O,O'-DIETHYL S-METHYL THIOPHOSPHATE

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]: 184.20

Physical Properties

Property code	Value	Unit	Source
hvap	58.69	kJ/mol	Cheméo Relay (1.0)
ie	8.93	eV	NIST Webbook
log10ws	-0.93		Cheméo Relay (1.0)
logp	2.530		Crippen Method
mcvol	135.730	ml/mol	McGowan Method
tb	508.70	K	Cheméo Relay (1.0)
tf	242.74	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2404059&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point