

Phosphorochloridothioic acid, O,O-dimethyl ester

Other names:	Chlorodimethoxyphosphine sulfide Dimethoxythiophosphonyl chloride Dimethyl chlorothionophosphate Dimethyl chlorothiophosphate Dimethyl chlorothiophosphonate Dimethyl thionophosphorochloridate Dimethyl thiophosphorochloridate O,O-Dimethyl chlorothionophosphate O,O-Dimethyl chlorothiophosphate O,O-Dimethyl phosphorochloridothioate O,O-Dimethyl phosphorochlorothioate O,O-Dimethyl phosphorothionochloridate O,O-Dimethyl thionophosphorochloridate O,O-Dimethyl thionophosphoryl chloride O,O-Dimethyl thiophosphoric acid chloride O,O-Dimethyl thiophosphoryl chloride (CH3O)2P(S)Cl Dimethyl phosphorochlorothioate Dimethylchlorthiofosfat Methyl PCT O,O-Dimethylester kyseliny chlorthiofosforecne Phosphonothioic acid, chloro-, O,O-dimethyl ester Dimethyl phosphorochloridothioate NA 2267 Dimethyl phosphochloridothioate Dimethyl phosphorochlorodithioate Dimethyl thiophosphoryl chloride MP-2 O,O-Dimethyl chlorophosphorothioate NSC 132984
Inchi:	InChI=1S/C2H6ClO2PS/c1-4-6(3,7)5-2/h1-2H3
InchiKey:	XFBJRFNXPUCPKU-UHFFFAOYSA-N
Formula:	C2H6ClO2PS
SMILES:	COP(=S)(Cl)OC
Mol. weight [g/mol]:	160.56
CAS:	2524-03-0

Physical Properties

Property code	Value	Unit	Source
log10ws	2.76		Crippen Method
logp	1.742		Crippen Method
mcvol	99.830	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2524030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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