

# Hydrocinnamic acid, 2-phosphono-, p,p-diisopropyl c-methyl ester

<b>Inchi:</b>	InChI=1S/C16H25O5P/c1-12(2)20-22(18,21-13(3)4)15(16(17)19-5)11-14-9-7-6-8-10-14/H
<b>InchiKey:</b>	UEXRQYHLWCJVSL-UHFFFAOYSA-N
<b>Formula:</b>	C16H25O5P
<b>SMILES:</b>	COC(=O)C(Cc1ccccc1)P(=O)(OC(C)C)OC(C)C
<b>Mol. weight [g/mol]:</b>	328.34
<b>CAS:</b>	116401-34-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.27		Crippen Method
logp	3.814		Crippen Method
mcvol	258.050	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401344&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401344&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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