

# Phosphonothioic acid, methyl-, o,o-dimethyl ester

Inchi:	InChI=1S/C3H9O2PS/c1-4-6(3,7)5-2/h1-3H3
InchiKey:	BHFOAIMSKFAWOU-UHFFFAOYSA-N
Formula:	C3H9O2PS
SMILES:	COP(C)(=S)OC
Mol. weight [g/mol]:	140.14
CAS:	681-06-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.48		Crippen Method
logp	1.218		Crippen Method
mcvol	101.680	ml/mol	McGowan Method

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C681061&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C681061&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/122-256-2/Phosphonothioic-acid-methyl-o-o-dimethyl-ester.pdf>

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