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

Inchi: InChI=1S/C15H23NO/c1-13(2)8-9-16-10-11-17-15(12-16)14-6-4-3-5-7-14/h3-7,13,15H,8-
InchiKey: SNCBWULAZWKWRJ-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CC(C)CCN1CCOC(c2ccccc2)C1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	3.106		Crippen Method
mcvol	203.440	ml/mol	McGowan Method
rinpol	1800.28		NIST Webbook
rinpol	1795.65		NIST Webbook
rinpol	1800.19		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=R293604&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