>>**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

$H_3CCH_2CH_2CH(NH_2)P(O)(OH)_2$

Molecular Formula: $C_4H_{12}NO_3P$
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%
General Statement: Free acid exists in dipolar forms

Aldrich: 36736-2
Sigma: A6537

>>**Variant:** (*S*)-form

CAS Registry Number: 82730-39-0
Molecular Formula: $C_4H_{12}NO_3P$
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: $C_8H_{20}NO_3P$
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: $Bp_{0.01}$ 130°
Optical Rotation: $[\alpha]_D^{20}$+4.83 (c, 1.48 in $CHCl_3$)

>>**Variant:** (±)-form

CAS Registry Number: 20263-10-9
Molecular Formula: $C_4H_{12}NO_3P$
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: pK_{a3} 10.32

>>**Derivative:** Di-Et ester
Synonym(s): Diethyl (1-aminobutyl)phosphonate

CAS Registry Number: 114299-27-3
Molecular Formula: $C_8H_{20}NO_3P$
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: $C_{11}H_{16}NO_4P$
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°