

Nicotinamide, N-(1-naphthyl)-

Inchi: InChI=1S/C16H12N2O/c19-16(13-7-4-10-17-11-13)18-15-9-3-6-12-5-1-2-8-14(12)15/h1-16
InchiKey: OZOFJVFVGZHBHV-UHFFFAOYSA-N
Formula: C16H12N2O
SMILES: O=C(Nc1cccc2ccccc12)c1cccnc1
Mol. weight [g/mol]: 248.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	3.487		Crippen Method
mcvol	190.850	ml/mol	McGowan Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		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=U308111&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/113-755-8/Nicotinamide-N-1-naphthyl.pdf>

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