



>>Entry Name: **Phosphonoacetic acid**, 9CI
Synonym(s): Dihydroxyphosphinylacetic acid, 9CI

CAS Registry Number: 4408-78-0
Related CAS Registry Numbers(s): 54870-27-8

$(\text{HO})_2\text{P}(\text{O})\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_2\text{H}_5\text{O}_5\text{P}$
Molecular Weight: 140.032
Accurate Mass: 139.987462
Percentage Composition: C 17.15%; H 3.60%; O 57.13%; P 22.12%

Use/Importance: Antiviral agent
Physical Description: Rhombs. (AcOH)
Melting Point: Mp 142-143°
Solubility: Insol. C_6H_6 , CHCl_3 , Et_2O
pKa Value: $\text{p}K_{\text{a}1}$ 1; $\text{p}K_{\text{a}2}$ 5.11; $\text{p}K_{\text{a}3}$ 8.69 (25°)
Calculated Log P Data: Log P -1.39 (uncertain value) (calc)

Aldrich: 28427-0
Sigma: P6909

>>Derivative: Di-Na salt
Synonym(s): Fosfonet sodium, INN, USAN. Abbott 38642

CAS Registry Number: 36983-81-0
Development Status: Never marketed

>>Derivative: C-Me ester
Synonym(s): Methyl dihydroxyphosphinylacetate. Methyl phosphonoacetate

CAS Registry Number: 40962-37-6

Molecular Formula: $\text{C}_3\text{H}_7\text{O}_5\text{P}$
Molecular Weight: 154.059
Accurate Mass: 154.003112
Percentage Composition: C 23.39%; H 4.58%; O 51.93%; P 20.11%
Physical Description: No data available

>>Derivative: C-Et ester
Synonym(s): Ethyl dihydroxyphosphinylacetate. Ethyl phosphonoacetate

CAS Registry Number: 35752-46-6

Molecular Formula: $\text{C}_4\text{H}_9\text{O}_5\text{P}$
Molecular Weight: 168.086
Accurate Mass: 168.018762
Percentage Composition: C 28.58%; H 5.40%; O 47.59%; P 18.43%
Physical Description: Viscous liq.
Solubility: Insol. C_6H_6 ; sl. sol. H_2O , EtOH, Et_2O

>>Derivative: Et ester, monoanilinium salt

Physical Description: Cryst. (Me_2CO)
Melting Point: Mp 134-136°

>>Derivative: C-tert-Butyl ester

Molecular Formula: $\text{C}_6\text{H}_{13}\text{O}_5\text{P}$
Molecular Weight: 196.139
Accurate Mass: 196.050062
Percentage Composition: C 36.74%; H 6.68%; O 40.79%; P 15.79%
Physical Description: Cryst. (Me_2CO) (as monoanilinium salt)
Melting Point: Mp 115-117°