

# Bis(1,2,2-trimethylpropyl) methylphosphonate

<b>Other names:</b>	Phosphonic acid, methyl-, bis(1,2,2-trimethylpropyl) ester Methylphosphonic acid, bis(1,2,2-trimethylpropyl) ester Dipinacolyl methylphosphonate Methylphosphonic acid, dipinacolyl ester
<b>Inchi:</b>	InChI=1S/C13H29O3P/c1-10(12(3,4)5)15-17(9,14)16-11(2)13(6,7)8/h10-11H,1-9H3
<b>InchiKey:</b>	XSQAITMTGIQAHD-UHFFFAOYSA-N
<b>Formula:</b>	C13H29O3P
<b>SMILES:</b>	CC(OP(C)(=O)OC(C)C(C)(C)C(C)C(C)C
<b>Mol. weight [g/mol]:</b>	264.34
<b>CAS:</b>	7040-58-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	4.712		Crippen Method
mcvol	232.100	ml/mol	McGowan Method
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook

## Sources

<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=C7040586&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7040586&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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