



>>Entry Name: (2-Aminoethyl)phosphonic acid, 9CI

Synonym(s): Ciliatine. AEP

CAS Registry Number: 2041-14-7

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

Molecular Formula: $\text{C}_2\text{H}_8\text{NO}_3\text{P}$

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%

Biological Source: Constit. as glyceryl esters of rumen protozoan, *Tetrahymena pyriformis*, sea anemones, bovine brain, mycobacteria, and a fungus *Pythium prolatum*

Physical Description: Rhombic cryst. or needles (EtOH aq.)

Melting Point: Mp 295-297 dec.°

pKa Value: $\text{p}K_{\text{a}1}$ 2.45; $\text{p}K_{\text{a}2}$ 7; $\text{p}K_{\text{a}3}$ 10.8 $\text{p}K_{\text{a}1}$ 1.3; $\text{p}K_{\text{a}2}$ 6.51; $\text{p}K_{\text{a}3}$ 11.5 (25°)

UV: [neutral] λ_{max} 0 (end) (ϵ) (H_2O) (Derep)

Other Data: The metastable rhombic form is difficult to prepare. First known natural compd. contg. the C-P bond

Aldrich: 26867-4

Sigma: A1508

>>Derivative: Di-Et ester

CAS Registry Number: 41468-36-4

Molecular Formula: $\text{C}_6\text{H}_{16}\text{NO}_3\text{P}$

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: Liq.

Boiling Point: $\text{Bp}_{0.025}$ 54-56°

>>Derivative: *N*-Benzoyl

Synonym(s): 2-(Benzoylamino)ethylphosphonic acid

Molecular Formula: $\text{C}_9\text{H}_{12}\text{NO}_4\text{P}$

Molecular Weight: 229.172

Accurate Mass: 229.050396

Percentage Composition: C 47.17%; H 5.28%; N 6.11%; O 27.93%; P 13.52%

Physical Description: Solid

Melting Point: Mp 191-192°

>>Derivative: *N*-Me

Synonym(s): *N*-Methylciliatine. 2-(Methylamino)ethylphosphonic acid

CAS Registry Number: 14596-55-5

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%

Biological Source: Isol. from the sea anemone *Anthopleura xanthogrammica*

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 291 dec.°

>>Derivative: *N,N*-Di-Me

Synonym(s): 2-Dimethylaminoethylphosphonic acid. *N,N*-Dimethylciliatine

CAS Registry Number: 14596-56-6

Molecular Formula: $\text{C}_4\text{H}_{12}\text{NO}_3\text{P}$

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%

Biological Source: Isol. from *Anthopleura xanthogrammica*

Physical Description: Pale-yellow cryst. (MeOH aq.)

Melting Point: Mp 249.5 dec.°