

Demeton S-sulfone

Other names:	Phosphorothioic acid, O,O-diethyl S-[2-(ethylsulfonyl)ethyl] ester Demeton sulfone Demeton thiol sulfone Isosystox sulfone O,O-Diethyl S-[2-(ethylsulfonyl)ethyl] phosphorothioate O,O-Diethyl S-(2-ethylsulfonylethyl)phosphorothioate Diethyl S-(2-ethylsulfonylethyl) thiophosphate O,O-Diethyl S-ethyl 2-ethylmercaptophosphorothiolate sulfone O,O-Diethyl 2-ethylmercaptoethyl thiophosphate, thiolo isomer Isodemeton-sulfone PO systox sulfone Thiol systox sulfone Disulfoton O-analog sulfone Disulfoton oxon sulfone
Inchi:	InChI=1S/C8H19O5PS2/c1-4-12-14(9,13-5-2)15-7-8-16(10,11)6-3/h4-8H2,1-3H3
InchiKey:	VMXCTQSDRPKAOA-UHFFFAOYSA-N
Formula:	C8H19O5PS2
SMILES:	CCOP(=O)(OCC)SCCS(=O)(=O)CC
Mol. weight [g/mol]:	290.34
CAS:	2496-91-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	2.335		Crippen Method
mvol	206.090	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=C2496915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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