

Isonicotinamide, N,N-didecyl-

Inchi: InChI=1S/C26H46N2O/c1-3-5-7-9-11-13-15-17-23-28(26(29)25-19-21-27-22-20-25)24-18
InchiKey: YDQMMWYGUPPADS-UHFFFAOYSA-N
Formula: C26H46N2O
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)c1ccncc1
Mol. weight [g/mol]: 402.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	7.805		Crippen Method
mcvol	374.970	ml/mol	McGowan Method
rinpol	2997.00		NIST Webbook
rinpol	2997.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308647&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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