

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

Latest version available from:

<https://www.chemeo.com/cid/65-694-0/Anatabine-N-acetyl.pdf>

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