

# Isobutyric acid, 3-dibutoxyphosphinyl, methyl ester

<b>Inchi:</b>	InChI=1S/C13H27O5P/c1-5-7-9-17-19(15,18-10-8-6-2)11-12(3)13(14)16-4/h12H,5-11H2
<b>InchiKey:</b>	FRMUDADDWKVTFZ-UHFFFAOYSA-N
<b>Formula:</b>	C13H27O5P
<b>SMILES:</b>	CCCCOP(=O)(CC(C)C(=O)OC)OCCCC
<b>Mol. weight [g/mol]:</b>	294.32
<b>CAS:</b>	116595-33-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	3.622		Crippen Method
mcvol	239.540	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=C116595336&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595336&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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