



>>Entry Name: Trimethyl phosphate, 9CI

Synonym(s): Trimethoxooxophosphorus(V)

CAS Registry Number: 512-56-1

(MeO)₃P=O

Molecular Formula: C₃H₉O₄P

Molecular Weight: 140.075

Accurate Mass: 140.023847

Percentage Composition: C 25.72%; H 6.48%; O 45.69%; P 22.11%

Use/Importance: Solvent for aromatic halogenations and nitrations. Methylating agent for nitrogen heterocyclic compds.

Physical Description: Pleasant smelling liq.

Boiling Point: Bp 196°. Bp₅₀ 110°. Bp₅ 62°

Solubility: Sol. H₂O, org. solvs.

Density: d₄²⁰ 1.21

Refractive Index: n_D²⁰ 1.3963

Hazard & Toxicity: Fl. p. 107°. Residue from a large-scale dist. at atm. pressure exploded. Dist. *in vacuo* recommended, in presence of MgO. LD₅₀ (rat, orl) 840 mg/kg

Aldrich: 24102-4

Fluka: 92720

Sigma: T8257

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 925C, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1495C, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 846D, (ir)
Evans, D.P. *et al.*, *J.C.S.*, 1930, 1310-1313, (synth)
Yamauchi, K. *et al.*, *J.C.S. Perkin I*, 1973, 391-392, (props, use)
Pearson, D.E. *et al.*, *Synthesis*, 1976, 621-623, (use)
Cowley, A.H. *et al.*, *Inorg. Chim. Acta*, 1977, **25**, L151-L152, (pe)
Burkhardt, W.D. *et al.*, *Z. Anorg. Allg. Chem.*, 1978, **442**, 19-25, (ir, Raman)
Lowe, G. *et al.*, *Chem. Comm.*, 1979, 733-735, (O-17 nmr, P-31 nmr)
Wolff, R. *et al.*, *Z. Phys. Chem. (Leipzig)*, 1980, **261**, 726-744, (struct)
Kawazoe, Y. *et al.*, *Chem. Pharm. Bull.*, 1982, **30**, 2077-2086, (props, use)
Cload, P.A. *et al.*, *Org. Mass Spectrom.*, 1983, **18**, 57-59, (ms)
Cowley, A.H. *et al.*, *Inorg. Chem.*, 1984, **23**, 3378-3383, (pe)
Cohen, J.S. *et al.*, *J. Magn. Reson.*, 1984, **59**, 181-187, (pmr)
Appling, J.R. *et al.*, *Org. Mass Spectrom.*, 1985, **20**, 343-350, (ms)
Yarkov, A.V. *et al.*, *Zh. Obshch. Khim.*, 1985, **55**, 50-53; *J. Gen. Chem. USSR (Engl. Transl.)*, 1985, **55**, 42-44, (ir, Raman, conformn)
Barcelo, D. *et al.*, *J. Chem. Res.*, 1989, **474**, 163-173, (hplc-ms)
Taga, K. *et al.*, *J. Mol. Struct.*, 1989, **212**, 157-168, (Raman, struct)
Thruston, A.D. *et al.*, *J. Am. Soc. Mass Spectrom.*, 1991, **2**, 419-426, (ms, anal)
D'Agostino, P.A. *et al.*, *CA*, 1995, **122**, 105971, (glc-ms, ms)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 1241
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992, 1289
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, TMD250