Disulfoton sulfone

Other names:	Phosphorodithioic acid, O,O-diethyl S-[2-(ethylsulfonyl)ethyl] ester
	Disyston sulfone
	Ethanethiol, 2-(ethylsulfonyl)-, S-ester with O,O-diethyl phosphorodithioate
	O,O-Diethyl S-(2-ethylsulfonylethyl) phosphorodithioate
	O,O-Diethyl S-(2-ethylsulfonylethyl) thionophosphate
	Phosphorodithioic acid, O,O-diethyl ester S-[2-(ethylsulfonyl)ethyl] ester
	O,O-Diethyl S-(2-ethsulfonylethyl) phosphorodithioate
	O,O-Diethyl S-(2-ethsulfonylethyl) thiothionophosphate
	O,O-Diethyl S-[2-(ethylsulfonyl)ethyl] dithiophosphate
Inchi:	InChI=1S/C8H19O4PS3/c1-4-11-13(14,12-5-2)15-7-8-16(9,10)6-3/h4-8H2,1-3H3
InchiKey:	BKVJOVPVLOJPKJ-UHFFFAOYSA-N
Formula:	C8H19O4PS3
SMILES:	CCOP(=S)(OCC)SCCS(=O)(=O)CC
Mol. weight [g/mol]:	306.40
CAS:	2497-06-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.68		Crippen Method
logp	2.452		Crippen Method
mcvol	216.570	ml/mol	McGowan Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2497065&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices