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

Other names: Phosphorothioic acid, O,O-diethyl O-[2-(ethylsulfinyl)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: HTXJPMPQYXHDOR-UHFFFAOYSA-N

Formula: C8H19O4PS2

SMILES: CCOP(=S)(OCC)OCCS(=O)CC

Mol. weight [g/mol]: 274.34

Physical Properties

Property code	Value	Unit	Source
hvap	89.98	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
logp	2.069		Crippen Method
mcvol	200.220	ml/mol	McGowan Method

Sources

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

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

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=C5286737&Units=SI

Legend

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume