

# Phosphonic acid, 2,4-hexadienoyl-, diethyl ester

<b>Inchi:</b>	InChI=1S/C10H17O4P/c1-4-7-8-9-10(11)15(12,13-5-2)14-6-3/h4,7-9H,5-6H2,1-3H3/b7-4
<b>InchiKey:</b>	KNBCPMPGYVYQRT-NUXDXBQRSA-N
<b>Formula:</b>	C10H17O4P
<b>SMILES:</b>	CC=CC=CC(=O)P(=O)(OCC)OCC
<b>Mol. weight [g/mol]:</b>	232.21
<b>CAS:</b>	109844-00-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	2.911		Crippen Method
mcvol	182.800	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=C109844000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109844000&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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