



>>Entry Name: Monophenyl phosphate, 9Cl, 8Cl

Synonym(s): Phenyl dihydrogen phosphate. Phenyl phosphoric acid. Dihydrogen phenyl phosphate

CAS Registry Number: 701-64-4

Related CAS Registry Numbers(s): 3279-54-7 57775-14-1

PhOP(O)(OH)₂

Molecular Formula: C₆H₇O₄P

Molecular Weight: 174.093

Accurate Mass: 174.008197

Percentage Composition: C 41.40%; H 4.05%; O 36.76%; P 17.79%

Physical Description: Cryst. (CHCl₃ or H₂O)

Melting Point: Mp 99.5-100°

pKa Value: pK_{a1} 0.48; pK_{a2} 5.7 (25°,H₂O) pK_{a1} 3.23; pK_{a2} 6.23 (50% EtOH aq.)

>>Derivative: Di-NH₄ salt

Physical Description: Solid

Melting Point: Mp 164-165 dec.°

>>Derivative: Monoanilinium salt

CAS Registry Number: 1992-39-8

Physical Description: Solid

Melting Point: Mp 169-170°

>>Derivative: Bis(cyclohexylammonium) salt

CAS Registry Number: 13798-39-5

Physical Description: Prisms (EtOH aq. or H₂O)

Melting Point: Mp 190°. Mp 214-215°

>>Derivative: Difluoride

>>Derivative: Dichloride

>>Derivative: Dianilide

References:

Miyano, M., *J.A.C.S.*, 1955, **77**, 3524, (*synth*)

Montgomery, H.A.C. *et al.*, *J.C.S.*, 1958, 1963, (*synth*)

Owen, G.R. *et al.*, *Synthesis*, 1974, 704, (*synth*)

Kodolov, V.I. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1977, 165; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1977, 142, (*pmr, pe*)

Blackburn, G.M. *et al.*, *J.C.S. Perkin 1*, 1980, 1150, (*pmr*)

Yamaguchi, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 1891, (*synth, ir, pmr*)

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