

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/ci9903071>
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

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