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

Other names: Diethyl S-ethsulfonylmethyl thiophosphate
O,O-Diethyl S-(ethylsulfonyl)methyl phosphorothioate
PO-Phorate sulfone
Phorate oxon sulfone
Phorate, O-analog sulfone
Phosphorothioic acid, O,O-diethyl S-[(ethylsulfonyl)methyl] ester

Inchi: InChI=1S/C7H17O5PS2/c1-4-11-13(8,12-5-2)14-7-15(9,10)6-3/h4-7H2,1-3H3

InchiKey: IIMUEPCADBPEMF-UHFFFAOYSA-N

Formula: C7H17O5PS2

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

Mol. weight [g/mol]: 276.32

Physical Properties

Property code	Value	Unit	Source
hvap	90.78	kJ/mol	Cheméo Relay (1.0)
ie	9.54	eV	Cheméo Relay (1.0)
log10ws	-1.61		Cheméo Relay (1.0)
logp	2.293		Crippen Method
mcvol	192.000	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=C2588069&Units=SI

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