

O,O,O-TRIETHYL PHOSPHOROTHIONATE

Other names: Triethylphosphorothioate
(C₂H₅O)₃PS
Phosphorothioic acid, O,O,O-triethyl ester
Ethyl phosphorothioate ((EtO)₃PS)
O,O,O-Triethyl phosphorothioate
O,O,O-Triethylester kyseliny thiofosforecne
O,O',O''-Triethyl phosphorothioate
Phosphine sulfide, triethoxy-
Thiophosphoric acid, tri-O-ethyl ester
Triethyl phosphorothionate
Triethyl thiophosphate
Triethylthiofosfat
O,O,O-Triethylthiofosfat
Ethyl thiophosphate, (C₂H₅O)₃PS
NSC 2650

Inchi: InChI=1S/C6H15O3PS/c1-4-7-10(11,8-5-2)9-6-3/h4-6H2,1-3H3

InchiKey: QTPJMTACJMLPLL-UHFFFAOYSA-N

Formula: C₆H₁₅O₃PS

SMILES: CCOP(=S)(OCC)OCC

Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
hvap	60.71	kJ/mol	Cheméo Relay (1.0)
ie	8.49 ± 0.02	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	-2.90		Cheméo Relay (1.0)
logp	2.320		Crippen Method
mcvol	149.820	ml/mol	McGowan Method
tb	509.88	K	Cheméo Relay (1.0)
tf	211.36	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	87.50	kJ/mol	320.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126681&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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