

# Di[1,1'-biphenyl]-2-yl 4-tert-butylphenyl phosphate

<b>Inchi:</b>	InChI=1S/C34H31O4P/c1-34(2,3)28-22-24-29(25-23-28)36-39(35,37-32-20-12-10-18-30)
<b>InchiKey:</b>	YBVDJFRGXXPYPS-UHFFFAOYSA-N
<b>Formula:</b>	C34H31O4P
<b>SMILES:</b>	CC(C)(C)c1ccc(OP(=O)(Oc2ccccc2-c2ccccc2)Oc2ccccc2-c2ccccc2)cc1
<b>Mol. weight [g/mol]:</b>	534.58

## Physical Properties

Property code	Value	Unit	Source
log10ws	-13.66		Crippen Method
logp	9.963		Crippen Method
mcvol	415.060	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=B6004019&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004019&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

Latest version available from:

<https://www.chemeo.com/cid/73-401-5/Di-1-1-biphenyl-2-yl-4-tert-butylphenyl-phosphate.pdf>

Generated by Cheméo on 2024-04-23 05:36:11.061141469 +0000 UTC m=+16139819.981718791.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.