

# Phosphorous acid, bis(2,2-dimethylpentyl) ester

<b>Inchi:</b>	InChI=1S/C14H31O3P/c1-7-9-13(3,4)11-16-18(15)17-12-14(5,6)10-8-2/h18H,7-12H2,1-6
<b>InchiKey:</b>	FFDNQLLGYMRACP-UHFFFAOYSA-N
<b>Formula:</b>	C14H31O3P
<b>SMILES:</b>	CCCC(C)(C)CO[PH](=O)OCC(C)(C)CCC
<b>Mol. weight [g/mol]:</b>	278.37
<b>CAS:</b>	116402-21-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	5.062		Crippen Method
mcvol	246.190	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=C116402212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402212&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

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