



>>Entry Name: (Trichloromethyl)phosphonic acid, 9CI

CAS Registry Number: 5994-41-2

$\text{Cl}_3\text{CP}(\text{O})(\text{OH})_2$

Molecular Formula: $\text{CH}_2\text{Cl}_3\text{O}_3\text{P}$

Molecular Weight: 199.357

Accurate Mass: 197.880713

Percentage Composition: C 6.02%; H 1.01%; Cl 53.35%; O 24.08%; P 15.54%

Physical Description: Cryst. + $2\text{H}_2\text{O}$

Melting Point: Mp 81-82°

pKa Value: $\text{p}K_{\text{a}1}$ 1.63; $\text{p}K_{\text{a}2}$ 4.81 (25°)

Rare Chemicals Library: S45877-5

>>Derivative: Mono-anilinium salt

Physical Description: Solid

Melting Point: Mp 262-263°

>>Derivative: Mono-imidazolium salt

Physical Description: Cryst. + $1\text{H}_2\text{O}$ (H_2O)

Melting Point: Mp 211.5-213.5°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl (trichloromethyl)phosphonate

CAS Registry Number: 29238-81-1

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

Molecular Weight: 227.41

Accurate Mass: 225.912013

Percentage Composition: C 15.84%; H 2.66%; Cl 46.77%; O 21.11%; P 13.62%

Boiling Point: Bp_{12} 121-122°

Density: d_0^{15} 1.46

Refractive Index: n_D^{14} 1.4580

>>Derivative: Di-Et ester

Synonym(s): Diethyl (trichloromethyl)phosphonate

CAS Registry Number: 866-23-9

Molecular Formula: $\text{C}_5\text{H}_{10}\text{Cl}_3\text{O}_3\text{P}$

Molecular Weight: 255.464

Accurate Mass: 253.943313

Percentage Composition: C 23.51%; H 3.95%; Cl 41.63%; O 18.79%; P 12.12%

Use/Importance: Converts carboxylic acids into their ethyl esters. With Li → anion of diethyl ester of (Dichloromethyl)phosphonic acid [DQK10-N](#)

Physical Description: Liq.

Boiling Point: Bp_{16} 129-130.5°

Density: d_0^{14} 1.37

Refractive Index: n_D^{14} 1.4585

Aldrich: 37452-0

Fluka: 91283

>>Derivative: Dipropyl ester

Synonym(s): Dipropyl (trichloromethyl)phosphonate

CAS Registry Number: 53582-73-3

Molecular Formula: $\text{C}_7\text{H}_{14}\text{Cl}_3\text{O}_3\text{P}$

Molecular Weight: 283.518

Accurate Mass: 281.974613

Percentage Composition: C 29.65%; H 4.98%; Cl 37.51%; O 16.93%; P 10.92%

Physical Description: Liq.

Boiling Point: Bp_7 123-125°

Density: d_4^{26} 1.31

Refractive Index: n