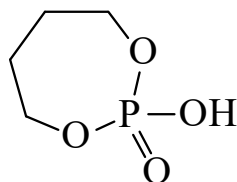




>>Entry Name: 2-Hydroxy-1,3,2-dioxaphosphhepane 2-oxide, 9Cl, 8Cl

ENTRY UNDER REVIEW

Synonym(s): Tetramethylene phosphoric acid. Tetramethylene hydrogen phosphate



CAS Registry Number: 51374-71-1

Molecular Formula: C₄H₉O₄P

Molecular Weight: 152.086

Accurate Mass: 152.023847

Percentage Composition: C 31.59%; H 5.96%; O 42.08%; P 20.37%

Physical Description: Cryst. (CH₂Cl₂), plates (C₆H₆)

Melting Point: Mp 129-131°

pKa Value: pK_a 1.58 (H₂O) pK_a 6.51 (EtOH) pK_a 10.02 (MeNO₂)

>>Derivative: 2-Ethoxy (Et ester)

Synonym(s): 2-Ethoxy-1,3,2-dioxaphosphhepane 2-oxide. Ethyl tetramethylene phosphate

CAS Registry Number: 18748-21-5

Molecular Formula: C₆H₁₃O₄P

Molecular Weight: 180.14

Accurate Mass: 180.055147

Percentage Composition: C 40.01%; H 7.27%; O 35.53%; P 17.19%

Physical Description: Liq.

Boiling Point: Bp_{0.001} 120-130°

Refractive Index: n_D²⁰ 1.4478

>>Derivative: 2-Phenoxy (Ph ester)

Synonym(s): 2-Phenoxy-1,3,2-dioxaphosphhepane 2-oxide. Phenyl tetramethylene phosphate

CAS Registry Number: 7191-26-6

Molecular Formula: C₁₀H₁₃O₄P

Molecular Weight: 228.184

Accurate Mass: 228.055147

Percentage Composition: C 52.64%; H 5.74%; O 28.05%; P 13.57%

Physical Description: Solid

Melting Point: Mp 62-64°

References:

Munoz, A. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 3343, (*ethyl ester*)

Coulter, C.L., *J.A.C.S.*, 1975, **97**, 4084, (*cryst struct*)

Penny, C.L. *et al.*, *Can. J. Chem.*, 1978, **56**, 2396, (*phenyl ester, pmr*)

Ramirez, F. *et al.*, *Tet. Lett.*, 1982, **23**, 5375, (*synth*)

Jankowska, J. *et al.*, *Synthesis*, 1984, 408-410, (*synth, cmr*)

Krychukov, A.A. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1987, 1244-1248; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1987, 1145, (*props*)