2H-1,3-Benzoxazine, 6-(1,1-dimethylethyl)-3,4-dihydro-3-phenyl-

Other names:	6-Tert-butyl-3-phenyl-3,4-dihydro-2h-1,3-benzoxazine
Inchi:	InChI=1S/C18H21NO/c1-18(2,3)15-9-10-17-14(11-15)12-19(13-20-17)16-7-5-4-6-8-16/h4
InchiKey:	INQHAWUMPJGNOM-UHFFFAOYSA-N
Formula:	C18H21NO
SMILES:	CC(C)(C)c1ccc2c(c1)CN(c1ccccc1)CO2
Mol. weight [g/mol]:	267.37
CAS:	55955-97-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.89		Crippen Method
logp	4.341		Crippen Method
mcvol	221.950	ml/mol	McGowan Method

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=C55955970&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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