6-Bromo-3-phenyl-3,4-dihydro-2h-1,3-benzoxazine

Inchi: InChI=1S/C14H12BrNO/c15-12-6-7-14-11(8-12)9-16(10-17-14)13-4-2-1-3-5-13/h1-8H,9-1
InchiKey: BPENDNNWTFWJPC-UHFFFAOYSA-N
Formula: C14H12BrNO
SMILES: Brc1ccc2c(c1)CN(c1ccccc1)CO2
Mol. weight [g/mol]: 290.15
CAS: 116495-83-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	3.806		Crippen Method
mcvol	183.090	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495831&Units=SI
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

Legend

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