

2-Pyrrolidinone, 3-hydroxy-1-methyl-5-(3-pyridinyl)-, (3R-trans)-

Other names:

trans-3-Hydroxycotinine

Hydroxycotinine

3-Hydroxycotinine

trans-3'-Hydroxycotinine

Inchi:

InChI=1S/C10H12N2O2/c1-12-8(5-9(13)10(12)14)7-3-2-4-11-6-7/h2-4,6,8-9,13H,5H2,1H

InchiKey:

XOKCJXZZNAUIQN-DTWKUNHWSA-N

Formula:

C10H12N2O2

SMILES:

CN1C(=O)C(O)CC1c1cccnc1

Mol. weight [g/mol]:

192.21

CAS:

34834-67-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	0.346		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rmpol	1812.60		NIST Webbook
rmpol	1812.60		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C34834678&Units=SI>

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>

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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