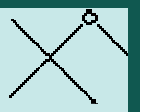
METHYL TERT-BUTYL ETHER



PRODUCT IDENTIFICATION

CAS NO.	1634-04-4
EINECS NO.	216-653-1
FORMULA	$(CH_3)_3COCH_3$
MOL WT.	88.15
H.S. CODE	2909.19
TOXICITY	Oral rat LD50: 4000 mg/kg
SYNONYMS	2-Methoxy-2-methylpropane; methyl t-butyl ether;

Tert-butyl methyl ether; Methyl Tertiary Butyl Ether; Methyl 1,1-dimethylethyl ether; 2-Methyl-2-methoxypropane;

DERIVATION CLASSIFICATION	

PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE	clear liquid
MELTING POINT	-109 C
BOILING POINT	55 - 56 C
SPECIFIC GRAVITY	0.74
SOLUBILITY IN WATER	slightly soluble (4.5 - 5.5 g/l at 25 C)
pH	
VAPOR DENSITY	
AUTOIGNITION	
NFPA RATINGS	Health: 2; Flammability: 3; Reactivity: 0
REFRACTIVE INDEX	
FLASH POINT	-28 C
STABILITY	Stable under ordinary conditions

GENERAL DESCRIPTION & APPLICATIONS

MTBE (Methyl-tert-Butyl Ether) is a volatile, low viscosity clear liquid at room temperature with an ether odour; boiling point 55.2 C; melting point -109 C. MTBE is flammable and can form explosive mixtures with air. It is slightly soluble in water and very soluble ethers and alcohol and in most organic solvents including hydro carbons. MTBE is an ether which contains an oxygen atom bonded to two carbon atoms. In Methyl-tert-Butyl Ether, one carbon atom is that of a methyl group and the other is the central atom in a tertiary butyl group. MTBE is prepared by reacting isobutylene contained in a mixed C4 stream with methanol in the presence of an acidic ion-exchange resin catalyst such as sulfonated styrene linked with divinyl benzene at 100 C. Isobutylene can also be prepared from TBA by dehydration and from n-butane by isomerization without dehydration. The most quantity produced worldwide is used as an oxygenate to gasoline. It is added both to increase octane enhancement to replace banned tetraethyl lead and to raise the oxygen content in gasoline. It is known that MTBE in fuel reduces exhaust emissions of VOC (volatile organic compounds: acetaldehyde, benzene, 1,3-butadiene, ethylbenzene, formaldehyde, toluene, xylenes, and particulate organic matter) except formaldehyde. Ozone is formed by the reaction of sunlight with NOx and VOCs. Some quantity of MTBE is used in the preparation of isobutene. With strong solvating capabilities for a wide variety of compounds including unsaturated hydrocarbons and steroids, MTBE is used as a reaction medium and extraction solvent to replace methylene chloride, aromatics, and other ethers. MTBE is a non-chlorinated process solvent. It is used as a solvent for chromotographic techniques. The sterically hindered tertiary butyl group imparts stability. It possesses a much lower tendency to form explosive organic peroxides than most ethers. It has

also an acid stability compare to other diether acetals. It forms azeotrope with water (52 - 53 C) and methanol (51 - 52 C). It is used as a solvent in Grignard synthesis and other organometallic reactions. It is used as an anionic and cationic polymerization solvent.

SALES SPECIFICATION	
APPEARANCE	clear liquid
ASSAY (G.C)	98.0% min
METHANOL	0.3% max
DIISOBUTYLENE	1.0% max
TRIISOBUTYLENE	1.0% max
T-BUTYL ALCOHOL	1.0% max
C4 C5 HYDROCARBONS	1.0% max
WATER	500ppm max
Cu CORROSION	Pass

TRANSPORTATION	
PACKING	
HAZARD CLASS	3 (Packing Group: II)
UN NO.	2398

OTHER INFORMATION

Hazard Symbols: XI F, Risk Phrases: 11-38, Safety Phrases: 9-16-33-37

GENERAL DESCRIPTION OF ETHER

Ether is any of a number of organic compounds characterized by an oxygen atom joined by two carbon atoms that are part of hydrocarbon groups. The general formula is ROR', where R and R' are alkyl groups. Ethers are formed by the condensation of two alcohols. They are similar to alcohols but are generally less dense, less soluble in water, and have lower boiling points. They are relatively unreactive chemically. This unreactive property makes ethers valuable as solvents. Common names of ethers simply list the alkyl groups in alphabetical order (ethyl methyl ether, IUPAC name is methoxyethane). Epoxides and crown ether are a special class of cyclic ethers. Epoxide (oxirane) is a three-membered cyclic ether in which an oxygen atom is joined to each of two carbon atoms that are already bonded to each other. Crown Ether is a macrocyclic polyether whose structure contains hydrogen, carbon and oxygen atoms. Each oxygen atoms are confined between two carbon atoms and exhibits a conformation with a hole (accordingly called "crown").