



>>Entry Name: 2-Ethylhexylphosphonic acid, 9CI, 8CI

CAS Registry Number: 14660-16-3

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

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%

>>Derivative: Me ester

Synonym(s): Methyl 2-ethylhexylphosphonate

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%

Boiling Point: Bp_{12} 131-133°

Refractive Index: n_D^{20} 1.4366

>>Derivative: (2-Ethylhexyl) ester

CAS Registry Number: 14802-03-0

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

Molecular Weight: 306.425

Accurate Mass: 306.232382

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

Physical Description: Liq.

Refractive Index: n_D^{25} 1.4471

>>Derivative: Bis(2-ethylhexyl) ester

CAS Registry Number: 126-63-6

Molecular Formula: $\text{C}_{24}\text{H}_{51}\text{O}_3\text{P}$

Molecular Weight: 418.639

Accurate Mass: 418.357582

Percentage Composition: C 68.86%; H 12.28%; O 11.47%; P 7.40%

Use/Importance: Intermed. for nerve gases

Physical Description: Liq.

Boiling Point: Bp_5 210°

Density: d_4^{20} 0.91

References:

U.S. Pat., 1953, 2 753 368; *CA*, **51**, 1246, (*bis(2-ethylhexyl) ester, synth*)

Van Wazer, J.R. *et al.*, *J.A.C.S.*, 1956, **78**, 5715, (*P-31 nmr*)

Peppard, D.F. *et al.*, *J. Inorg. Nucl. Chem.*, 1959, **12**, 60, (*2-ethylhexyl ester, synth, ir*)

Ferraro, J.R. *et al.*, *J. Chem. Phys.*, 1963, **67**, 2639, (*P-31 nmr*)

Rabillourd, G., *Bull. Soc. Chim. Fr.*, 1966, 1145, (*Me ester, synth*)

Nishiwaki, T., *Tetrahedron*, 1966, **22**, 1383, (*ms*)

Kertes, A.S., *J. Inorg. Nucl. Chem.*, 1972, **34**, 796, (*props*)

Katzin, L.I. *et al.*, *Spectrochim. Acta A*, 1978, **34**, 57, (*ir*)