Isonicotinamide, N,N-dioctyl-

Inchi: InChI=1S/C22H38N2O/c1-3-5-7-9-11-13-19-24(20-14-12-10-8-6-4-2)22(25)21-15-17-23-
InchiKey: SQSMOCDVJZOEHJ-UHFFFAOYSA-N
Formula: C22H38N2O
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)c1ccncc1
Mol. weight [g/mol]: 346.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.24		Crippen Method
logp	6.245		Crippen Method
mcvol	318.610	ml/mol	McGowan Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		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=U308645&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

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