

2H-1,3-Benzoxazine, 6-chloro-3,4-dihydro-3-phenyl-

Other names:	6-Chloro-3-phenyl-3,4-dihydro-2h-1,3-benzoxazine
Inchi:	InChI=1S/C14H12ClNO/c15-12-6-7-14-11(8-12)9-16(10-17-14)13-4-2-1-3-5-13/h1-8H,9-
InchiKey:	ANDMOXODDHVMFN-UHFFFAOYSA-N
Formula:	C14H12ClNO
SMILES:	Clc1ccc2c(c1)CN(c1ccccc1)CO2
Mol. weight [g/mol]:	245.70
CAS:	51892-04-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.696		Crippen Method
mcvol	177.830	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C51892047&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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