

# 1,3-Propanediol, 2,2-dimethyl-, cyclic 2,2-dichloro-vinyl phosphonate

<b>Inchi:</b>	InChI=1S/C7H11Cl2O4P/c1-7(2)4-12-14(10,13-5-7)11-3-6(8)9/h3H,4-5H2,1-2H3
<b>InchiKey:</b>	FFWIVYNETUDCQC-UHFFFAOYSA-N
<b>Formula:</b>	C7H11Cl2O4P
<b>SMILES:</b>	CC1(C)COP(=O)(OC=C(Cl)Cl)OC1
<b>Mol. weight [g/mol]:</b>	261.04
<b>CAS:</b>	116402-11-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Crippen Method
logp	3.461		Crippen Method
mcvol	162.750	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=C116402110&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402110&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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