

# Bis(2-chloro-1-methylethyl) 2-chloropropyl phosphate

<b>Other names:</b>	Phosphoric acid, bis(2-chloro-1-methylethyl) 2-chloropropyl ester
<b>Inchi:</b>	InChI=1S/C9H18Cl3O4P/c1-7(12)6-14-17(13,15-8(2)4-10)16-9(3)5-11/h7-9H,4-6H2,1-3H
<b>InchiKey:</b>	NISNGFDWYZNPT-UHFFFAOYSA-N
<b>Formula:</b>	C9H18Cl3O4P
<b>SMILES:</b>	CC(Cl)COP(=O)(OC(C)CCl)OC(C)CCl
<b>Mol. weight [g/mol]:</b>	327.57
<b>CAS:</b>	76025-08-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	4.026		Crippen Method
mcvol	218.330	ml/mol	McGowan Method
rinpol	1828.00		NIST Webbook
rinpol	1831.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C76025086&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C76025086&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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
<b>rinpol:</b>	Non-polar retention indices

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