

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

Inchi: InChI=1S/C23H41NO3/c1-2-3-4-5-6-7-8-12-19-27-23(26)21-15-17-24(18-16-21)22(25)20
InchiKey: SUROJKDVSBNTHS-UHFFFAOYSA-N
Formula: C23H41NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]: 379.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	5.489		Crippen Method
mcvol	332.200	ml/mol	McGowan Method
rinsol	3076.00		NIST Webbook
rinsol	3076.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361033&Units=SI>
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>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/45-599-8/Isonipecotic-acid-N-cyclohexylcarbonyl-decyl-ester.pdf>

Generated by Cheméo on 2024-04-19 17:42:04.626713067 +0000 UTC m=+15837773.547290382.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.