



>>Entry Name: Tris(trimethylsilyl) phosphate

Synonym(s): Trimethylsilanol 3:1 phosphate, 9Cl

CAS Registry Number: 10497-05-9

$(\text{Me}_3\text{SiO})_3\text{P}=\text{O}$

Molecular Formula: $\text{C}_9\text{H}_{27}\text{O}_4\text{PSi}_3$

Molecular Weight: 314.54

Accurate Mass: 314.095478

Percentage Composition: C 34.37%; H 8.65%; O 20.35%; P 9.85%; Si 26.79%

Source/Synthesis: Synth. from $\text{H}_3\text{PO}_4 + \text{Me}_3\text{SiCl} + \text{Et}_3\text{N}$

Use/Importance: Commercially available. Reagent for Beckmann rearrangement

Physical Description: Liq.

Boiling Point: Bp 232°. Bp₅ 93-94°

Density: d_4^{20} 0.96

Refractive Index: n_D^{20} 1.4100

Other Data: Viscosity 1.4090 cP

Hazard & Toxicity: Fl. p. 110°C. LD₅₀ (rat, orl) 3440 mg/kg

Aldrich: 27579-4

Fluka: 93409

Other: Gelest

>>Derivative: Methoiodide

Synonym(s): Methoxytris(trimethylsilyloxy)phosphonium iodide

Molecular Formula: $\text{C}_{10}\text{H}_{30}\text{IO}_4\text{PSi}_3$

Molecular Weight: 456.479

Accurate Mass: 456.023426

Percentage Composition: C 26.31%; H 6.62%; I 27.80%; O 14.02%; P 6.79%; Si 18.46%

Physical Description: Solid

Melting Point: Mp 95-96°

Solubility: Sol. CH_2Cl_2

>>Derivative: Me_3SiI adduct

Synonym(s): Tetrakis(trimethylsilyloxy)phosphonium iodide

Molecular Formula: $\text{C}_{12}\text{H}_{36}\text{IO}_4\text{PSi}_4$

Molecular Weight: 514.634

Accurate Mass: 514.047303

Percentage Composition: C 28.01%; H 7.05%; I 24.66%; O 12.44%; P 6.02%; Si 21.83%

Source/Synthesis: Synth. from the parent phosphate + Me_3SiI

Physical Description: Solid

Melting Point: Mp 151°

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 700B, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1664A, (ir)

Voronkov, M.G. *et al.*, *Zh. Obshch. Khim.*, 1972, **42**, 2030; *J. Gen. Chem. USSR (Engl. Transl.)*, 1972, **42**, 2027, (synth)

Schmidbaur, H. *et al.*, *Chem. Ber.*, 1974, **107**, 1731, (synth, derivs, ir, pmr)

Lebedev, E.P. *et al.*, *Zh. Obshch. Khim.*, 1974, **44**, 787; 1769; *J. Gen. Chem. USSR (Engl. Transl.)*, 1974, **44**, 759; 1736, (synth)

Kolodyaznyi, Yu.V. *et al.*, *Zh. Obshch. Khim.*, 1975, **45**, 749; *J. Gen. Chem. USSR (Engl. Transl.)*, 1975, **45**, 738, (struct)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, PHE750