



>>Entry Name: 2-Amino-2-phosphonoacetic acid, 8CI

Synonym(s): 2-Phosphonoglycine

CAS Registry Number: 59679-89-9

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

Molecular Formula: $\text{C}_2\text{H}_6\text{NO}_5\text{P}$

Molecular Weight: 155.047

Accurate Mass: 154.998361

Percentage Composition: C 15.49%; H 3.90%; N 9.03%; O 51.60%; P 19.98%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 230-232°

>>Derivative: Tri-Et ester

Molecular Formula: $\text{C}_8\text{H}_{18}\text{NO}_5\text{P}$

Molecular Weight: 239.208

Accurate Mass: 239.092261

Percentage Composition: C 40.17%; H 7.58%; N 5.86%; O 33.44%; P 12.95%

Boiling Point: $\text{Bp}_{0.1}$ 140°

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

Molecular Formula: $\text{C}_{12}\text{H}_{16}\text{NO}_7\text{P}$

Molecular Weight: 317.235

Accurate Mass: 317.066441

Percentage Composition: C 45.43%; H 5.08%; N 4.42%; O 35.30%; P 9.76%

Physical Description: Cryst.

Melting Point: Mp 87-88°

>>Derivative: *N*-Benzyloxycarbonyl, tri-Me ester

CAS Registry Number: 88568-95-0

Molecular Formula: $\text{C}_{13}\text{H}_{18}\text{NO}_7\text{P}$

Molecular Weight: 331.261

Accurate Mass: 331.082091

Percentage Composition: C 47.14%; H 5.48%; N 4.23%; O 33.81%; P 9.35%

Physical Description: Cryst. (hexane/EtOAc)

Melting Point: Mp 80°

Aldrich: 37635-3

Fluka: 97040

Sigma: C9794

References:

Schmidt, V. *et al.*, *Synthesis*, 1984, 53, (*synth, derivs, pmr*)