O,O-Diethyl S-eththionylmethyl phosphorothioate

Other names: Phosphorothioic acid, O,O-diethyl S-[(ethylsulfinyl)methyl] ester
Phoratoxon sulfoxide
Diethyl S-eththionylmethyl thiophosphate
Phorate O-analog sulfoxide
Phorate sulfoxide oxon

Inchi: InChI=1S/C7H17O4PS2/c1-4-10-12(8,11-5-2)13-7-14(9)6-3/h4-7H2,1-3H3

InchiKey: RCRHKXGEYNVPDK-UHFFFAOYSA-N

Formula: C7H17O4PS2

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

Mol. weight [g/mol]: 260.31

CAS: 2588-05-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	2.627		Crippen Method
mcvol	186.130	ml/mol	McGowan Method

Sources

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

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2588058&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume