

Methylthiophosphorylchloride

Inchi: InChI=1S/CH3Cl2OPS/c1-6-5(2,3)4/h1H3
InchiKey: XKEDDHKQRMGTDD-UHFFFAOYSA-N
Formula: CH3Cl2OPS
SMILES: CSP(=O)(Cl)Cl
Mol. weight [g/mol]: 164.98
CAS: 18281-76-0

Physical Properties

Property code	Value	Unit	Source
ie	9.82	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
log10ws	-3.70		Crippen Method
logp	2.935		Crippen Method
mcvol	92.110	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18281760&Units=SI&Mask=3FFF>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/101-298-9/Methylthiophosphorylchloride.pdf>

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