

Nornicotine, N-hexanoyl

Inchi:	InChI=1S/C15H22N2O/c1-2-3-4-9-15(18)17-11-6-8-14(17)13-7-5-10-16-12-13/h5,7,10,12
InchiKey:	NKXYWVGCISTJDE-UHFFFAOYSA-N
Formula:	C15H22N2O
SMILES:	CCCCCC(=O)N1CCCC1c1cccnc1
Mol. weight [g/mol]:	246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.09		Crippen Method
logp	3.325		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
rinpola	2159.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R44839&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
rinpola:	Non-polar retention indices

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