

# Phosphonic acid, chloro, cyclic 2-ethyl-2-hydroxy-methyltrimethylene ester

<b>Inchi:</b>	InChI=1S/C6H12ClO4P/c1-2-6(3-8)4-10-12(7,9)11-5-6/h8H,2-5H2,1H3
<b>InchiKey:</b>	UGXGXCYCELZNRBM-UHFFFAOYSA-N
<b>Formula:</b>	C6H12ClO4P
<b>SMILES:</b>	CCC1(CO)COP(=O)(Cl)OC1
<b>Mol. weight [g/mol]:</b>	214.58

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	1.769		Crippen Method
mcvol	140.720	ml/mol	McGowan Method

## Sources

<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=B6001546&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001546&amp;Units=SI</a>
<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>

## 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

Latest version available from:

<https://www.chemeo.com/cid/92-126-0/Phosphonic-acid-chloro-cyclic-2-ethyl-2-hydroxy-methyltrimethylene-ester.pdf>

Generated by Cheméo on 2024-04-28 21:54:35.501807913 +0000 UTC m=+16630524.422385224.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.