



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

CAS Registry Number: 13138-36-8

Related CAS Registry Numbers(s): 82730-39-0 82730-40-3 83245-93-6

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

Molecular Formula: $\text{C}_4\text{H}_{12}\text{NO}_3\text{P}$

Molecular Weight: 153.117

Accurate Mass: 153.055481

Percentage Composition: C 31.38%; H 7.90%; N 9.15%; O 31.35%; P 20.23%

Aldrich: 36736-2

Sigma: A6537

>>Variant: (S)-form

CAS Registry Number: 82730-39-0

Molecular Formula: $\text{C}_4\text{H}_{12}\text{NO}_3\text{P}$

Molecular Weight: 153.117

Accurate Mass: 153.055481

Percentage Composition: C 31.38%; H 7.90%; N 9.15%; O 31.35%; P 20.23%

>>Derivative: Di-Et ester

CAS Registry Number: 104549-65-7

Molecular Formula: $\text{C}_8\text{H}_{20}\text{NO}_3\text{P}$

Molecular Weight: 209.225

Accurate Mass: 209.118081

Percentage Composition: C 45.93%; H 9.63%; N 6.69%; O 22.94%; P 14.80%

Physical Description: Oil

Boiling Point: $\text{Bp}_{0.01}$ 130°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +4.83$ (c, 1.48 in CHCl_3)

>>Variant: (±)-form

CAS Registry Number: 20263-10-9

Molecular Formula: $\text{C}_4\text{H}_{12}\text{NO}_3\text{P}$

Molecular Weight: 153.117

Accurate Mass: 153.055481

Percentage Composition: C 31.38%; H 7.90%; N 9.15%; O 31.35%; P 20.23%

Physical Description: Solid

Melting Point: Mp 262-264°. Mp 298-299°

pKa Value: $\text{pK}_{\text{a}3}$ 10.32

>>Derivative: Di-Et ester

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

CAS Registry Number: 114299-27-3

Molecular Formula: $\text{C}_8\text{H}_{20}\text{NO}_3\text{P}$

Molecular Weight: 209.225

Percentage Composition: C 45.93%; H 9.63%; N 6.69%; O 22.94%; P 14.80%

Physical Description: Characterised spectroscopically

>>Derivative: N-Benzoyl

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

Molecular Formula: $\text{C}_{11}\text{H}_{16}\text{NO}_4\text{P}$

Molecular Weight: 257.225

Accurate Mass: 257.081696

Percentage Composition: C 51.36%; H 6.27%; N 5.45%; O 24.88%; P 12.04%

Physical Description: Solid

Melting Point: Mp 186-187°