



>>Entry Name: 2-Methoxy-2-methylpropane, 9CI

Synonym(s): *tert*-Butyl methyl ether, 8CI. Methyl (2-methyl-2-propyl) ether. Methyl *tert*-butyl ether. MTBE

CAS Registry Number: 1634-04-4

(H₃C)₃COMe

Molecular Formula: C₅H₁₂O

Molecular Weight: 88.149

Accurate Mass: 88.088815

Percentage Composition: C 68.13%; H 13.72%; O 18.15%

Use/Importance: Reagent for esterifications and formation of sugar methyl glycosides. Important industrial chemical, 18th in order of volume for USA in 1994 (production 6.83 million tons/year). Less hazardous than Diethyl ether BGW51-U with little tendency to form peroxides. Dissolves cholesterol, and has been used in treatment of gallstones. Fuel additive

Biological Use/Importance: Cholelitholytic agent

Melting Point: Mp -109°

Boiling Point: Bp 54°

Solubility: Spar. sol. H₂O

Density: d₄²⁰ 0.741

Refractive Index: n_D²⁰ 1.3689

Hazard & Toxicity: Highly flammable, fl. p. -28°. Irritating to eyes and mucous membranes. Anaesthetic properties

Aldrich: 44380-8

Fluka: 20252

Sigma: B9281

Supelco: 4-8027

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 319B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 266D, (*ir*)

U.S. Pat., 1934, 1 968 601; *CA*, **28**, 5831

Derevitskaya, V.A. *et al.*, *Tet. Lett.*, 1969, 4769; 1970, 4269, (*use*)

Konno, C. *et al.*, *Tetrahedron*, 1976, **32**, 325, (*cmr*)

Allen, M.J. *et al.*, *Gastroenterology*, 1985, **88**, 122-125; **89**, 1097-1103, (*pharmacol*)

Suwa, A. *et al.*, *J. Mol. Struct.*, 1988, **172**, 275, (*mol struct, ir*)

Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **9**, 860

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 1888

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MHV859

Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 465