

Nicotinamide, N,N-dihexyl-

Inchi:	InChI=1S/C18H30N2O/c1-3-5-7-9-14-20(15-10-8-6-4-2)18(21)17-12-11-13-19-16-17/h11
InchiKey:	QYZSGTMURONPKY-UHFFFAOYSA-N
Formula:	C18H30N2O
SMILES:	CCCCCN(CCCCC)C(=O)c1cccnc1
Mol. weight [g/mol]:	290.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.57		Crippen Method
logp	4.684		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
rinpol	2232.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308472&Units=SI
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

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/10-765-1/Nicotinamide-N-N-dihexyl.pdf>

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