



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

Synonym(s): Diethyl (carboxymethyl)phosphonate

CAS Registry Number: 3095-95-2

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

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%

Use/Importance: Esters are Wittig-Horner reagents for the synth. of esters of $\alpha\beta$ -unsat. carboxylic acids

Physical Description: Oil or cryst.

Melting Point: Mp 18°. Mp 27-28°

Density: d_4^{20} 1.25

pKa Value: $\text{p}K_a$ 4.66 (25°, 50% EtOH aq.)

Aldrich: 26812-7

>>Derivative: Cyclohexylammonium salt

Physical Description: Cryst. ($\text{Me}_2\text{CO}/\text{Et}_2\text{O}$)

Melting Point: Mp 107-108°

>>Derivative: Me ester

Synonym(s): Diethyl (methoxycarbonylmethyl)phosphonate

CAS Registry Number: 1067-74-9

Molecular Formula: $\text{C}_7\text{H}_{15}\text{O}_5\text{P}$

Molecular Weight: 210.166

Accurate Mass: 210.065712

Percentage Composition: C 40.00%; H 7.19%; O 38.06%; P 14.74%

Physical Description: Liq.

Boiling Point: Bp₉ 131.5-132.5°

Density: d_4^{20} 1.14

Refractive Index: n_D^{20} 1.4335

Aldrich: 15876-3

Fluka: 79517

>>Derivative: Et ester

Synonym(s): Diethyl (ethoxycarbonylmethyl)phosphonate. Triethyl phosphonoacetate

CAS Registry Number: 867-13-0

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%

Use/Importance: Used in Wittig-Horner reactions

Physical Description: Liq.

Boiling Point: Bp₂₀ 152-153°. Bp₉ 142-145°

Refractive Index: n_D^{20} 1.4320

Aldrich: T6130-1

Fluka: 79525

Sigma: T4263