O,O',S-TRIETHYL THIOPHOSPHATE

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

Physical Properties

Property code	Value	Unit	Source
hvap	60.09	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	-1.36		Cheméo Relay (1.0)
logp	2.921		Crippen Method
mcvol	149.820	ml/mol	McGowan Method
tb	525.45	K	Cheméo Relay (1.0)
tf	225.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	76.30	kJ/mol	332.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1186090&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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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