



>>Entry Name: 4-(Diethoxyphosphinyl)butanoic acid, 9CI

CAS Registry Number: 38694-48-3

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

Molecular Formula: $\text{C}_8\text{H}_{17}\text{O}_5\text{P}$

Molecular Weight: 224.193

Accurate Mass: 224.081362

Percentage Composition: C 42.86%; H 7.64%; O 35.68%; P 13.82%

Physical Description: Cryst. (Et_2O)

Melting Point: Mp 46.5-47.5°

Boiling Point: Bp_{0.03} 140-145°

pKa Value: pK_{a1} 4.57 (25°, H₂O) pK_{a1} 5.67 (25°, 50% EtOH aq.)

>>Derivative: Me ester

Synonym(s): Methyl 4-(diethoxyphosphinyl)butanoate

CAS Registry Number: 2327-68-6

Molecular Formula: $\text{C}_9\text{H}_{19}\text{O}_5\text{P}$

Molecular Weight: 238.22

Accurate Mass: 238.097012

Percentage Composition: C 45.38%; H 8.04%; O 33.58%; P 13.00%

Physical Description: Liq.

Boiling Point: Bp_{0.01} 104-105°

Refractive Index: n_D²⁵ 1.4376

>>Derivative: Et ester

Synonym(s): Ethyl 4-(diethoxyphosphinyl)butanoate. Triethyl 4-phosphonobutanoate

CAS Registry Number: 2327-69-7

Molecular Formula: $\text{C}_{10}\text{H}_{21}\text{O}_5\text{P}$

Molecular Weight: 252.247

Accurate Mass: 252.112662

Percentage Composition: C 47.62%; H 8.39%; O 31.71%; P 12.28%

Physical Description: Liq.

Boiling Point: Bp₄ 144-145°

Density: d₄²⁰ 1.09

Refractive Index: n_D²⁰ 1.4378

>>Derivative: Benzyl ester

Synonym(s): Benzyl 4-(diethoxyphosphinyl)butanoate

Molecular Formula: $\text{C}_{15}\text{H}_{23}\text{O}_5\text{P}$

Molecular Weight: 314.317

Accurate Mass: 314.128312

Percentage Composition: C 57.32%; H 7.38%; O 25.45%; P 9.85%

Physical Description: Liq.

Boiling Point: Bp_{0.005} 136-140°

Refractive Index: n_D²⁵ 1.4933

>>Derivative: Amide

Molecular Formula: $\text{C}_8\text{H}_{18}\text{NO}_4\text{P}$

Molecular Weight: 223.208

Accurate Mass: 223.097346

Percentage Composition: C 43.05%; H 8.13%; N 6.28%; O 28.67%; P 13.88%

Physical Description: Cryst. ($\text{C}_6\text{H}_6/\text{Et}_2\text{O}$)

Melting Point: Mp 58-61°