

Phoratoxon sulfone

Other names:	Phosphorothioic acid, O,O-diethyl S-[(ethylsulfonyl)methyl] ester O,O-Diethyl S-(ethylsulfonyl)methyl phosphorothioate Phorate oxon sulfone PO-Phorate sulfone Diethyl S-ethylsulfonylmethyl thiophosphate Phorate, O-analog sulfone
Inchi:	InChI=1S/C7H17O5PS2/c1-4-11-13(8,12-5-2)14-7-15(9,10)6-3/h4-7H2,1-3H3
InchiKey:	IIMUEPCADBPEMF-UHFFFAOYSA-N
Formula:	C7H17O5PS2
SMILES:	CCOP(=O)(OCC)SCS(=O)(=O)CC
Mol. weight [g/mol]:	276.31
CAS:	2588-06-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.293		Crippen Method
mcvol	192.000	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=C2588069&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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