

Phosphorothioic acid, O,O-diethyl S-methyl ester

Other names:	O,O-Diethyl S-methyl phosphorothioate O,O'-Diethyl S-methyl thiophosphate Phosphorothioic acid, O,O'-diethyl S-methyl ester
Inchi:	InChI=1S/C5H13O3PS/c1-4-7-9(6,10-3)8-5-2/h4-5H2,1-3H3
InchiKey:	GWEDODYYNURODY-UHFFFAOYSA-N
Formula:	C5H13O3PS
SMILES:	CCOP(=O)(OCC)SC
Mol. weight [g/mol]:	184.19
CAS:	2404-05-9

Physical Properties

Property code	Value	Unit	Source
ie	8.93	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	2.530		Crippen Method
mcvol	135.730	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2404059&Units=SI

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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