

Isonipecotic acid, N-(cyclohexylcarbonyl)-, undecyl ester

Inchi: InChI=1S/C24H43NO3/c1-2-3-4-5-6-7-8-9-13-20-28-24(27)22-16-18-25(19-17-22)23(26)
InchiKey: PGDNHCJMGBMHDJ-UHFFFAOYSA-N
Formula: C24H43NO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]: 393.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.38		Crippen Method
logp	5.879		Crippen Method
mcvol	346.290	ml/mol	McGowan Method
rmpol	3182.00		NIST Webbook
rmpol	3182.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U361034&Units=SI>

Legend

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

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