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

Inchi: InChI=1S/C13H19NO/c1-2-8-14-9-10-15-13(11-14)12-6-4-3-5-7-12/h3-7,13H,2,8-11H2,1
InchiKey: VYAMLADJSHKTKB-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CCCN1CCOC(c2ccccc2)C1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	2.470		Crippen Method
mcvol	175.260	ml/mol	McGowan Method
rinpol	1605.80		NIST Webbook
rinpol	1608.80		NIST Webbook
rinpol	1602.10		NIST Webbook
rinpol	1605.80		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=R293639&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: