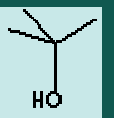
tert-BUTYL ALCOHOL



PRODUCT IDENTIFICATION

CAS NO.	75-65-0
EINECS NO.	200-889-7
FORMULA	$(CH_3)_3COH$
MOL WT.	74.12
H.S. CODE	2905.14
TOXICITY	Oral rat LD50: 2743 mg/kg
SYNONYMS	2-Methyl-2-propanol; 1,1-Dimethylethanol; Trimethylcarbinol; 2-Methylpropan-2-ol; tert-Butanol; TBA; t-butyl hydroxide; trimethyl methanol; Dimethylethanol; Methyl-2-propanol; tertiary-butyl alcohol;
DERIVATION	
CLASSIFICATION	

PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE	clear, noncorrosive liquid
MELTING POINT	25 C
BOILING POINT	83 C
SPECIFIC GRAVITY	0.78 - 0.79
SOLUBILITY IN WATER	Soluble
SOLVENT SOLUBILITY	
pH	
VAPOR DENSITY	
AUTOIGNITION	343 C
NFPA RATINGS	Health: 1; Flammability: 3; Reactivity: 0
REFRACTIVE INDEX	
FLASH POINT	37 C
STABILITY	Stable under ordinary conditions

GENERAL DESCRIPTION & APPLICATIONS

Tert-butyl alcohol (TBA) is a clear, noncorrosive liquid. It is miscible with water as well as most common organic solvents and forms azeotrope. The sterically hindered tertiary butyl group imparts stability compare to primary and secondary alcohols. In result, the solubility and oxidative stability characteristics provide many industrial applications as a reaction and process solvent and chemical intermediate. It is used as a non-reactive solvent for chemical reactions, a non-surfactant compatibilizer for many solvent blends, and a non-corrosive solvent. It is used in free radical polymerizations to dissolve monomers. TBA is a main raw material of tert-butyl functional group in organic synthesis. It is used as a coupling aid for formulating pesticides and fertilizers in aqueous solutions without generating an emulsion. TBA was used as a fuel additive for high octane component to replace tetraethyl lead. TBA is used as a reaction solvent as well as an intermediate for the product of organic peroxides, metal alkoxides. Tert-butyl group is readily cleaved under strongly acidic conditions. TBA is a source to produce alkylated aromatic and nitrogen compounds in mid acidic conditions. Dehydration reaction of TBA yields isobutylene which is the main raw material of MTBE, the mostly used fuel oxygenates.

SALES SPECIFICATION

APPEARANCE	colorless, non-corrosive liquid
TBA	99.3% min
WATER	0.15% max
ACIDITY	0.003% max (as ACETIC ACID)

SPECIFIC GRAVITY	0.781 - 0.785 at 26/26 C
DISTILLATION RANGE	81.5 C min (IBP) , 83.0 C max (DP)
NON-VOLATILE MATTER	0.001 max (g/100ml)
COLOR (Pt-Co)	10 max

TRANSPORTATION

PACKING	
HAZARD CLASS	3
UN NO.	1120

OTHER INFORMATION

European Hazard Symbols: XN F, Risk Phrases: 11-20, Safety Phrases: 9-10

GENERAL DESCRIPTION OF ALCOHOL

Alcohols are widely used as solvents, fuels and chemical raw materials. Generally, hydroxyl group compounds are polar, which trends to promote solubility in water. But the carbon chain resist to solubility in water. Short chain alcohols (methanol, ethanol, and propanol) in which the hydroxyl group predominates are miscible in water. Butanol is moderately soluble because of the balance between the two opposing solubility trends. Higher alcohols are practically insoluble in water because of the hydrocarbon chain's trend is stronger. Alcohols are "protic" solvents. Protic refers to a hydrogen atom attached to an electronegative atom, oxygen. Polar protic solvents are compounds that can be represented by the general formula ROH of which water (H_2O), methanol (CH_3OH) and acetic acid (CH_3COOH) are examples. Water-soluble alcohols, low-molecular weight products, are solvents for the manufacture of coatings, dyes and inks, plastics, flavorings, personal-care products, pharmaceuticals, and cleaners. The higher alcohols, slightly soluble in water or insoluble, can provide the proper balance of target properties when solvent-based solvents are formulated for desired viscosity, flowing and leveling, and curing rate and can be used as coupling agents in waterborne coatings.

Alcohols are very weak acids as they lose H^+ in the hydroxyl group. Alcohols undergoes dehydration reaction which means the elimination of water molecule replaced by a pi bond between two adjacent carbon atoms to form alkenes under heating in the presence of strong acids like hydrocloric acid or phosphoric acid. Primary and secondary alcohols can be oxidized to aldehydes and ketones respectively. Carboxylic acids are obtained from oxidation of aldehydes. Oxidation in organic chemistry can be considered to be the loss of hydrogen or gain of oxygen and reduction to gain hydrogen or loss of oxygen. Tertiary alcohols do not react to give oxidation products as they have no H attached to the alcohol carbon. Alcohols undergoes important reactions called nucleophilic substitution in which an electron donor replaces a leaving group, generally conjugate bases of strong acids, as a covalent substitute of some atom. One of important reaction of alcohol is condensation. Ethers are formed by the condensation of two alcohols by heating with sulfuric acid; the reaction is one of dehydration. Almost infinite esters are formed through condensation reaction called esterification between carboxylic acid and alcohol, which produces water. Alcohols are important solvents and chemical raw materials. Alcohols are intermediates for the production of target compounds, such as pharmaceuticals, veterinary medicines, plasticizers, surfactants, lubricants, ore floatation agents, pesticides, hydraulic fluids, and detergents.

Carbinol is a primary alcohol with general formula RCH_2OH. In carbinol nomenclature system, the term of carbinol is methanol itself and other groups are considered to have replaced one of the methanol hydrogen atoms to describe larger alcohols as derivatives of carbinol. This nomenclature system is particularly useful when the groups attached to the methanol carbon are large, aromatic, and cyclo groups. Benzyl alcohol is called phenylcarbinol or benzenecarbinol whilebenzyl carbinol is phenylethyl alcohol.