8,8'-Methylene bis-(6-chloro-3,4-dihydro-3-phenyl-2h, 1,3-benzoxazine)

Inchi: InChI=1S/C29H24Cl2N2O2/c30-24-12-20(28-22(14-24)16-32(18-34-28)26-7-3-1-4-8-26)1

InchiKey: HVGXMJWHXMQBLQ-UHFFFAOYSA-N

Formula: C29H24Cl2N2O2

SMILES: Clc1cc(Cc2cc(Cl)cc3c2OCN(c2ccccc2)C3)c2c(c1)CN(c1ccccc1)CO2

Mol. weight [g/mol]: 503.42

CAS: 103269-23-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.16		Crippen Method
logp	7.297		Crippen Method
mcvol	358.890	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103269234&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume