



>>Entry Name: Phenylphosphonic acid, 9Cl, 8Cl

Synonym(s): Benzenephosphonic acid

CAS Registry Number: 1571-33-1

PhP(O)(OH)₂

Molecular Formula: C₆H₇O₃P

Molecular Weight: 158.093

Accurate Mass: 158.013282

Percentage Composition: C 45.58%; H 4.46%; O 30.36%; P 19.59%

Use/Importance: Fire retardant. Used as aq. soln. for pptn. of rare earth elements. Used as a 2% aq. soln. for detn. of lanthanides

Physical Description: Plates (H₂O or EtOAc)

Melting Point: Mp 162-164°

Solubility: Sol. H₂O

pKa Value: pK_{a1} 1.83; pK_{a2} 7.45 (25°)

Other Data: Titrates as a monobasic acid in Me₂CO or ROH but as dibasic in DMF

Hazard & Toxicity: LD₅₀ (mus, ipr) 110 mg/kg

Aldrich: P2900-6

Fluka: 78913

>>Derivative: Bis(triethylammonium) salt

Physical Description: Cryst. (EtOH/EtOAc)

Melting Point: Mp 112-114°

>>Derivative: Mono-Me ester

>>Derivative: Di-Me ester

>>Derivative: Mono-Et ester

>>Derivative: Di-Et ester

>>Derivative: Monopropyl ester

>>Derivative: Dipropyl ester

Synonym(s): Dipropyl phenylphosphonate

CAS Registry Number: 20677-03-6

Molecular Formula: C₁₂H₁₉O₃P

Molecular Weight: 242.254

Accurate Mass: 242.107182

Percentage Composition: C 59.50%; H 7.90%; O 19.81%; P 12.79%

Physical Description: Liq.

Boiling Point: Bp₁ 106-108°

Refractive Index: n_D²⁰ 1.4895