HANDBOOK of ORGANIC SOLVENTS

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INTRODUCTION

A solvent may be defined in rough terms as any liquid that serves as a carrier for another substance, as a medium for conducting a chemical reaction, or as a means of extracting or separating other substances. Whatever the precise definition used, solvents are a ubiquitous feature of both modern industry and everyday life. Solvents serve as carriers for paints, reagents, medications, cleaning agents, and a host of other active ingredients. Many of the most important industrial processes take place in a solvent medium. Solvents find wide application for cleaning and for separations of all kinds. In terms of either production bulk or dollar value, solvents form one of the leading categories of products of the chemical industry.

The most common solvent is water, but next in importance comes a group of organic liquids and their mixtures. This book presents data on 564 organic compounds which are now used (or are potentially useful) as solvents. The selection of a limited set of substances from the extremely large universe of organic compounds must necessarily be somewhat arbitrary. Manufacturers' catalogs and other books on solvents have been consulted, as well as the general chemical literature. In some cases, the complete set of isomers of a compound has been covered, even though not all of the isomers find current use. This has been done in the hope that new ideas for replacement solvents may emerge. Emphasis has also been given to environmentally benign compounds which are finding increasing use as replacements for more hazardous solvents such as chlorinated hydrocarbons.

In practice, many solvents are mixtures rather than pure compounds. It would be a formidable task to compile data on all the mixtures of industrial significance. However, the pure compound data in this book form a basis for estimating properties of mixed solvents. A few useful references to mixture properties and estimation methods are given in the Bibliography (Ref. 8, 10, 35-37).

The properties covered fall into the following categories:

- Identifying information such as name, synonyms, and various registry numbers which are helpful in accessing other reference sources.
- Common physical properties: melting point, normal boiling point, critical constants, density, index of refraction, and solubility in water and other substances.
- Thermodynamic properties, including heat capacity; heats of formation, fusion, and vaporization; surface tension; and vapor pressure as a function of temperature.

- Transport properties: viscosity and thermal conductivity as a function of temperature.
- Electrical properties: dipole moment, dielectric constant, and ionization potential.
- Spectral data: mass spectra, infrared, Raman, ultraviolet, and nuclear magnetic resonance.
- Health and safety information, including flammability, permissible airborne concentration, carcinogenicity, and pertinent information from government regulatory lists concerning use and disposal of the substance. The latter information provides an indication of toxicity and other health hazards of the substance.

The data presented in this book have been taken from evaluated sources whenever possible, rather than the primary literature. Space and format limitations prevent giving detailed references to each piece of data, but the major sources consulted are listed in the bibliography. In addition, reviews and compilations in the *Journal of Physical and Chemical Reference Data* and in other publications of the Standard Reference Data Program of the National Institute of Standards and Technology have been heavily used. Where there were discrepancies between different sources, the author used his judgment on selecting the most likely value.

The compounds are arranged alphabetically by the most frequently used name. Again, the choice of primary name is somewhat arbitrary, but an effort has been made to strike a balance between names that are easily recognizable and names that are chemically informative. A systematic name, generally the Chemical Abstracts Service Index Name, is also given, as well as other synonyms. Each compound is assigned an ID number, which serves as the key in the indexes.

Four indexes are provided to aid in location of a compound. These are the **Name Index**, which includes the primary name, systematic name, and all listed synonyms for each solvent; a **Compound Class Index**, in which the compounds are arranged by chemical class; a **Molecular Formula Index**, and a **CAS Registry Number Index**. There are four additional indexes which list compounds in order of **Normal Boiling Point**, **Melting Point**, **Density**, and **Dielectric Constant**.

Explanation of the Data Fields

The following data items appear for each solvent when the information is available. The principal references used as sources for this book are indicated in brackets.

Syst. name: Generally, the Index Name from the *8th or 9th Collective Index* of Chemical Abstracts Service (CAS). [Ref. 2]

Synonyms: One or more synonyms in common use. [Ref. 2]

CASRN: The Chemical Abstracts Registry Number assigned by CAS as the unique identifier for the specific isomer of the compound. [Ref. 2]

Rel. CASRN's: Related CAS Registry Numbers under which the compound is sometimes listed. In most cases these are "generic" Registry Numbers assigned to a compound without specification of the particular isomer. The number may refer to a mixture of isomers or simply to a substance for which the isomer is unidentified. Such numbers are often used in Government regulatory lists instead of the CASRN's for the individual isomers. [Ref. 31, 32]

Merck No: Monograph Number in *The Merck Index, Eleventh Edition.* It should be noted that this is not a unique identifier for a single compound, since several derivatives or isomers of a compound may be included in the same Monograph. [Ref 3]

DOT No: Registry number assigned by the Department of Transportation for labeling hazardous substances when they are shipped. [Ref. 31]

Beil RN: The Beilstein Registry Number used as a unique identifier in the *Beilstein Database*. [Ref. 9]

Beil Ref: Citation to the printed *Beilstein Handbook of Organic Chemistry.* An entry of 5-18-11-01234, for example, indicates that the compound may be found in the 5th Series, Volume 18, Subvolume 11, page 1234. [Ref. 9]

MF: The molecular formula written in the Hill Order, in which C appears first, H second (if present), and then the other element symbols in alphabetical order. [Ref. 2]

MW: Molecular weight (relative molar mass) as calculated with the 1993 IUPAC Standard Atomic Weights. [Ref. 2]

MP: Normal melting point in ^{o}C. Although some values are quoted to 0.1^{o}C, uncertainties are typically several degrees Celsius. [Ref. 1-6, 9, 10, 12, 13, 17]

BP: Normal boiling point in ^{o}C. This is the temperature at which the liquid phase is in equilibrium with the vapor at a pressure of 760 mmHg (101.325 kPa). [Ref. 1-6, 9, 10, 12, 13, 17]

Den: Density (mass per unit volume) in g/cm^3 for the liquid phase. The superscript indicates the temperature in ^{o}C. All values are true densities, not specific gravities. The number of decimal places gives a rough estimate of the accuracy of the value. [Ref. 1-6, 10, 13, 17]

***n*$_D$**: Refractive index of the liquid, at the temperature in ^{o}C indicated by the superscript. All values refer to a wavelength of 589 nm (sodium D line). [Ref. 2, 3]

Vap. pres: Vapor pressure in kPa at the temperature indicated by the superscript (in ^{o}C). Note that 1 kPa = 7.50 mmHg and 101.325 kPa = 1 atmos. [Ref. 1, 4, 5, 10, 13]

Therm. prop: This field gives the molar enthalpy (heat) of fusion ($\Delta_{fus}H$) at the melting point, enthalpy of vaporization ($\Delta_{vap}H$) at the normal boiling point, and standard enthalpy of formation from the elements in their standard reference states ($\Delta_f H°$). All values are in kJ/mol. [Ref. 1, 4, 5, 11, 12, 14, 15, 17]

***C*$_p$ (liq)**: Molar heat capacity of the liquid phase in J/mol ^{o}C at the temperature indicated by the superscript. [Ref. 1, 4, 5, 10, 14, 16]

γ: Surface tension in mN/m (equivalent to dyn/cm) at the temperature indicated by the superscript. When available, the change in surface tension with temperature, $d\gamma/dT$, is also given. [Ref. 1, 4, 10, 18]

Sol: Solubility on a relative scale: 1 = insoluble; 2 = slightly soluble; 3 = soluble; 4 = very soluble; 5 = miscible; 6 = decomposes. See List of Abbreviations for the solvent abbreviations. [Ref. 2, 3]

Elec. prop: This field includes:
-Electric dipole moment μ in debye units (1 D = 1.33564 X 10^{-30} C m). Values measured in the gas phase are given when available. If there is no gas-phase measurement, a value determined in the liquid phase or in solution is given in parentheses; such values are much less reliable. [Ref. 1, 22, 23]

-Dielectric constant ε (also called relative permittivity) at the temperature in ^{o}C indicated by the superscript. Information on the temperature dependence of the dielectric constant may be found in the references. [Ref. 1, 24]
-First ionization potential **IP** of the substance. [Ref. 1, 25]

η: Viscosity of the liquid in mPa s (equivalent to centipoise, cP). The temperature is indicated by the superscript. [Ref. 1, 4, 5, 10, 19-21]

***k*:** Thermal conductivity of the liquid in W/m ^{o}C at the temperature indicated by the superscript. [Ref. 1, 5, 7, 10, 20]

MS: The m/e values of the most abundant peaks in the mass spectrum. Relative intensities are given in parentheses, with the most abundant peak assigned an intensity of (100). [Ref. 2]

IR: Major infrared peaks in cm^{-1}. Values are given to the nearest 10 cm^{-1}. [Ref. 2]

Raman: Most significant peaks in the Raman spectrum, in cm^{-1}. [Ref. 2]

UV: Strongest ultraviolet bands, in nm (1 nm = 10 Å). When available, the molar absorption coefficient follows the wavelength (in parentheses). Solvents are specified in some cases. [Ref. 2]

^{13}C NMR: Chemical shifts in ppm for specific carbon atoms or recognizable groups, referenced to tetramethylsilane (TMS). If known, the solvent in which the spectrum was obtained is given (see List of Abbreviations). [Ref. 2]

^{1}H NMR: Proton chemical shifts in ppm for specific protons or recognizable groups, referenced to tetramethylsilane (TMS). [Ref. 2]

Flammability: This field includes:
-Flash point, which is the minimum temperature at which the vapor pressure of a liquid is sufficient to form an ignitable mixture with air near the surface of the liquid. Flash point is not an intrinsic physical property but depends on the conditions of measurement. See Ref. 29 for details. [Ref. 4, 5, 29]
-Ignition temperature (also called autoignition temperature), which is the minimum temperature required for self-sustained combustion in the absence of an external ignition source. As in the case of flash point, the value depends on specified test conditions. [Ref. 29]
-Flammable limits (often called explosive limits), which specify the range of concentration of the vapor in air (in percent by volume) for which a flame can propagate. Below the lower flammable limit, the gas mixture is too lean to

burn; above the upper flammable limit, the mixture is too rich. Values refer to ambient temperature and pressure and are dependent on the precise test conditions. [Ref. 29]

TLV/TWA: The threshold limit value, expressed as a time weighted average airborne concentration over a normal 8-hour workday and 40-hour workweek, to which most workers can be exposed without adverse effects. The values given here are the recommendations of the American Conference of Governmental Industrial Hygienists (ACGIH), based in part on regulations issued by the Occupational Safety and Health Administration (OSHA). Values conform to the 1993-94 adoptions of ACGIH; intended changes for 1993-94 are not included, since these are still tentative. Changes are issued annually. [Ref. 28, 31]

Reg. lists: The following information has been extracted from Government regulations regarding safe use and disposal of hazardous substances:
-CERCLA indicates the compound is on the list of hazardous substances issued under the Comprehensive Emergency Response, Compensation, and Liability Act of 1980. Any release of such a substance into the environment within a 24-hour period that equals or exceeds the specified Reportable Quantity (RQ) must be reported to the National Response Center (800-424-8802). The RQ value in pounds is given here for each solvent on the CERCLA list. The information is believed to be current as of July 1993. [Ref. 31, 34]
-SARA 313 indicates that the compound appears on the list of toxic chemicals for which reporting standards have been set under Section 313 of the Superfund Amendments and Reauthorization Act of 1986. Anyone using a compound on this list in an amount of 10,000 pounds per year or greater must report the fact to the Environmental Protection Agency. The percentage figure given in parentheses is the threshold concentration of the compound in a mixture below which the reporting requirement is waived. The information is believed to be current as of July 1993. [Ref. 31, 34]
-RCRA indicates that the compound is on the list of hazardous wastes released under Section 3010 of the Resource Conservation and Recovery Act. Hazardous waste containers that contain such a compound must be labeled with the RCRA number given here. A number preceded by "P" indicates a compound that is considered acutely hazardous, while "U" indicates a compound deemed toxic. The information is believed to be current as of July 1993. [Ref. 31, 34]
-If the compound is a confirmed or suspected human carcinogen, this fact is indicated. The information is based on the designations of the International Agency for Research on Cancer (IARC), the National Toxicology Program (NTP), and the Occupational Safety and Health Administration (OSHA); it is believed to be current as of January 1993. All substances so designated by at

