

Phosphorothioo thionate, o,o-diethyl-s-(1-ethoxy-2-methylpropyl)-

Inchi:	InChI=1S/C11H25O3PS2/c1-6-12-11(9-10(4)5)17-15(16,13-7-2)14-8-3/h10-11H,6-9H2,1
InchiKey:	BQCBPZZPIHENQN-UHFFFAOYSA-N
Formula:	C11H25O3PS2
SMILES:	CCOC(CC(C)C)SP(=S)(OCC)OCC
Mol. weight [g/mol]:	300.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	4.426		Crippen Method
mcvol	236.620	ml/mol	McGowan Method

Sources

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=B6000639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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