

Isonicotinamide, N,N-dinonyl-

Inchi: InChI=1S/C24H42N2O/c1-3-5-7-9-11-13-15-21-26(22-16-14-12-10-8-6-4-2)24(27)23-17-
InchiKey: YRWSROYVIOPCRR-UHFFFAOYSA-N
Formula: C24H42N2O
SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)c1ccncc1
Mol. weight [g/mol]: 374.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.08		Crippen Method
logp	7.025		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
rinpol	2761.00		NIST Webbook
rinpol	2761.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308646&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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