



>>Entry Name: 2-(Diethoxyphosphinyl)butanoic acid, 9CI

Related CAS Registry Numbers(s): 17145-91-4 81376-66-1 87180-46-9 111948-07-3
(EtO)₂P(O)CH(COOH)CH₂CH₃

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%

>>Variant: (±)-form

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%

>>Derivative: Me ester

Synonym(s): Methyl 2-(diethoxyphosphinyl)butanoate

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%

Physical Description: Liq.

Boiling Point: Bp_{0.25} 86°

>>Derivative: Et ester

Synonym(s): Ethyl 2-(diethoxyphosphinyl)butanoate. Triethyl 2-phosphonobutanoate

CAS Registry Number: 17145-91-4

Molecular Formula: C₁₀H₂₁O₅P

Molecular Weight: 252.247

Accurate Mass: 252.112662

Percentage Composition: C 47.62%; H 8.39%; O 31.71%; P 12.28%

Use/Importance: Wittig-Horner reagent for the synth. of enoic ethyl esters

Physical Description: Liq.

Boiling Point: Bp_{0.6} 117-118°

Density: d₄²⁰ 1.11

Refractive Index: n_D²⁰ 1.4310 n_D²⁰ 1.4530

Aldrich: 41746-7

>>Derivative: Ph ester

Synonym(s): Phenyl 2-(diethoxyphosphinyl)butanoate

CAS Registry Number: 53327-49-4

Molecular Formula: C₁₄H₂₁O₅P

Molecular Weight: 300.291

Accurate Mass: 300.112662

Percentage Composition: C 56.00%; H 7.05%; O 26.64%; P 10.31%

Physical Description: Cryst. (cyclohexane)

Melting Point: Mp 97-98°

References:

Berry, J.P. *et al.*, *J.O.C.*, 1972, **37**, 4396, (*synth*)

Rachon, J. *et al.*, *Z. Chem.*, 1974, **14**, 152, (*synth, ir, pmr*)

Runge, W. *et al.*, *Annalen*, 1975, 1361, (*use*)

Moskva, V.V. *et al.*, *Zh. Obshch. Khim.*, 1976, **46**, 536; *J. Gen. Chem. USSR (Engl. Transl.)*, 1976, **46**, 529, (*synth*)

Huston, R. *et al.*, *Helv. Chim. Acta*, 1982, **65**, 1563, (*use*)

Kandil, A.A. *et al.*, *Synthesis*, 1987, 411, (*Me ester, ir, pmr*)

Tay, M.K. *et al.*, *Synth. Commun.*, 1988, **18**, 1349, (*Et ester, synth, P-31 nmr*)

Henin, F. *et al.*, *Tetrahedron*, 1989, **45**, 6171, (*methyl ester, synth, ir, ms, pmr, reactions*)

Nakano, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1990, **63**, 2224, (*ester, synth, pmr*)