

# 3,4-Dihydro-3,3-dimethyl-2-p-tolyl-2H-1,4,2-benzox

<b>Inchi:</b>	InChI=1S/C16H18NO2P/c1-12-8-10-13(11-9-12)20(18)16(2,3)17-14-6-4-5-7-15(14)19-20
<b>InchiKey:</b>	ZVVGPFDOIWVWL-UHFFFAOYSA-N
<b>Formula:</b>	C16H18NO2P
<b>SMILES:</b>	Cc1ccc(P2(=O)Oc3ccccc3NC2(C)C)cc1
<b>Mol. weight [g/mol]:</b>	287.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.28		Crippen Method
logp	4.139		Crippen Method
mcvol	220.100	ml/mol	McGowan Method
rinpol	2468.00		NIST Webbook

## 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=R566868&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R566868&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
<b>rinpol:</b>	Non-polar retention indices

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