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

Inchi: InChI=1S/C13H19NO/c1-11(2)14-8-9-15-13(10-14)12-6-4-3-5-7-12/h3-7,11,13H,8-10H2,
InchiKey: CHHFZVOTWWUPDQ-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CC(C)N1CCOC(c2ccccc2)C1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	2.468		Crippen Method
mcvol	175.260	ml/mol	McGowan Method
rinpol	1598.75		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1595.83		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R293619&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices