Phosphorothioic acid, O,O-diethyl S-methyl ester

Other names: O,O-Diethyl S-methyl phosphorothioate
O,O'-Diethyl S-methyl thiophosphate
Phosphorothioic acid, O,O'-diethyl S-methyl ester

Inchi: InChI=1S/C5H13O3PS/c1-4-7-9(6,10-3)8-5-2/h4-5H2,1-3H3

InchiKey: GWEDODYYNURODY-UHFFFAOYSA-N

Formula: C5H13O3PS

SMILES: CCOP(=O)(OCC)SC

Mol. weight [g/mol]: 184.19

CAS: 2404-05-9

Physical Properties

Property code	Value	Unit	Source
ie	8.93	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	2.530		Crippen Method
mcvol	135.730	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=C2404059&Units=SI

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume