



>>Entry Name: (Chloromethyl)phosphonic acid, 9Cl

CAS Registry Number: 2565-58-4

ClCH2P(O)(OH)2

Molecular Formula: CH₄ClO₃P

Molecular Weight: 130.467

Accurate Mass: 129.958659

Percentage Composition: C 9.21%; H 3.09%; Cl 27.17%; O 36.79%; P 23.74%

Physical Description: Needles (C₆H₆/MeNO₂)

Melting Point: Mp 90-91°

pKa Value: pK_{a1} 1.04; pK_{a2} 6.59 (25°) pK_{a1} 1.4; pK_{a2} 6.3

>>Derivative: Mono-anilinium salt

Physical Description: Cryst. (EtOH)

Melting Point: Mp 187-188 dec.°

>>Derivative: Bis(cyclohexylammonium) salt

CAS Registry Number: 23896-97-1

Physical Description: Cryst. (EtOH)

Melting Point: Mp 199-200°

>>Derivative: Mono-Me ester

Synonym(s): Methyl hydrogen (chloromethyl)phosphonate

CAS Registry Number: 1929-41-5

Molecular Formula: C₂H₆ClO₃P

Molecular Weight: 144.494

Accurate Mass: 143.974309

Percentage Composition: C 16.62%; H 4.19%; Cl 24.54%; O 33.22%; P 21.44%

Physical Description: Liq.

Boiling Point: Bp_{0.006} 130-135°

Density: d₄²⁰ 1.48

Refractive Index: n_D²⁰ 1.4595

>>Derivative: Di-Me ester

Synonym(s): Dimethyl (chloromethyl)phosphonate

CAS Registry Number: 6346-15-2

Molecular Formula: C₃H₈ClO₃P

Molecular Weight: 158.521

Accurate Mass: 157.989959

Percentage Composition: C 22.73%; H 5.09%; Cl 22.36%; O 30.28%; P 19.54%

Physical Description: Liq.

Boiling Point: Bp₄ 79.5-80°

Density: d₄²⁰ 1.33

Refractive Index: n_D²⁰ 1.4450

>>Derivative: Mono-Et ester

Synonym(s): Monoethyl (chloromethyl)phosphonate. Ethyl hydrogen (chloromethyl)phosphonate

Molecular Formula: C₃H₈ClO₃P

Molecular Weight: 158.521

Accurate Mass: 157.989959

Percentage Composition: C 22.73%; H 5.09%; Cl 22.36%; O 30.28%; P 19.54%

Boiling Point: Bp_{2.5} 86-87°

Density: d₂₀²⁰ 1.19

Refractive Index: n_D²⁰ 1.4360