



>>Entry Name: 3-Phosphonopropanoic acid, 9CI

Synonym(s): (2-Carboxyethyl)phosphonic acid

CAS Registry Number: 5962-42-5

Related CAS Registry Numbers(s): 81582-16-3 81582-17-4 131328-38-6

HOOCCH2CH2P(O)(OH)2

Molecular Formula: C₃H₇O₅P

Molecular Weight: 154.059

Accurate Mass: 154.003112

Percentage Composition: C 23.39%; H 4.58%; O 51.93%; P 20.11%

Physical Description: Cryst. (AcOH/CHCl₃)

Melting Point: Mp 167°. Mp 178°

pKa Value: pK_{a1} 2.26; pK_{a2} 4.63; pK_{a3} 7.75 (25°,H₂O)

Hazard & Toxicity: May be cytotoxic

Aldrich: 22855-9

>>Derivative: Mono-*p*-toluidinium salt

Physical Description: Cryst. (EtOH)

Melting Point: Mp 158°

>>Derivative: Et ester

Synonym(s): Ethyl 3-phosphonopropanoate

CAS Registry Number: 72563-46-3

Molecular Formula: C₅H₁₁O₅P

Molecular Weight: 182.113

Accurate Mass: 182.034412

Percentage Composition: C 32.98%; H 6.09%; O 43.93%; P 17.01%

Physical Description: Plates (C₆H₆)

Melting Point: Mp 64.5°

>>Derivative: Triethyl ester

>>Derivative: *P,P*-Dibutyl *O*-Me triester

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

Molecular Formula: C₁₂H₂₅O₅P

Molecular Weight: 280.3

Accurate Mass: 280.143962

Percentage Composition: C 51.42%; H 8.99%; O 28.54%; P 11.05%

Physical Description: Liq.

Boiling Point: Bp_{0.001} 78-90°

Density: d₄²⁰ 1.06

Refractive Index: n_D²⁰ 1.4383

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 918D, (*ir*)

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Bochwic, B. *et al.*, *Pol. J. Chem. (Rocz. Chem.)*, 1951, **25**, 338, (*synth, derivs*)

Ginsberg, V.A. *et al.*, *Zh. Obshch. Khim.*, 1960, **30**, 3987; *J. Gen. Chem. USSR (Engl. Transl.)*, 1960, **30**, 3944, (*synth*)

Kreutzkamp, N. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1962, **295**, 773, (*synth*)

Heubel, P.H.C. *et al.*, *J. Solution Chem.*, 1979, **8**, 615, (*props*)

Jaeggi, K.A. *et al.*, *Phosphorus, Sulfur, Silicon, Relat. Elem.*, 1990, **54**, 197, (*salts, synth, pmr, cmr*)

Robitaille, P.M.L. *et al.*, *J. Magn. Reson.*, 1991, **92**, 73-84, (*P-31 nmr, props*)