least one of the above agencies are indicated as carcinogenic in this book. [Ref. 28, 31, 32, 34]

List of Abbreviations

abs	absolute
ac	acid
ace	acetone
AcOEt	ethyl acetate
alk	alkali
aq	aqueous
Bu	butyl
bz	benzene
CERCLA	Comprehensive Emergency Response, Compensation, and Liability Act of 1980
chl	chloroform
con	concentrated
ctc	carbon tetrachloride
cyhex	cyclohexane
dil	dilute
diox	dioxane
Et	ethyl
eth	ethyl ether
EtOH	ethyl alcohol
HOAc	acetic acid
hp	heptane
hx	hexane
iso	isooctane
lig	ligroin
liq	liquid
MeCN	acetonitrile
MeOH	methyl alcohol
os	organic solvents
peth	petroleum ether
$PhNH_2$	aniline
ppm	parts per million
pres	pressure
PrOH	propyl alcohol
py	pyridine
RCRA	Resource Conservation and Recovery Act
SARA	Superfund Amendments and Reauthorization Act of 1986
sat	saturated, saturation

sulf	sulfuric acid
tol	toluene
TLV	threshold limit value
TMS	tetramethylsilane
TWA	time weighted average

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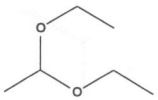
1. Acetal

Syst. Name: Ethane, 1,1-diethoxy-
Synonyms: 1,1-Diethoxyethane; Acetylene diethyl acetal



CASRN: 105-57-7 **DOT No.**: 1088
Merck No.: 31 **Beil Ref.**: 4-01-00-03103
Beil RN: 1098310
MF: $C_6H_{14}O_2$ **MP[°C]**: -100 **Den.[g/cm^3]**: 0.8254^{20}
MW: 118.18 **BP[°C]**: 102.2 n_D: 1.3834^{20}
Sol.: H_2O 3; EtOH 5; eth 5; ace 4; chl 3
Crit. Const.: T_c = 254°C
Vap. Press. [kPa]: 0.777^{0}; 3.68^{25}; 13.2^{50}; 38.1^{75}; 93.9^{100}
Therm. Prop.[kJ/mol]: $\Delta_{vap}H$ = 36.3; $\Delta_fH°$(l, 25°C) = -491.4
C_p (liq.) [J/mol °C]: 238.0^{25}
γ [mN/m]: 20.89^{25}; $d\gamma/dT$ = 0.1030 mN/m °C
Elec. Prop.: μ = (1.4 D); ε = 3.80^{25}; IP = 9.78 eV
MS: 44(100) 43(92) 29(77) 31(76) 45(74) 27(52) 72(48) 73(23) 28(17) 46(15)
IR [cm^{-1}]: 2940 2860 1450 1370 1330 1140 1100 1040 950 850
Raman [cm^{-1}]: 2980 2940 2880 2800 2760 2730 2660 1490 1410 1400 1370 1340 1280 1170 1140 1100 1060 1030 960 920 860 840 810 660 530 470 450 360 230
UV [nm]: 286(0) 264(0)
^{13}C NMR [ppm]: 15.3 19.9 60.6 99.5 $CDCl_3$
^{1}H NMR [ppm]: 1.2 1.3 3.5 3.7 4.7 $CDCl_3$
Flammability: Flash pt. = -21°C; ign. temp. = 230°C; flam. lim. = 1.6-10.4%