TETRAHYDROFURAN

PRODUCT IDENTIFICATION

CAS NO. 109-99-9
EINECS NO. 203-726-8
FORMULA C4H8O
MOL WT. 72.11
H.S. CODE 2932.11

TOXICITY Oral rat LD50: 890 mg/kg

SYNONYMS

Cyclotetramethylene oxide; THF; Butylene Oxide; Furanidine;
Butane ¥á,¥ä-oxide; 1,4-Epoxy-Butane; Oxacyclopentane; Oxolane; Tetrahydrofuran;
Tetramethylene oxide; Diethylene oxide; Hydrofuran; Tetrahydrofuraan; Tetrahydrofuranne;

Tetraidrofurano;

PRICE U\$2,450/mt CFR (fcl quantity basis)

CLASSIFICATION

GENERAL DESCRIPTION OF FURAN AND THE

Furan; One of a class of heterocyclic aromatic compounds characterized by five-membered ring structure consisting of four CH2 groups and one oxygen atom. The simplest furan compound is furan itself; a clear, volatile and mildly toxic liquid; melts at -86 C, boils at 32 C, insoluble in water, soluble in alcohol and ether. In the absence of inhibitors, it may form peroxides and and accumulate peroxides which may explode when subjected to heat or shock. It may discolor on exposure to air. This material is hazardous when peroxide levels are concentrated by distillation or evaporation. It can be stabilized with BHT. It can be obtained from wood oils. It is used as a solvent as well as in the synthesis of furfural and other organic compounds. It is converted to more important solvent, tetrahydrofuran by hydrogenation. Niitro-substituted furan derivatives are used as biocides or fungicides to inhibit bacterial growth. Sulfur-substituted furan derivatives are used as flavouring agents. Furfural (Furfuraldehyde), a derivative of furan, is a viscous, colorless liquid that has a pleasant aromatic odor; upon exposure to air it turns dark brown or black; boils at about 160 C; soluble in ethanol, ether and somewhat in water. It is commonly used as a solvent. Furfural is the aldehyde of pyromucic acid; it has properties similar to those of benzaldehyde. It is prepared commercially by dehydration of pentose sugars obtained from cornstalks and corncobs, husks of oat and peanut, and other waste products. The major application of furfural is being use as a feedstock for furfuryl alcohol. The most commercial quantity of furfuryl alcohol is used in the production of thermosetting furan resin and furan cement, strong adhesive, in which the furan ring is an integral part of the polymer chain providing highly resistance to chemicals. Furfural is used as a solvent for refining lubricating oils and butadiene extraction. It is used as a fungicide and weed killer. It is used in the production of tetrahydrofuran (THF), saturated form of furan. THF is one of the most polar ethers. It is used as an important industrial solvent recognized for its unique combination of useful properties. It is a colorless, volatile cycloaliphatic (5-membered) ether with a characteristic odor; boiling point at 66 C; soluble in water and organic solvents. THF is unstable at room temperature due to possibility of peroxide formation; stabilized sometimes with BHT. Its unhindered oxygen atom carries two unshared pairs of electrons - a structure which favors the formation of coordination complexes and the solvation of cations. THF is made also by eliminating water from 1,4-butanediol. THF is used as an useful chemical intermediate especially as a starting materials for the preparation of nylon.

PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE Clear, mobile liquid, ether odor

MELTING POINT -65 C BOILING POINT 65 - 66 C SPECIFIC GRAVITY 0.885 - 0.895 SOLUBILITY IN WATER Miscible

-1 7

VAPOR DENSITY 2.5
AUTOIGNITION 321 C

NFPA RATINGS Health: 2; Flammability: 3; Reactivity: 1

REFRACTIVE INDEX

FLASH POINT -21 C

STABILITY Peroxide formation may occur

APPLICATIONS

- Adhesives and sealants industry
- Solvent welding agent for PVC
- Extracting agent, reaction medium
- Surface coating of films and textiles with PVC or PUR solutions
- Special printing inks
- Magnetizable information carriers
- Chemical intermediate

SALES	SPECIFICATION

APPEARANCE	Clear liquid
PURITY	99.9% min
PEROXIDE	50ppm max
SPECIFIC GRAVITY	0.885 - 0.895
VISCOSITY	0.48 cP at 25 C
COLOR (APHA)	10 max

TRANSPORTATION

PACKING 180kgs in drum

HAZARD CLASS 3 UN NO. 2056

OTHER INFORMATION

European Hazard Symbols: XI F, Risk Phrases: 11-19-36/37, Safety Phrases: 16-29-33

GENERAL DESCRIPTION OF SOLVENT

Solvent is a substance, usually a liquid, that acts as a dissolving agent or that is capable of dissolving another substance. In solutions of solids or gases in a liquid, the liquid is the solvent. In all other homogeneous mixtures (i.e., liquids, solids, or gases dissolved in liquids; solids in solids; and gases in gases), solvent is the component of the greatest amount. The minor proportion substances are called solutes. The solvent offers several functions during a chemical reaction. It solves not only the substance that reacts with another one to produce a new set of substances (reactant) but also the compound that supplies the molecule, ion, or free radical, which is considered as the attacking species in a chemical reaction (reagent). The solvent is conductive to collisions between the reactants and reagents to transform the reactants to new products. The solvent also takes roll of temperature control, either to provide the energy of the colliding particles for speedy reaction and to absorb heat in exothermic reaction. The appropriate solvent should be selected based on the inactivity in the reaction conditions, dissolving the reagents as well as reactants, appropriate boiling point and easy removal at the end of the reaction.

Polarity

The most common solvent is water. Other common solvents which dissolve substances that are insoluble (or nearly insoluble) in water are acetone, alcohol, formic acid, acetic acid, formamide. BTX, carbon disulfide, diemthyl sulfoxide, carbon tetrachloride, chloroform, ether, tetrahydrofuran,

furfural, hexane and turpentine. They may be classified as polar and non-polar. Polar solvents, like water, have molecules whose electric charges are unequally distributed, leaving one end of each molecule more positive than the other. Usually polar solvent has O-H bond of which water (HOH), (CH₃OH) and acetic acid (CH₃COOH) are examples. Propanol, butanol, formic acid, formamide are polar solvents. Dipolar solvents which contain a C-O solid bond without O-H bond are acetone [(CH3)2C=O], ethyl acetate (CH3COOCH2CH3), methyl ethyl ketone, acetonitrile, N,Ndimethylformamide and diemthyl sulfoxide. Nonpolar solvents, like carbon tetrachloride (CCI $_4$), benzene (C6H6), and diethyl ether (CH3CH2OCH2CH3), have molecules whose electric charges are equally distributed and are not miscible with water. Hexane, tetrahydrofuran and methylene chloride are non-polar solvents. Polar solvents are hydrophilic but non-polar solvents are lipophilic. Polar reactants will dissolve in polar solvents. Non-polar solvents dissolve non-polar compounds best. Oil and water don't mix but separate into two layers. There are three measures of the polarity as "dipole moment", "dielectric constant" and "miscibility with water". Though low dipole moments and small dielectric constants indicates non-polar solvents, sharp boundaries between polar and nonpolar solvents are not available. The polarity reflects the balance between a polar component (OH) and a non-polar hydrocarbon component, existing in the same molecule. If hydrocarbon character increases relatively, the polarity decreases. On an operational basis, solvents that are miscible with water are polar.

Polar Protic and Dipolar Aprotic

Protic refers to a hydrogen atom attached to an electronegative atom. Protic solvents can donate an H+ (proton) since they contain dissociable H+, such as hydrogen attached to oxygen as in a hydroxyl group, nitrogen as in a amine group. Examples are water, methanol, ethanol, formic acid, hydrogen fluoride and ammonia. Aprotic solvents don't has O-H bond but a C=O bond typically. Examples are acetone [(CH₃)₂C=O] and ethyl acetate (CH₃COOCH₂CH₃). Polar protic solvents are useful in S_N1 reaction, while polar aprotic solvents are S_N2 reaction.