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

Inchi: InChI=1S/C15H23NO/c1-2-3-7-10-16-11-12-17-15(13-16)14-8-5-4-6-9-14/h4-6,8-9,15H,2
InchiKey: MZCPNUOUBRLOEF-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CCCCCN1CCOC(c2ccccc2)C1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	3.250		Crippen Method
mcvol	203.440	ml/mol	McGowan Method
rinpol	1803.10		NIST Webbook
rinpol	1802.60		NIST Webbook
rinpol	1800.30		NIST Webbook
rinpol	1803.10		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=R293624&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

Latest version available from: