

O,O-Diethyl S-eththionylmethyl phosphorothioate

Other names:	Phosphorothioic acid, O,O-diethyl S-[(ethylsulfinyl)methyl] ester Phoratoxon sulfoxide Diethyl S-eththionylmethyl thiophosphate Phorate O-analog sulfoxide Phorate sulfoxide oxon
Inchi:	InChI=1S/C7H17O4PS2/c1-4-10-12(8,11-5-2)13-7-14(9)6-3/h4-7H2,1-3H3
InchiKey:	RCRHKXGEYNVPDK-UHFFFAOYSA-N
Formula:	C7H17O4PS2
SMILES:	CCOP(=O)(OCC)SCS(=O)CC
Mol. weight [g/mol]:	260.31
CAS:	2588-05-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	2.627		Crippen Method
mcvol	186.130	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=C2588058&Units=SI

Legend

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

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