



>>Entry Name: Propylphosphonic acid, 9CI

Synonym(s): 1-Propanephosphonic acid

CAS Registry Number: 4672-38-2

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

Molecular Formula: $\text{C}_3\text{H}_9\text{O}_3\text{P}$

Molecular Weight: 124.076

Accurate Mass: 124.028932

Percentage Composition: C 29.04%; H 7.31%; O 38.68%; P 24.96%

Use/Importance: Monoalkyl esters control plant growth and fruit ripening

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 73°

pKa Value: $\text{p}K_{\text{a}1}$ 2.49; $\text{p}K_{\text{a}2}$ 8.06 (25° , H_2O)

Aldrich: 30568-5

>>Derivative: Di-Me ester

Synonym(s): Dimethyl propylphosphonate

CAS Registry Number: 18755-43-6

Molecular Formula: $\text{C}_5\text{H}_{13}\text{O}_3\text{P}$

Molecular Weight: 152.13

Accurate Mass: 152.060232

Percentage Composition: C 39.48%; H 8.61%; O 31.55%; P 20.36%

Boiling Point: Bp_{14} $80-82^\circ$

Refractive Index: n_{D}^{20} 1.4210

>>Derivative: Di-Et ester

Synonym(s): Diethyl propylphosphonate

CAS Registry Number: 18812-51-6

Molecular Formula: $\text{C}_7\text{H}_{17}\text{O}_3\text{P}$

Molecular Weight: 180.183

Accurate Mass: 180.091532

Percentage Composition: C 46.66%; H 9.51%; O 26.64%; P 17.19%

Physical Description: Liq.

Boiling Point: Bp_9 $88-89^\circ$

Density: d_4^{20} 1.01

Refractive Index: n_{D}^{20} 1.4172

>>Derivative: Dipropyl ester

Synonym(s): Dipropyl propylphosphonate

CAS Registry Number: 1789-95-3

Molecular Formula: $\text{C}_9\text{H}_{21}\text{O}_3\text{P}$

Molecular Weight: 208.237

Accurate Mass: 208.122832

Percentage Composition: C 51.91%; H 10.16%; O 23.05%; P 14.87%

Physical Description: Liq.

Boiling Point: Bp_{18} 126°

>>Derivative: Dibutyl ester

Synonym(s): Dibutyl propylphosphonate

CAS Registry Number: 4628-12-0

Molecular Formula: $\text{C}_{11}\text{H}_{25}\text{O}_3\text{P}$

Molecular Weight: 236.29

Accurate Mass: 236.154132

Percentage Composition: C 55.91%; H 10.66%; O 20.31%; P 13.11%

Physical Description: Liq.

Boiling Point: Bp_{10} $133-137^\circ$

Density: d_4^{20} 0.96

Refractive Index: n