Anatabine, N-formyl

Inchi: InChI=1S/C11H12N2O/c14-9-13-7-2-1-5-11(13)10-4-3-6-12-8-10/h1-4,6,8-9,11H,5,7H2
InchiKey: IIXFXMGADSMCLR-UHFFFAOYSA-N
Formula: C11H12N2O
SMILES: O=CN1CC=CCC1c1cccnc1
Mol. weight [g/mol]: 188.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	1.541		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	1858.00		NIST Webbook
rinpol	1858.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R44786&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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