

# Bis(4-tert-butylphenyl) 4-cyclohexylphenyl phosphate

<b>Inchi:</b>	InChI=1S/C32H41O4P/c1-31(2,3)26-14-20-29(21-15-26)35-37(33,36-30-22-16-27(17-23
<b>InchiKey:</b>	MHCOFIPYRBTZJP-UHFFFAOYSA-N
<b>Formula:</b>	C32H41O4P
<b>SMILES:</b>	CC(C)(C)c1ccc(OP(=O)(Oc2ccc(C3CCCCC3)cc2)Oc2ccc(C(C)(C)C)cc2)cc1
<b>Mol. weight [g/mol]:</b>	520.64
<b>CAS:</b>	116295-50-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.10		Crippen Method
logp	9.974		Crippen Method
mcvol	423.540	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=C116295502&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295502&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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