

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-
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/ci9903071
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

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