

# Phosphorothioic acid, O,O-diethyl O-[2-(ethylthio)ethyl] ester

<b>Other names:</b>	Demetonthione Demeton thiono Demeton-O O,O-Diethyl O-[2-(ethylthio)ethyl] phosphorothionate O,O-Diethyl O-2-(ethylthio)ethyl phosphorothioate Di-Septon Diethyl (2-(ethylthio)ethyl) thionophosphate Diethyl (2-(ethylthio)ethyl) phosphorothionate Ethanol, 2-(ethylthio)-, O-ester with O,O-diethyl phosphorothioate Thiolmecaptophos Diaethylthiophosphorsaureester des aethylthioglykol Demethon-O NSC 8928 Phosphorothioic acid, O,O-diethyl ester O-[2-(ethylthio)ethyl] ester O,O-diethyl-O-[2-(ethylthio)ethyl] thiophosphate
<b>Inchi:</b>	InChI=1S/C8H19O3PS2/c1-4-9-12(13,10-5-2)11-7-8-14-6-3/h4-8H2,1-3H3
<b>InchiKey:</b>	DGLIBALSRMUQDD-UHFFFAOYSA-N
<b>Formula:</b>	C8H19O3PS2
<b>SMILES:</b>	CCOP(=S)(OCC)OCCSCC
<b>Mol. weight [g/mol]:</b>	258.34
<b>CAS:</b>	298-03-3

## Physical Properties

Property code	Value	Unit	Source
hvap	78.70	kJ/mol	NIST Webbook
log10ws	1.43		Crippen Method
logp	3.054		Crippen Method
mcvol	194.350	ml/mol	McGowan Method
rinpol	1598.00		NIST Webbook
rinpol	1621.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C298033&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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