Methylphosphonothioic dichloride

Other names:
Methylthiophosphonic dichloride
Phosphonothioic dichloride, methyl-
Phosphine, dichloro-methyl-thioxo-
Dichloromethylphosphine sulfide
Methanephosphonothioic dichloride
Methyldichlorophosphine sulfide
Methylphosphonothioyl dichloride
Methylthionophosphonic dichloride
Methylthiophosphonic acid dichloride
Methylphosphonothiodichloride

Inchi: InChI=1S/CH3Cl2PS/c1-4(2,3)5/h1H3
InchiKey: TUNCWCIKOHOGJX-UHFFFAOYSA-N
Formula: CH3Cl2PS
SMILES: CP(=S)(Cl)Cl
Mol. weight [g/mol]: 148.98
CAS: 676-98-2

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	NIST Webbook
ie	9.75	eV	NIST Webbook
ie	9.73	eV	NIST Webbook
log10ws	2.19		Crippen Method
logp	2.403		Crippen Method
mcvol	86.240	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C676982&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

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https://www.chemeo.com/cid/25-904-0/Methylphosphonothioic-dichloride.pdf

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