

# O-Ethyl S-2-diethylaminoethyl ethylphosphonothiolate

<b>Other names:</b>	S-[2-(Diethylamino)ethyl] o-ethyl ethylphosphonothioate Ethyl-phosphonothioic acid S-(2-diethylamino-ethyl) ester O-ethyl ester VE
<b>Inchi:</b>	InChI=1S/C10H24NO2PS/c1-5-11(6-2)9-10-15-14(12,8-4)13-7-3/h5-10H2,1-4H3
<b>InchiKey:</b>	QXRUNSUMQBTCQS-UHFFFAOYSA-N
<b>Formula:</b>	C10H24NO2PS
<b>SMILES:</b>	CCOP(=O)(CC)SCCN(CC)CC
<b>Mol. weight [g/mol]:</b>	253.34
<b>CAS:</b>	21738-25-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	3.311		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
rinpol	1622.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1670.90		NIST Webbook
rinpol	1671.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21738250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21738250&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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