



>>Entry Name: 3-(Diethoxyphosphinyl)propanoic acid, 9CI

CAS Registry Number: 3095-96-3

(EtO)2P(O)CH2CH2COOH

Molecular Formula: C₇H₁₅O₅P

Molecular Weight: 210.166

Accurate Mass: 210.065712

Percentage Composition: C 40.00%; H 7.19%; O 38.06%; P 14.74%

Physical Description: Cryst. (Et₂O/pentane)

Melting Point: Mp 37.5-38.5°

pKa Value: pK_{a1} 4.28 (25°,H₂O) pK_{a1} 5.26 (25°,50% EtOH aq.)

>>Derivative: Me ester

Synonym(s): Methyl 3-(diethoxyphosphinyl)propanoate

CAS Registry Number: 1112-94-3

Molecular Formula: C₈H₁₇O₅P

Molecular Weight: 224.193

Accurate Mass: 224.081362

Percentage Composition: C 42.86%; H 7.64%; O 35.68%; P 13.82%

Physical Description: Liq.

Boiling Point: Bp₁₄ 154-155°. Bp₃ 115-117°

Density: d₄²⁰ 1.12

Refractive Index: n_D²⁰ 1.4346

>>Derivative: Et ester

Synonym(s): Ethyl 3-(diethoxyphosphinyl)propanoate. Triethyl 3-phosphonopropanoate

CAS Registry Number: 3699-67-0

Molecular Formula: C₉H₁₉O₅P

Molecular Weight: 238.22

Accurate Mass: 238.097012

Percentage Composition: C 45.38%; H 8.04%; O 33.58%; P 13.00%

Boiling Point: Bp₁₂ 156-158°. Bp_{0.2} 110-111°

Density: d₄²⁰ 1.1

Refractive Index: n_D²⁰ 1.4315

Aldrich: 39188-3

>>Derivative: Amide

Molecular Formula: C₇H₁₆NO₄P

Molecular Weight: 209.181

Accurate Mass: 209.081696

Percentage Composition: C 40.19%; H 7.71%; N 6.70%; O 30.59%; P 14.81%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 74.5-76°. Mp 60-63°

>>Derivative: Nitrile

Synonym(s): 3-(Diethoxyphosphinyl)propanenitrile

Molecular Formula: C₇H₁₄NO₃P

Molecular Weight: 191.166

Accurate Mass: 191.071131

Percentage Composition: C 43.98%; H 7.38%; N 7.33%; O 25.11%; P 16.20%

Physical Description: Liq.

Boiling Point: Bp₁₀ 160°. Bp_{0.1} 110°

Other Data: n_D 1.4382

References: