

Angustureine

Inchi: InChI=1S/C15H23N/c1-3-4-5-9-14-12-11-13-8-6-7-10-15(13)16(14)2/h6-8,10,14H,3-5,9,11H
InchiKey: KSQZVAWGIAAZHJ-CQSZACIVSA-N
Formula: C15H23N
SMILES: CCCCCC1CCc2ccccc2N1C
Mol. weight [g/mol]: 217.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	4.018		Crippen Method
mcvol	197.570	ml/mol	McGowan Method
rinpol	1770.00		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=R398313&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:

<https://www.chemeo.com/cid/60-857-4/Angustureine.pdf>

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