

# Bis-2-chloroethyl-2-chloroethylphosphonate

<b>Other names:</b>	Bis(«beta»-chloroethyl)-«beta»-chloroethyl phosphonate Phosphonic acid, (2-chloroethyl)-, bis(2-chloroethyl) ester
<b>Inchi:</b>	InChI=1S/C6H12Cl3O3P/c7-1-4-11-13(10,6-3-9)12-5-2-8/h1-6H2
<b>InchiKey:</b>	XXIDKSWYSYEFAG-UHFFFAOYSA-N
<b>Formula:</b>	C6H12Cl3O3P
<b>SMILES:</b>	O=P(CCCl)(OCCCl)OCCCl
<b>Mol. weight [g/mol]:</b>	269.49
<b>CAS:</b>	6294-34-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.929		Crippen Method
mcvol	170.190	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=C6294344&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6294344&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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