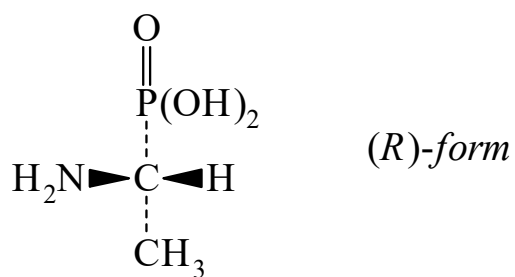




>>Entry Name: (1-Aminoethyl)phosphonic acid, 9CI

Synonym(s): Phosphoalanine



CAS Registry Number: 6323-97-3

Related CAS Registry Numbers(s): 54788-35-1 66068-76-6 73270-41-4

Molecular Formula: C₂H₈NO₃P

Molecular Weight: 125.064

Accurate Mass: 125.024181

Percentage Composition: C 19.21%; H 6.45%; N 11.20%; O 38.38%; P 24.77%

General Statement: Exists in dipolar form

Aldrich: 26866-6

Sigma: A7509

>>Variant: (R)-form

CAS Registry Number: 60687-36-7

Molecular Formula: C₂H₈NO₃P

Molecular Weight: 125.064

Accurate Mass: 125.024181

Percentage Composition: C 19.21%; H 6.45%; N 11.20%; O 38.38%; P 24.77%

Use/Importance: Component of Alafosfalin [BQM80-W](#)

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 263 dec.°. Mp 294-295 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -166$ (c, 2 in 1M NaOH)

Aldrich: 36754-0

Fluka: 6655

Sigma: A6801

>>Derivative: Di-Et ester

CAS Registry Number: 84173-53-5

Molecular Formula: C₆H₁₆NO₃P

Molecular Weight: 181.171

Accurate Mass: 181.086781

Percentage Composition: C 39.78%; H 8.90%; N 7.73%; O 26.49%; P 17.10%

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{20} -5.2$ (c, 1 in CHCl₃)

>>Derivative: Di-Et ester; hydrochloride

CAS Registry Number: 98820-85-0

Physical Description: Solid

Melting Point: Mp 107°

>>Variant: (S)-form

CAS Registry Number: 66068-76-6

Molecular Formula: C₂H₈NO₃P

Molecular Weight: 125.064

Accurate Mass: 125.024181

Percentage Composition: C 19.21%; H 6.45%; N 11.20%; O 38.38%; P 24.77%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 278-279°. Mp 295-296 dec.°. Mp 290°