

2',3-N-Methylpyrrolidinyhygrine

Other names: 2',3-N-Methylpyrrolidinyhygrine
Inchi: InChI=1S/C13H24N2O/c1-10(16)9-13-11(6-8-15(13)3)12-5-4-7-14(12)2/h11-13H,4-9H2,1
InchiKey: SZBJLDZJDLLKKT-BPCQOVAHSA-N
Formula: C13H24N2O
SMILES: CC(=O)CC1C(C2CCCN2C)CCN1C
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	1.380		Crippen Method
mcvol	193.840	ml/mol	McGowan Method
rinpol	1577.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1580.00		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=R274316&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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