

# 4-Tert-butylphenyl bis(2-methylphenyl) phosphate

<b>Inchi:</b>	InChI=1S/C24H27O4P/c1-18-10-6-8-12-22(18)27-29(25,28-23-13-9-7-11-19(23)2)26-21-
<b>InchiKey:</b>	UTVBYAZNJDVVSU-UHFFFAOYSA-N
<b>Formula:</b>	C24H27O4P
<b>SMILES:</b>	Cc1ccccc1OP(=O)(Oc1ccc(C(C)(C)C)cc1)Oc1ccccc1C
<b>Mol. weight [g/mol]:</b>	410.44
<b>CAS:</b>	116402-07-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.40		Crippen Method
logp	7.246		Crippen Method
mcvol	321.680	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402074&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402074&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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