

Cuscohygrine

Inchi: InChI=1S/C13H24N2O/c1-14-7-3-5-11(14)9-13(16)10-12-6-4-8-15(12)2/h11-12H,3-10H2
InchiKey: ZEBIACKKLGVLVLFZ-UHFFFAOYSA-N
Formula: C13H24N2O
SMILES: CN1CCCC1CC(=O)CC1CCCN1C
Mol. weight [g/mol]: 224.34
CAS: 454-14-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	1.524		Crippen Method
mcvol	193.840	ml/mol	McGowan Method
rinpol	1650.00		NIST Webbook
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rinpol	1650.00		NIST Webbook
rinpol	1650.00		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=C454148&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/22-045-7/Cuscohygrine.pdf>

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