

# Di[1,1'-biphenyl]-2-yl 4-(1-phenylethyl)phenyl phosphate

<b>Inchi:</b>	InChI=1S/C38H31O4P/c1-29(30-15-5-2-6-16-30)31-25-27-34(28-26-31)40-43(39,41-37-2
<b>InchiKey:</b>	NSGMZQQTTMQEMW-UHFFFAOYSA-N
<b>Formula:</b>	C38H31O4P
<b>SMILES:</b>	CC(c1ccccc1)c1ccc(OP(=O)(Oc2ccccc2-c2ccccc2)Oc2ccccc2-c2ccccc2)cc1
<b>Mol. weight [g/mol]:</b>	582.62
<b>CAS:</b>	116402-02-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-14.83		Crippen Method
logp	10.817		Crippen Method
mcvol	447.660	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402029&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402029&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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