

# Phorate sulfone

<b>Other names:</b>	Phosphorodithioic acid, O,O-diethyl S-[(ethylsulfonyl)methyl] ester O,O-Diethyl S-ethylsulfonylmethyl phosphorodithioate O,O-Diethyl S-ethylsulfonylmethyl dithiophosphate O,O-Diethyl S-ethylsulfonylmethyl thiothionophosphate Methanethiol, (ethylsulfonyl)-, S-ester with O,O-diethyl phosphorodithioate Thimet sulfone
<b>Inchi:</b>	InChI=1S/C7H17O4PS3/c1-4-10-12(13,11-5-2)14-7-15(8,9)6-3/h4-7H2,1-3H3
<b>InchiKey:</b>	YVPSNUIHHFTTRL-UHFFFAOYSA-N
<b>Formula:</b>	C7H17O4PS3
<b>SMILES:</b>	CCOP(=S)(OCC)SCS(=O)(=O)CC
<b>Mol. weight [g/mol]:</b>	292.38
<b>CAS:</b>	2588-04-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.61		Crippen Method
logp	2.409		Crippen Method
mcvol	202.480	ml/mol	McGowan Method

## Sources

<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>
<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=C2588047&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2588047&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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