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

Inchi: 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
InchiKey: ZVVGPWFDOIWWQL-UHFFFAOYSA-N
Formula: C16H18NO2P
SMILES: Cc1ccc(P2(=O)Oc3ccccc3NC2(C)C)cc1
Mol. weight [g/mol]: 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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R566868&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices