Phosphonothioic acid, methyl-, S-(2-diethylaminoethyl), O-2-methylpropyl ester

Othernames: O-(iso-Butyl) S-(2-diethylaminoethyl) methylphosphonothiolate
P-methylphosphonothioic acid, S-[2(diethylamino)ethyl] O-(2-methylpropyl) ester
Inchi: InChI=1S/C11H26NO2PS/c1-6-12(7-2)8-9-16-15(5,13)14-10-11(3)4/h11H,6-10H2,1-5H3
InchiKey: MNLAVFKVRUQAKW-UHFFFAOYSA-N
Formula: C11H26NO2PS
SMILES: CCN(CC)CCSP(C)(=O)OCC(C)C
Mol. weight [g/mol]: 267.37
CAS: 159939-87-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	3.557		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	76.60	kJ/mol	324.00	NIST Webbook

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=C159939874&Units=SI

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices