

Demeton S-sulfoxide

Other names:	Phosphorothioic acid, O,O-diethyl S-[2-(ethylsulfanyl)ethyl] ester Isosystox sulfoxide O,O-Diethyl S-(2-eththionylethyl) phosphorothioate Diethyl S-(2-eththionylethyl) thiophosphate O,O-Diethyl S-ethyl-2-ethylmercaptophosphorothiolate sulfoxide Isodemeton-sulfoxide PO systox sulfoxide Thiol systox sulfoxide
Inchi:	InChI=1S/C8H19O4PS2/c1-4-11-13(9,12-5-2)14-7-8-15(10)6-3/h4-8H2,1-3H3
InchiKey:	RWRHZQVSYSDUSM-UHFFFAOYSA-N
Formula:	C8H19O4PS2
SMILES:	CCOP(=O)(OCC)SCCS(=O)CC
Mol. weight [g/mol]:	274.34
CAS:	2496-92-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	2.669		Crippen Method
mvol	200.220	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=C2496926&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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