

# Mono-octyl phosphate

<b>Other names:</b>	octyl dihydrogen phosphate
<b>Inchi:</b>	InChI=1S/C8H19O4P/c1-2-3-4-5-6-7-8-12-13(9,10)11/h2-8H2,1H3,(H2,9,10,11)
<b>InchiKey:</b>	WRKCIHRWQZQBOL-UHFFFAOYSA-N
<b>Formula:</b>	C8H19O4P
<b>SMILES:</b>	CCCCCCCCOP(=O)(O)O
<b>Mol. weight [g/mol]:</b>	210.21
<b>CAS:</b>	3991-73-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	2.456		Crippen Method
mcvol	167.520	ml/mol	McGowan Method

## Sources

<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>
<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=C3991739&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3991739&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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