Phosphorothioic acid, O,O-diethyl S-[2-(ethylsulfonyl)ethyl] ester

Other names: Demeton sulfone
Demeton thiol sulfone
Diethyl S-(2-ethsulfonylethyl) thiophosphate
Disulfoton O-analog sulfone
Disulfoton oxon sulfone
Isodemeton-sulfone
Isosystox sulfone
O,O-Diethyl 2-ethylmercaptoethyl thiophosphate, thiolo isomer
O,O-Diethyl S-(2-ethsulfonylethyl)phosphorothioate
O,O-Diethyl S-[2-(ethylsulfonyl)ethyl] phosphorothioate
O,O-Diethyl S-ethyl 2-ethylmercaptophosphorothiolate sulfone
PO systox sulfone
Phosphorothioic acid, O,O-diethyl S-[2-(ethylsulfonyl)ethyl] ester
Thiol systox 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: VMXCTQSDRPKAOC-UHFFFAOYSA-N

Formula: C8H19O5PS2

SMILES: CCOP(=O)(OCC)SCCS(=O)(=O)CC

Mol. weight [g/mol]: 290.34

Physical Properties

Property code	Value	Unit	Source
hvap	101.72	kJ/mol	Cheméo Relay (1.0)
ie	9.08	eV	Cheméo Relay (1.0)
log10ws	-1.25		Cheméo Relay (1.0)
logp	2.335		Crippen Method
mcvol	206.090	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2496915&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume