



>>Entry Name: (Dimethoxyphosphinyl)acetic acid, 9CI

Synonym(s): Dimethyl (carboxymethyl)phosphonate

CAS Registry Number: 34159-46-1

Type of Compound Code(s): AC5040

(MeO)₂P(O)CH₂COOH

Molecular Formula: C₄H₉O₅P

Molecular Weight: 168.086

Accurate Mass: 168.018762

Percentage Composition: C 28.58%; H 5.40%; O 47.59%; P 18.43%

Use/Importance: Both the acid and its esters form carbanions used in Wittig-Horner reactions for synth. of α,β-unsaturated acids and esters

Physical Description: Hygroscopic cryst. (butanone)

Melting Point: Mp 40-41°

pKa Value: pK_{a1} 3.34 (25°,H₂O) pK_{a1} 4.45 (25°,50% EtOH aq.)

>>Derivative: K salt

Physical Description: Cryst. (MeOH)

Melting Point: Mp 122-123°

>>Derivative: Me ester

Synonym(s): Methyl (dimethoxyphosphinyl)acetate. Trimethyl phosphonoacetate

CAS Registry Number: 5927-18-4

Type of Compound Code(s): AC5040

Molecular Formula: C₅H₁₁O₅P

Molecular Weight: 182.113

Accurate Mass: 182.034412

Percentage Composition: C 32.98%; H 6.09%; O 43.93%; P 17.01%

Physical Description: Liq.

Boiling Point: Bp₅ 117-118°. Bp_{0.2} 87-90°

Density: d₄²⁰ 1.264

Refractive Index: n_D²⁰ 1.4373

Aldrich: T7975-8

Fluka: 79527

>>Derivative: Et ester

Synonym(s): Ethyl (dimethoxyphosphinyl)acetate

CAS Registry Number: 311-46-6

Type of Compound Code(s): AC5040

Molecular Formula: C₆H₁₃O₅P

Molecular Weight: 196.139

Accurate Mass: 196.050062

Percentage Composition: C 36.74%; H 6.68%; O 40.79%; P 15.79%

Physical Description: Liq.

Boiling Point: Bp₁₀ 134.5-135°. Bp_{0.4} 91-92°

Density: d₄²⁰ 1.21

Refractive Index: n_D²⁰ 1.4348

Aldrich: 36526-2

Fluka: 2610

Sigma: D4664

>>Derivative: Ph ester

Synonym(s): Phenyl (dimethoxyphosphinyl)acetate

CAS Registry Number: 17604-67-0

Type of Compound Code(s): AC5040

Molecular Formula: C₁₀H₁₃O₅P

Molecular Weight: 244.183

Accurate Mass: 244.050062

Percentage Composition: C 49.19%; H 5.37%; O 32.76%; P 12.68%

Physical Description: Liq.

Boiling Point: Bp_{0.07} 136-137°

Density: d₄²⁰ 1.34

Refractive Index: n_D²⁰ 1.5260

References: