

Phosphorothioic acid, O,O,S-triethyl ester

Other names:	O,O-Diethyl S-ethyl phosphorothioate O,O,S-Triethyl phosphorothioate O,O,S-Triethyl thiophosphate O,O',S-Triethyl thiophosphate Phosphorothioic acid, o,o',s-triethyl ester
Inchi:	InChI=1S/C6H15O3PS/c1-4-8-10(7,9-5-2)11-6-3/h4-6H2,1-3H3
InchiKey:	YEXTYUIZRKSYHA-UHFFFAOYSA-N
Formula:	C6H15O3PS
SMILES:	CCOP(=O)(OCC)SCC
Mol. weight [g/mol]:	198.22
CAS:	1186-09-0

Physical Properties

Property code	Value	Unit	Source
ie	8.63	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	-3.66		Crippen Method
logp	2.921		Crippen Method
mvol	149.820	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	76.30	kJ/mol	332.00	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=C1186090&Units=SI

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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