

Nornicotine, N-acetyl

Inchi:	InChI=1S/C11H14N2O/c1-9(14)13-7-3-5-11(13)10-4-2-6-12-8-10/h2,4,6,8,11H,3,5,7H2,1
InchiKey:	SSABMTSCLQGWB-BUHFFFAOYSA-N
Formula:	C11H14N2O
SMILES:	CC(=O)N1CCCC1c1cccnc1
Mol. weight [g/mol]:	190.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	1.765		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
rinsol	1827.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R44807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinsol:	Non-polar retention indices

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