



>>Entry Name: (2-Oxopropyl)phosphonic acid, 9CI

Synonym(s): Acetonylphosphonic acid. Phosphonoacetone

CAS Registry Number: 6913-02-6

Related CAS Registry Numbers(s): 30386-62-0 41162-13-4 53372-31-9 93412-27-2 93412-28-3

$\text{H}_3\text{CCOCH}_2\text{P}(\text{O})(\text{OH})_2$

Molecular Formula: $\text{C}_3\text{H}_7\text{O}_4\text{P}$

Molecular Weight: 138.06

Accurate Mass: 138.008197

Percentage Composition: C 26.10%; H 5.11%; O 46.36%; P 22.44%

Use/Importance: Esters form anions which may be alkylated, and which act as Wittig-Horner reagents

Other Data: When heated, the mono-Na salt $\rightarrow \text{Me}_2\text{CO}$. Esters exist almost entirely in the keto form but form Mg enolates. Ester anions exist as *Z*- and *E*-forms in soln

>>Derivative: Mono(dicyclohexylammonium) salt

CAS Registry Number: 68064-33-5

Physical Description: Solid

Melting Point: Mp 173-175°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl (2-oxopropyl)phosphonate. Dimethyl acetonylphosphonate

CAS Registry Number: 4202-14-6

Molecular Formula: $\text{C}_5\text{H}_{11}\text{O}_4\text{P}$

Molecular Weight: 166.113

Accurate Mass: 166.039497

Percentage Composition: C 36.15%; H 6.67%; O 38.53%; P 18.65%

Physical Description: Liq.

Boiling Point: Bp₁₀ 123-124°. Bp_{0.5} 85-88°

Refractive Index: n_D²⁰ 1.4338

Aldrich: 18069-6

Fluka: 75948

Sigma: D6641

>>Derivative: Di-Et ester

Synonym(s): Diethyl (2-oxopropyl)phosphonate. Diethyl acetonylphosphonate

CAS Registry Number: 1067-71-6

Molecular Formula: $\text{C}_7\text{H}_{15}\text{O}_4\text{P}$

Molecular Weight: 194.167

Accurate Mass: 194.070797

Percentage Composition: C 43.30%; H 7.79%; O 32.96%; P 15.95%

Boiling Point: Bp_{0.5} 88-90°

Refractive Index: n_D²² 1.4335

Other Data: Aq. Ba(OH)₂ $\rightarrow \text{Me}_2\text{CO}$

Aldrich: 37047-9

>>Derivative: Diisopropyl ester

Synonym(s): Bis(1-methylethyl) (2-oxopropyl)phosphonate. Diisopropyl acetonylphosphonate

CAS Registry Number: 67257-36-7

Molecular Formula: $\text{C}_9\text{H}_{19}\text{O}_4\text{P}$

Molecular Weight: 222.22

Accurate Mass: 222.102097

Percentage Composition: C 48.64%; H 8.62%; O 28.80%; P 13.94%

Physical Description: Liq.

Boiling Point: Bp_{0.5} 92-96°

Refractive Index: n_D²² 1.4301