

Isonicotinamide, N-heptyl-N-octyl-

Inchi: InChI=1S/C21H36N2O/c1-3-5-7-9-11-13-19-23(18-12-10-8-6-4-2)21(24)20-14-16-22-17-
InchiKey: VKVQNQNWKVDQOV-UHFFFAOYSA-N
Formula: C21H36N2O
SMILES: CCCCCCCN(CCCCCC)C(=O)c1ccncc1
Mol. weight [g/mol]: 332.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	5.855		Crippen Method
mcvol	304.520	ml/mol	McGowan Method
rinpola	2471.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308644&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/40-543-4/Isonicotinamide-N-heptyl-N-octyl.pdf>

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