

Isonicotinamide, N-decyl-N-methyl-

Inchi: InChI=1S/C17H28N2O/c1-3-4-5-6-7-8-9-10-15-19(2)17(20)16-11-13-18-14-12-16/h11-14
InchiKey: SRGUWNCOTIABDR-UHFFFAOYSA-N
Formula: C17H28N2O
SMILES: CCCCCCCCCN(C)C(=O)c1cncc1
Mol. weight [g/mol]: 276.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Crippen Method
logp	4.294		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
rinsol	2209.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308642&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/68-271-6/Isonicotinamide-N-decyl-N-methyl.pdf>

Generated by Cheméo on 2024-04-27 10:21:26.699191434 +0000 UTC m=+16502535.619768756.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.