

Methyl dichlorophosphate

Other names:	Methyl phosphorodichloridate Phosphorodichloridic acid, methyl ester
Inchi:	InChI=1S/CH3Cl2O2P/c1-5-6(2,3)4/h1H3
InchiKey:	SNVCRNWSNUUGEA-UHFFFAOYSA-N
Formula:	CH3Cl2O2P
SMILES:	COP(=O)(Cl)Cl
Mol. weight [g/mol]:	148.91
CAS:	677-24-7

Physical Properties

Property code	Value	Unit	Source
ie	11.50	eV	NIST Webbook
log10ws	-2.90		Crippen Method
logp	2.218		Crippen Method
mcvol	81.630	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.50 ± 1.50	K	2.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C677247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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