

Phorate oxon

Other names:	O,O-Diethyl-S-ethylthiomethyl phosphorothioate Phosphorothioic acid, O,O-diethyl-s-(ethylthiomethyl) ester
Inchi:	InChI=1S/C7H17O3PS2/c1-4-9-11(8,10-5-2)13-7-12-6-3/h4-7H2,1-3H3
InchiKey:	FMXFZNGITFNSAG-UHFFFAOYSA-N
Formula:	C7H17O3PS2
SMILES:	CCOP(=O)(OCC)SCSCC
Mol. weight [g/mol]:	244.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	3.611		Crippen Method
mcvol	180.260	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U289841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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/55-089-3/Phorate-oxon.pdf>

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