

# 3,4-Dihydro-3-phenyl-6-(1,1,3,3-tetramethylbutyl)-2H-1,3-benzoxazine

**Inchi:** InChI=1S/C22H29NO/c1-21(2,3)15-22(4,5)18-11-12-20-17(13-18)14-23(16-24-20)19-9-7  
**InchiKey:** VERSMYMNMADGSM-UHFFFAOYSA-N  
**Formula:** C22H29NO  
**SMILES:** CC(C)(C)CC(C)(C)c1ccc2c(c1)CN(c1ccccc1)CO2  
**Mol. weight [g/mol]:** 323.47

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.33		Crippen Method
logp	5.757		Crippen Method
mcvol	278.310	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=B6003974&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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