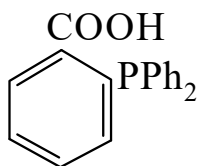




>>Entry Name: 2-(Diphenylphosphino)benzoic acid, 9CI

Synonym(s): (2-Carboxyphenyl)diphenylphosphine



CAS Registry Number: 17261-28-8

Type of Compound Code(s): AC0300

Molecular Formula: C₁₉H₁₅O₂P

Molecular Weight: 306.3

Accurate Mass: 306.080967

Percentage Composition: C 74.51%; H 4.94%; O 10.45%; P 10.11%

Physical Description: Light-yellow needles (EtOH aq. or MeOH)

Melting Point: Mp 187-188° (174-177°)

Aldrich: 45488-5

>>Derivative: Methiodide

Synonym(s): (2-Carboxyphenyl)methyldiphenylphosphonium iodide

Type of Compound Code(s): AC0310

Molecular Formula: C₂₀H₁₈IO₂P

Molecular Weight: 448.239

Accurate Mass: 448.008915

Percentage Composition: C 53.59%; H 4.05%; I 28.31%; O 7.14%; P 6.91%

Physical Description: Cryst. (Me₂CO/C₆H₆)

Melting Point: Mp 169-173 dec.°

>>Derivative: Me ester

CAS Registry Number: 79932-99-3

Type of Compound Code(s): AC0600 AC0300

Molecular Formula: C₂₀H₁₇O₂P

Molecular Weight: 320.327

Accurate Mass: 320.096617

Percentage Composition: C 74.99%; H 5.35%; O 9.99%; P 9.67%

Physical Description: Cryst.

Melting Point: Mp 96-97°

>>Derivative: Anilide

CAS Registry Number: 91410-02-5

Type of Compound Code(s): AC0300

Molecular Formula: C₂₅H₂₀NOP

Molecular Weight: 381.413

Accurate Mass: 381.128251

Percentage Composition: C 78.73%; H 5.29%; N 3.67%; O 4.19%; P 8.12%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 87-88°

>>Derivative: Oxide

CAS Registry Number: 2572-40-9

Type of Compound Code(s): AC0310

Molecular Formula: C₁₉H₁₅O₃P

Molecular Weight: 322.299

Accurate Mass: 322.075882

Percentage Composition: C 70.81%; H 4.69%; O 14.89%; P 9.61%

Physical Description: Cryst. (EtOH, EtOH aq., or AcOH aq.)

Melting Point: Mp 252-254°. Mp 262-264 274-275°°

pKa Value: pK_a 5.37 (50% EtOH aq.)