



>>Entry Name: (Aminomethyl)phosphonic acid, 9CI

CAS Registry Number: 1066-51-9

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

Molecular Formula: $\text{CH}_6\text{NO}_3\text{P}$

Molecular Weight: 111.037

Accurate Mass: 111.008531

Percentage Composition: C 10.82%; H 5.45%; N 12.61%; O 43.23%; P 27.90%

General Statement: Free acid exists in dipolar form

Use/Importance: Metab. of Glyphosine [DLC43-C](#) and Glyphosate [DLC41-A](#)

Physical Description: Cryst.

Melting Point: Mp 308-310°

pKa Value: $\text{p}K_{\text{a}1}$ 0.44; $\text{p}K_{\text{a}2}$ 5.39; $\text{p}K_{\text{a}3}$ 10.05 (25°, H_2O) $\text{p}K_{\text{a}1}$ 1.85; $\text{p}K_{\text{a}2}$ 5.35; $\text{p}K_{\text{a}3}$ 10

Aldrich: 32481-7

Fluka: 8385

Sigma: A7759

>>Derivative: Di-Et ester

Synonym(s): Diethyl (aminomethyl)phosphonate

CAS Registry Number: 50917-72-1

Molecular Formula: $\text{C}_5\text{H}_{14}\text{NO}_3\text{P}$

Molecular Weight: 167.144

Accurate Mass: 167.071131

Percentage Composition: C 35.93%; H 8.44%; N 8.38%; O 28.72%; P 18.53%

Physical Description: Yellowish liq.

Other Data: Dec. on attempted distn.

>>Derivative: Diamide

see *P*-(Aminomethyl)phosphonic diamide, [MLH97-P](#)

>>Derivative: *N*-Ac, di-Me ester

Synonym(s): Dimethyl [(*N*-acetylamino)methyl]phosphonate

Molecular Formula: $\text{C}_5\text{H}_{12}\text{NO}_4\text{P}$

Molecular Weight: 181.128

Accurate Mass: 181.050396

Percentage Composition: C 33.16%; H 6.68%; N 7.73%; O 35.33%; P 17.10%

Physical Description: Solid

Melting Point: Mp 46-47°

Boiling Point: $\text{Bp}_{0.008}$ 117-120°

>>Derivative: *N*-Ac, di-Et ester

Synonym(s): Diethyl [(*N*-acetylamino)methyl]phosphonate

Molecular Formula: $\text{C}_7\text{H}_{16}\text{NO}_4\text{P}$

Molecular Weight: 209.181

Accurate Mass: 209.081696

Percentage Composition: C 40.19%; H 7.71%; N 6.70%; O 30.59%; P 14.81%

Physical Description: Solid

Melting Point: Mp 38-39°

Boiling Point: $\text{Bp}_{0.006}$ 122-123°