



>>Entry Name: Hexylphosphonic acid, 9CI

Synonym(s): 1-Phosphonohexane. 1-Hexanephosphonic acid

CAS Registry Number: 4721-24-8

$\text{H}_3\text{C}(\text{CH}_2)_5\text{P}(\text{O})(\text{OH})_2$

Molecular Formula: $\text{C}_6\text{H}_{15}\text{O}_3\text{P}$

Molecular Weight: 166.156

Accurate Mass: 166.075882

Percentage Composition: C 43.37%; H 9.10%; O 28.89%; P 18.64%

Physical Description: Cryst. (petrol)

Melting Point: Mp 105-106°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl hexylphosphonate

CAS Registry Number: 6172-92-5

Molecular Formula: $\text{C}_8\text{H}_{19}\text{O}_3\text{P}$

Molecular Weight: 194.21

Accurate Mass: 194.107182

Percentage Composition: C 49.48%; H 9.86%; O 24.71%; P 15.95%

Physical Description: Liq.

Boiling Point: Bp₁₀ 121-123°

Refractive Index: n_D²⁰ 1.4276

>>Derivative: Di-Et ester

Synonym(s): Diethyl hexylphosphonate

CAS Registry Number: 16165-66-5

Molecular Formula: $\text{C}_{10}\text{H}_{23}\text{O}_3\text{P}$

Molecular Weight: 222.264

Accurate Mass: 222.138482

Percentage Composition: C 54.04%; H 10.43%; O 21.60%; P 13.94%

Boiling Point: Bp₁₆ 195-200°. Bp₂ 103°

Refractive Index: n_D¹⁷ 1.4311

>>Derivative: Diisopropyl ester

Synonym(s): Diisopropyl hexylphosphonate

Molecular Formula: $\text{C}_{12}\text{H}_{27}\text{O}_3\text{P}$

Molecular Weight: 250.317

Accurate Mass: 250.169782

Percentage Composition: C 57.58%; H 10.87%; O 19.17%; P 12.37%

Boiling Point: Bp₂ 111.5-113°

Refractive Index: n_D²⁰ 1.4328

>>Derivative: Difluoride

CAS Registry Number: 14576-59-1

Molecular Formula: $\text{C}_6\text{H}_{13}\text{F}_2\text{OP}$

Molecular Weight: 170.139

Accurate Mass: 170.067208

Percentage Composition: C 42.36%; H 7.70%; F 22.33%; O 9.40%; P 18.21%

Physical Description: Liq.

Boiling Point: Bp 176-177°. Bp₇ 58-60°

Density: d₄²⁰ 1.07

>>Derivative: Dichloride