

2H-1,3-Benzoxazine, 6-chloro-3-cyclohexyl-3,4-dihydro-8-methyl-

Other names:	6-Chloro-3-cyclohexyl-3,4-dihydro-8-methyl-2H-1,3-benzoxazine
Inchi:	InChI=1S/C15H20ClNO/c1-11-7-13(16)8-12-9-17(10-18-15(11)12)14-5-3-2-4-6-14/h7-8,1
InchiKey:	HLFBMVRLQWNGLY-UHFFFAOYSA-N
Formula:	C15H20ClNO
SMILES:	<chem>Cc1cc(Cl)cc2c1OCN(C1CCCCC1)C2</chem>
Mol. weight [g/mol]:	265.78
CAS:	6640-34-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.11		Crippen Method
logp	4.133		Crippen Method
mcvol	204.820	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=C6640342&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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