



>>Entry Name: (3-Aminopropyl)phosphonic acid, 9Cl, 8Cl

CAS Registry Number: 13138-33-5

$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{P}(\text{O})(\text{OH})_2$

Molecular Formula: $\text{C}_3\text{H}_{10}\text{NO}_3\text{P}$

Molecular Weight: 139.091

Accurate Mass: 139.039831

Percentage Composition: C 25.91%; H 7.25%; N 10.07%; O 34.51%; P 22.27%

General Statement: Free acid probably exists in dipolar form

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 282-288°. Mp 274°

Aldrich: 26861-5

Sigma: A7884

>>Derivative: Di-Et ester

Synonym(s): Diethyl (3-aminopropyl)phosphonate

CAS Registry Number: 4402-24-8

Molecular Formula: $\text{C}_7\text{H}_{18}\text{NO}_3\text{P}$

Molecular Weight: 195.198

Accurate Mass: 195.102431

Percentage Composition: C 43.07%; H 9.29%; N 7.18%; O 24.59%; P 15.87%

Physical Description: Liq.

Boiling Point: Bp_{0.0075} 68-75° (lit. gives a pressure range). Bp_{0.01} 92-95°

>>Derivative: Diisopropyl ester

Synonym(s): Diisopropyl (3-aminopropyl)phosphonate

CAS Registry Number: 53253-56-8

Molecular Formula: $\text{C}_9\text{H}_{22}\text{NO}_3\text{P}$

Molecular Weight: 223.251

Accurate Mass: 223.133731

Percentage Composition: C 48.42%; H 9.93%; N 6.27%; O 21.50%; P 13.87%

Physical Description: Liq.

Boiling Point: Bp_{0.018} 74°

>>Derivative: N-Ac, Di-Et ester

Molecular Formula: $\text{C}_9\text{H}_{20}\text{NO}_4\text{P}$

Molecular Weight: 237.235

Accurate Mass: 237.112996

Percentage Composition: C 45.57%; H 8.50%; N 5.90%; O 26.98%; P 13.06%

Physical Description: Liq.

Boiling Point: Bp_{0.05} 125°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 1477C, (nmr)
Kosolapoff, G.M., *J.A.C.S.*, 1947, **69**, 2112, (synth)
Harvey, D.J. *et al.*, *J. Chromatogr.*, 1973, **79**, 65, (derivs, glc, ms)
Collins, D.J. *et al.*, *Aust. J. Chem.*, 1974, **27**, 1759, (diethyl ester, ir, pmr, deriv)
Cassaigne, A. *et al.*, *C. R. Hebd. Seances Acad. Sci. Ser. D*, 1976, **282**, 1637, (metab)
Brigot, D. *et al.*, *Tetrahedron*, 1979, **35**, 1345, (synth, pmr)
Glowiak, T. *et al.*, *Acta Cryst. B*, 1980, **36**, 961, (cryst struct)
Fabre, G. *et al.*, *Can. J. Chem.*, 1981, **59**, 864, (synth, ir, pmr)
Appleton, T.G. *et al.*, *Aust. J. Chem.*, 1984, **37**, 1833, (pmr, cmr, P-31 nmr, struct)
Rosowski, A. *et al.*, *J. Med. Chem.*, 1988, **31**, 1326, (diethyl ester, synth, ir)
Wasielewski, C. *et al.*, *J. Prakt. Chem.*, 1989, **331**, 507, (synth, ir, pmr)
Harris, R.K. *et al.*, *Magn. Reson. Chem.*, 1989, **27**, 470, (P-31 nmr, ms)
Glowacki, Z. *et al.*, *Magn. Reson. Chem.*, 1989, **27**, 897, (cmr)
Wasielewski, C. *et al.*, *Synthesis*, 1989, 52, (synth, ir, pmr)
Glowacki, R.K. *et al.*, *Phosphorus, Sulfur, Silicon, Relat. Elem.*, 1991, **60**, 67, (P-31 nmr)
Cameron, D.G. *et al.*, *Phosphorus, Sulfur, Silicon, Relat. Elem.*, 1993, **83**, 21, (ms, pmr, cmr, P-31 nmr)