



>>Entry Name: (1-Aminopentyl)phosphonic acid, 9CI

CAS Registry Number: 13138-37-9

Related CAS Registry Numbers(s): 77526-42-2 80125-38-8 80125-40-2

$\text{H}_3\text{C}(\text{CH}_2)_3\text{CH}(\text{NH}_2)\text{P}(\text{O})(\text{OH})_2$

Molecular Formula: $\text{C}_5\text{H}_{14}\text{NO}_3\text{P}$

Molecular Weight: 167.144

Accurate Mass: 167.071131

Percentage Composition: C 35.93%; H 8.44%; N 8.38%; O 28.72%; P 18.53%

>>Variant: (±)-form

CAS Registry Number: 33439-83-7

Molecular Formula: $\text{C}_5\text{H}_{14}\text{NO}_3\text{P}$

Molecular Weight: 167.144

Accurate Mass: 167.071131

Percentage Composition: C 35.93%; H 8.44%; N 8.38%; O 28.72%; P 18.53%

Physical Description: Solid

Melting Point: Mp 263-264°. Mp 285-287°

pKa Value: $\text{p}K_{\text{a}2}$ 5.7; $\text{p}K_{\text{a}3}$ 10.29 (25°)

>>Derivative: Di-Et ester

Synonym(s): Diethyl (1-aminopentyl)phosphonate

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: Characterised spectroscopically

>>Derivative: N-Benzoyl

Synonym(s): [1-(Benzoylamino)pentyl]phosphonic acid

Molecular Formula: $\text{C}_{12}\text{H}_{18}\text{NO}_4\text{P}$

Molecular Weight: 271.252

Accurate Mass: 271.097346

Percentage Composition: C 53.14%; H 6.69%; N 5.16%; O 23.59%; P 11.42%

Physical Description: Solid

Melting Point: Mp 106-107°

>>Derivative: N-Benzyl

Synonym(s): [1-(Benzylamino)pentyl]phosphonic acid

Molecular Formula: $\text{C}_{12}\text{H}_{20}\text{NO}_3\text{P}$

Molecular Weight: 257.269

Accurate Mass: 257.118081

Percentage Composition: C 56.02%; H 7.84%; N 5.44%; O 18.66%; P 12.04%

Physical Description: Solid

Melting Point: Mp 205-207°

References:

- Tyka, R., *Tet. Lett.*, 1970, 677, (*synth, deriv*)
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Constantin, E. *et al.*, *Org. Mass Spectrom.*, 1986, **21**, 431, (*ms*)
Kudzin, Z.H. *et al.*, *J. Organomet. Chem.*, 1989, **376**, 245, (*synth, tlc, P-31 nmr*)
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