

O,O-Diethyl O-2-ethylsulfinyethyl phosphorothioate

Other names:	Phosphorothioic acid, O,O-diethyl O-[2-(ethylsulfiny)ethyl] ester Disulfoton O-analog sulfoxide O,O-Diethyl O-(2-eththionylethyl)phosphorothioate Diethyl 2-eththionylethyl thionophosphate Systox sulfoxide Demeton-O-sulfoxide
Inchi:	InChI=1S/C8H19O4PS2/c1-4-10-13(14,11-5-2)12-7-8-15(9)6-3/h4-8H2,1-3H3
InchiKey:	HTXJPMQYXHDOR-UHFFFAOYSA-N
Formula:	C8H19O4PS2
SMILES:	CCOP(=S)(OCC)OCCS(=O)CC
Mol. weight [g/mol]:	274.34
CAS:	5286-73-7

Physical Properties

Property code	Value	Unit	Source
log10ws	2.68		Crippen Method
logp	2.069		Crippen Method
mcvol	200.220	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=C5286737&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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