

Phosphorodithioic acid, O,O-diethyl ester

Other names:	Diethyl dithiophosphate Diethyl phosphorodithioate Diethyl ester of phosphorodithioic acid Dithiophosphoric acid, O,O-diethyl ester O,O-Diethyl dithiophosphate O,O-Diethyl dithiophosphoric acid O,O-Diethyl hydrogen phosphorodithioate O,O-Diethyl phosphorodithioic acid O,O-Diethyl-S-hydrogen phosphorodithioate O,O'-Diethyl dithiophosphate O,O'-Diethyl hydrogen dithiophosphate Kyselina O,O-diethyldithiofosforecna O,O-Diethylphosphorodithioate Phosphorodithioic acid, O,O'-diethyl ester Phosphorothiothionic acid, O,O-diethyl ester Di-O-ethyl dithiophosphate NSC 171184 O,O-Diethyl dithiophosphoric acid ester O,O-Diethyl thiolothionophosphate
Inchi:	InChI=1S/C4H11O2PS2/c1-3-5-7(8,9)6-4-2/h3-4H2,1-2H3,(H,8,9)
InchiKey:	IRDLUHRVLVEUHA-UHFFFAOYSA-N
Formula:	C4H11O2PS2
SMILES:	CCOP(=S)(S)OCC
Mol. weight [g/mol]:	186.23
CAS:	298-06-6

Physical Properties

Property code	Value	Unit	Source
hvap	67.70	kJ/mol	NIST Webbook
ie	9.14	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	2.00		Crippen Method
logp	2.214		Crippen Method
mvol	132.120	ml/mol	McGowan Method

Sources

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=C298066&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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