



>>Entry Name: 4-(Diphenylphosphino)benzoic acid, 9CI

Synonym(s): (4-Carboxyphenyl)diphenylphosphine

CAS Registry Number: 2129-31-9

Related CAS Registry Numbers(s): 78952-89-3 101630-35-7

Type of Compound Code(s): AC0300

Structure by analogy with 2-(Diphenylphosphino)benzoic acid, [DPW08-T](#)

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%

Use/Importance: Ligand for Pd, Ru

Physical Description: Cryst. (AcOH)

Melting Point: Mp 156-158°

pKa Value: pK_a 5.39 (50% EtOH aq.)

Aldrich: 40159-5

>>Derivative: Me ester

Synonym(s): Methyl 4-(diphenylphosphino)benzoate

CAS Registry Number: 5032-51-9

Type of Compound Code(s): 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. (MeOH)

Melting Point: Mp 98-99°

>>Derivative: Oxide

Synonym(s): 4-(Diphenylphosphinyl)benzoic acid

CAS Registry Number: 2272-04-0

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. (MeOH aq. or dioxan aq.)

Melting Point: Mp 273-274°

pKa Value: pK_a 4.88 (50% EtOH aq.)

>>Derivative: Oxide, Me ester

Synonym(s): Methyl 4-(diphenylphosphinyl)benzoate

Type of Compound Code(s): AC0310

Molecular Formula: C₂₀H₁₇O₃P

Molecular Weight: 336.326

Accurate Mass: 336.091532

Percentage Composition: C 71.42%; H 5.09%; O 14.27%; P 9.21%

Physical Description: Cryst. (MeOH aq. or Et₂O/hexane)

Melting Point: Mp 113-116°

>>Derivative: Sulfide

Synonym(s): *p*-(Diphenylphosphinothiioyl)benzoic acid

CAS Registry Number: 5068-24-6

Type of Compound Code(s): AC0330

Molecular Formula: C₁₉H₁₅O₂PS

Molecular Weight: 338.366

Accurate Mass: 338.053037

Percentage Composition: C 67.44%; H 4.47%; O 9.46%; P 9.15%; S 9.48%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 177-178.5°

pKa Value: pK_a 4.97 (50% EtOH aq.)