

# 1,3-Propanediol, 2,2-dimethyl-, cyclic phosphorochloridate

Other names:	2-chloro-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide
Inchi:	InChI=1S/C5H10ClO3P/c1-5(2)3-8-10(6,7)9-4-5/h3-4H2,1-2H3
InchiKey:	VZMUCIBBVMLEKC-UHFFFAOYSA-N
Formula:	C5H10ClO3P
SMILES:	CC1(C)COP(=O)(Cl)OC1
Mol. weight [g/mol]:	184.56
CAS:	4090-55-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.406		Crippen Method
mcvol	120.760	ml/mol	McGowan Method

## Sources

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>
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=C4090555&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4090555&amp;Units=SI</a>

## Legend

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

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