

# Phosphonic acid, phenyl-, di-isobutyl ester

<b>Inchi:</b>	InChI=1S/C14H23O3P/c1-12(2)10-16-18(15,17-11-13(3)4)14-8-6-5-7-9-14/h5-9,12-13H,
<b>InchiKey:</b>	PGYHLMXGZNLMIK-UHFFFAOYSA-N
<b>Formula:</b>	C14H23O3P
<b>SMILES:</b>	CC(C)COP(=O)(OCC(C)C)c1ccccc1
<b>Mol. weight [g/mol]:</b>	270.30
<b>CAS:</b>	64470-42-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.14		Crippen Method
logp	3.850		Crippen Method
mcvol	222.430	ml/mol	McGowan Method

## 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=C64470424&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C64470424&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
<b>mcvol:</b>	McGowan's characteristic volume

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