Anatabine, N-acetyl

Inchi: InChI=1S/C12H14N2O/c1-10(15)14-8-3-2-6-12(14)11-5-4-7-13-9-11/h2-5,7,9,12H,6,8H2
InchiKey: CAYYVQDGGHLYMO-UHFFFAOYSA-N
Formula: C12H14N2O
SMILES: CC(=O)N1CC=CCC1c1cccnc1
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	1.931		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
rinpol	1902.00		NIST Webbook

Sources

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=R44772&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices