106
12	0.259	0.539	0.873	1.356	1.782	2.179	2.681	3.055
13	0.259	0.538	0.870	1.350	1.771	2.160	2.650	3.012
14	0.258	0.537	0.868	1.345	1.761	2.145	2.624	2.977
15	0.258	0.536	0.866	1.341	1.753	2.131	2.602	2.947
16	0.258	0.535	0.865	1.337	1.746	2.120	2.583	2.921
17	0.257	0.534	0.863	1.333	1.740	2.110	2.567	2.898
18	0.257	0.534	0.862	1.330	1.734	2.101	2.552	2.878
19	0.257	0.533	0.861	1.328	1.729	2.093	2.539	2.861
20	0.257	0.533	0.860	1.325	1.725	2.086	2.528	2.845
21	0.257	0.532	0.859	1.323	1.721	2.080	2.518	2.831
22	0.256	0.532	0.858	1.321	1.717	2.074	2.508	2.819
23	0.256	0.532	0.858	1.319	1.714	2.069	2.500	2.807
24	0.256	0.531	0.857	1.318	1.711	2.064	2.492	2.797
25	0.256	0.531	0.856	1.316	1.708	2.060	2.485	2.787
26	0.256	0.531	0.856	1.315	1.706	2.056	2.479	2.799
27	0.256	0.531	0.855	1.314	1.703	2.052	2.473	2.771
28	0.256	0.530	0.855	1.313	1.701	2.048	2.467	2.763
29	0.256	0.530	0.854	1.311	1.699	2.045	2.462	2.756
30	0.256	0.530	0.854	1.310	1.697	2.042	2.457	2.750
40	0.255	0.529	0.851	1.303	1.684	2.021	2.423	2.704
60	0.254	0.527	0.848	1.296	1.671	2.000	2.390	2.660
120	0.254	0.526	0.845	1.289	1.658	1.980	2.358	2.617
∞	0.253	0.524	0.842	1.282	1.645	1.960	2.326	2.576
df*	$-t_{.40}$	$-t_{.30}$	$-t_{.20}$	$-t_{.10}$	$-t_{.05}$	$-t_{.025}$	$-t_{.01}$	$-t_{.006}$

*When the table is read from the foot, the table values should be prefixed with a negative sign. Interpolation should be performed using the reciprocals of the degrees of freedom.

Source: Perry, Chilton, and Kirkpatrick, *Chemical Engineers' Handbook*, 4th ed., McGraw-Hill, New York (1963).

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