



>>Entry Name: (3-Aminopropyl)phosphonic acid, 9CI, 8CI

CAS Registry Number: 13138-33-5

$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{P}(\text{O})(\text{OH})_2$

Molecular Formula: $\text{C}_3\text{H}_{10}\text{NO}_3\text{P}$

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: Prisms (EtOH aq.)

Melting Point: Mp 282-288°. Mp 274°

Aldrich: 26861-5

Sigma: A7884

>>Derivative: Di-Et ester

Synonym(s): Diethyl (3-aminopropyl)phosphonate

CAS Registry Number: 4402-24-8

Molecular Formula: $\text{C}_7\text{H}_{18}\text{NO}_3\text{P}$

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_{0.0075} 68-75° (lit. gives a pressure range). Bp_{0.01} 92-95°

>>Derivative: Diisopropyl ester

Synonym(s): Diisopropyl (3-aminopropyl)phosphonate

CAS Registry Number: 53253-56-8

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: Liq.

Boiling Point: Bp_{0.018} 74°

>>Derivative: N-Ac, Di-Et ester

Molecular Formula: $\text{C}_9\text{H}_{20}\text{NO}_4\text{P}$

Molecular Weight: 237.235

Accurate Mass: 237.112996

Percentage Composition: C 45.57%; H 8.50%; N 5.90%; O 26.98%; P 13.06%

Physical Description: Liq.

Boiling Point: Bp_{0.05} 125°

References:

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