



CAS Registry Number: 1754-47-8

Molecular Formula: C₂₂H₃₉O₃P

Molecular Weight: 382.522

Accurate Mass: 382.263682

Percentage Composition: C 69.08%; H 10.28%; O 12.55%; P 8.10%

Physical Description: Liq.

Boiling Point: Bp₄ 204-207°. Bp_{0.001} 200°

Refractive Index: n_D²⁵ 1.4765

Aldrich: 41342-9

Fluka: 12584

Rare Chemicals Library: S57593-3

Sigma: D3399

>> **Derivative:** Mono-Ph ester

Synonym(s): Phenyl hydrogen phenylphosphonate

CAS Registry Number: 2310-87-4

Molecular Formula: C₁₂H₁₁O₃P

Molecular Weight: 234.191

Accurate Mass: 234.044582

Percentage Composition: C 61.54%; H 4.73%; O 20.50%; P 13.23%

Physical Description: Needles (EtOH aq. or hexane)

Melting Point: Mp 78-79°

Boiling Point: Bp_{0.001} 170-178°

pKa Value: pK_{a1} 0.68 (20°, 0.1M NaClO₄)

>> **Derivative:** Di-Ph ester

Synonym(s): Diphenyl phenylphosphonate

CAS Registry Number: 3049-24-9

Molecular Formula: C₁₈H₁₅O₃P

Molecular Weight: 310.288

Accurate Mass: 310.075882

Percentage Composition: C 69.68%; H 4.87%; O 15.47%; P 9.98%

Physical Description: Cryst. (petrol)

Melting Point: Mp 75-75.5°

Boiling Point: Bp_{0.45} 163-165°

>> **Derivative:** Bis(4-nitrophenyl) ester

CAS Registry Number: 38873-91-5

Molecular Formula: C₁₈H₁₃N₂O₇P

Molecular Weight: 400.284

Accurate Mass: 400.04604

Percentage Composition: C 54.01%; H 3.27%; N 7.00%; O 27.98%; P 7.74%

Use/Importance: Peptide coupling agent causing little racemization

Physical Description: Cryst. (CCl₄)

Melting Point: Mp 94-96°

>> **Derivative:** Bis(trimethylsilyl) ester

CAS Registry Number: 42449-24-1

Molecular Formula: C₁₂H₂₃O₃PSi₂

Molecular Weight: 302.457

Accurate Mass: 302.092336

Percentage Composition: C 47.65%; H 7.66%; O 15.87%; P 10.24%; Si 18.57%

Physical Description: Liq.

Boiling Point: Bp_{0.06} 77°

Density: d₄²⁰ 1.02

Refractive Index: n_D²⁰ 1.4703

>> **Derivative:** Difluoride