

2-phenyl-4-butyl-tetrahydro-1,4-oxazine

Inchi: InChI=1S/C14H21NO/c1-2-3-9-15-10-11-16-14(12-15)13-7-5-4-6-8-13/h4-8,14H,2-3,9-12
InchiKey: WTHGQPVOMHFJIL-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCC1CCOC(c2ccccc2)C1
Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	2.860		Crippen Method
mcvol	189.350	ml/mol	McGowan Method
rinpol	1706.80		NIST Webbook
rinpol	1704.40		NIST Webbook
rinpol	1700.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R293580&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
rinpol: Non-polar retention indices

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