



>>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.  $\text{C}_6\text{H}_6$ ,  $\text{CHCl}_3$ ,  $\text{Et}_2\text{O}$   
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.  $\text{C}_6\text{H}_6$ ; sl. sol.  $\text{H}_2\text{O}$ , EtOH,  $\text{Et}_2\text{O}$

>>Derivative: Et ester, monoanilinium salt

Physical Description: Cryst. ( $\text{Me}_2\text{CO}$ )  
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. ( $\text{Me}_2\text{CO}$ ) (as monoanilinium salt)  
Melting Point: Mp 115-117°