



>>Entry Name: Octylphosphonic acid, 9CI

Synonym(s): 1-Octanephosphonic acid

CAS Registry Number: 4724-48-5

$\text{H}_3\text{C}(\text{CH}_2)_7\text{P}(\text{O})(\text{OH})_2$

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: Plates (petrol)

Melting Point: Mp 102-102.5°

>>Derivative: Mono-anilinium salt

Physical Description: Cryst. ( $\text{H}_2\text{O}$ )

Melting Point: Mp 143-145°

>>Derivative: Mono-cyclohexylammonium salt

Physical Description: Solid

Melting Point: Mp 187-188°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl octylphosphonate

CAS Registry Number: 6172-97-0

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%

Physical Description: Liq.

Boiling Point: Bp<sub>14</sub> 156°

Density:  $d_4^{20}$  0.98

Refractive Index:  $n_D^{20}$  1.4350

>>Derivative: Di-Et ester

Synonym(s): Diethyl octylphosphonate

CAS Registry Number: 1068-07-1

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%

Physical Description: Liq.

Boiling Point: Bp<sub>1</sub> 119°

Density:  $d_4^{20}$  0.95

Refractive Index:  $n_D^{16}$  1.4360

>>Derivative: Dibutyl ester

Synonym(s): Dibutyl octylphosphonate

Molecular Formula:  $\text{C}_{16}\text{H}_{35}\text{O}_3\text{P}$

Molecular Weight: 306.424

Accurate Mass: 306.232382

Percentage Composition: C 62.72%; H 11.51%; O 15.66%; P 10.11%

Physical Description: Liq.

Boiling Point: Bp<sub>2</sub> 159-161°

Density:  $d_4^{20}$  0.93

Refractive Index:  $n_D^{25}$  1.4391

>>Derivative: Di-Ph ester

Synonym(s): Diphenyl octylphosphonate