

Nornicotine, N-butanoyl

Inchi:	InChI=1S/C13H18N2O/c1-2-5-13(16)15-9-4-7-12(15)11-6-3-8-14-10-11/h3,6,8,10,12H,2,
InchiKey:	MIRXCTXDBCQAAR-UHFFFAOYSA-N
Formula:	C13H18N2O
SMILES:	CCCC(=O)N1CCCC1c1cccnc1
Mol. weight [g/mol]:	218.29
CAS:	69730-91-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	2.545		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
rinpol	1961.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C69730912&Units=SI

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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<https://www.chemeo.com/cid/31-548-9/Nornicotine-N-butanoyl.pdf>

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