

# Phosphonic acid, methyl-, dihexyl ester

<b>Other names:</b>	Phosphonic acid, methyl-, O,O-dihexyl ester Methylphosphonic acid, dihexyl ester Phosphonic acid, P-methyl-, dihexyl ester
<b>Inchi:</b>	InChI=1S/C13H29O3P/c1-4-6-8-10-12-15-17(3,14)16-13-11-9-7-5-2/h4-13H2,1-3H3
<b>InchiKey:</b>	XMEOPSOYUNXCJQ-UHFFFAOYSA-N
<b>Formula:</b>	C13H29O3P
<b>SMILES:</b>	CCCCCOP(C)(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	264.34
<b>CAS:</b>	77304-63-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.71		Crippen Method
logp	5.003		Crippen Method
mcvol	232.100	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=C77304633&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C77304633&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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