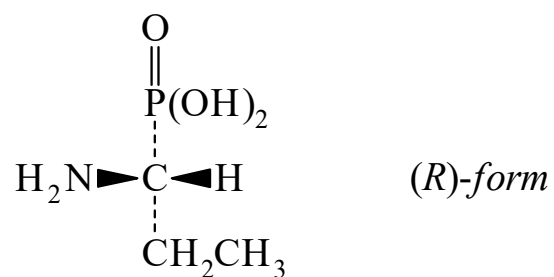




>>Entry Name: (1-Aminopropyl)phosphonic acid, 9CI

Synonym(s): Ampropylfos, BSI. Appa



CAS Registry Number: 14047-23-5

Related CAS Registry Numbers(s): 20459-54-5 80993-32-4 97147-68-7 98049-00-4

Molecular Formula: C₃H₁₀NO₃P

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 exists in dipolar form

Aldrich: 36739-7

Sigma: A6662

>>Variant: (*R*)-form

CAS Registry Number: 98049-00-4

Molecular Formula: C₃H₁₀NO₃P

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%

Physical Description: Solid

Melting Point: Mp 277°

Optical Rotation: $[\alpha]_{578}^{20} -18.7$ (c, 1 in 1M NaOH)

Aldrich: 47188-7

>>Variant: (*S*)-form

CAS Registry Number: 98048-99-8

Molecular Formula: C₃H₁₀NO₃P

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%

Physical Description: Solid

Melting Point: Mp 274-275° (265-266°)

Optical Rotation: $[\alpha]_{\text{D}}^{17} -3.3$ (c, 1.1 in 1M NaOH)

Aldrich: 47189-5

>>Derivative: Di-Et ester

CAS Registry Number: 104549-64-6

Molecular Formula: C₇H₁₈NO₃P

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_{0.01} 110°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +7.18$ (c, 1.66 in CHCl₃)