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

Inchi: InChI=1S/C14H21NO/c1-12(2)10-15-8-9-16-14(11-15)13-6-4-3-5-7-13/h3-7,12,14H,8-11
InchiKey: NVQGZBNFGIADTH-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CC(C)CN1CCOC(c2ccccc2)C1
Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	2.716		Crippen Method
mcvol	189.350	ml/mol	McGowan Method
rinpol	1699.12		NIST Webbook
rinpol	1698.64		NIST Webbook
rinpol	1695.55		NIST Webbook
rinpol	1699.12		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R293595&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
rinpol: Non-polar retention indices

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