

# Phosphorodithioic acid, O,O,S-trimethyl ester

<b>Other names:</b>	O,O,S-Trimethyl dithiophosphate O,O,S-Trimethyl phosphorodithioate
<b>Inchi:</b>	InChI=1S/C3H9O2PS2/c1-4-6(7,5-2)8-3/h1-3H3
<b>InchiKey:</b>	ILDHFYGNIDICFB-UHFFFAOYSA-N
<b>Formula:</b>	C3H9O2PS2
<b>SMILES:</b>	COP(=S)(OC)SC
<b>Mol. weight [g/mol]:</b>	172.21
<b>CAS:</b>	2953-29-9

## Physical Properties

Property code	Value	Unit	Source
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	2.61		Crippen Method
logp	1.867		Crippen Method
mcvol	118.030	ml/mol	McGowan Method

## Sources

<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=C2953299&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2953299&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>ie:</b>	Ionization energy
<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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