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

Inchi: InChI=1S/C22H39NO3/c1-2-3-4-5-6-7-11-18-26-22(25)20-14-16-23(17-15-20)21(24)19-1
InchiKey: JUATXFKFQIKUOR-UHFFFAOYSA-N
Formula: C22H39NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]: 365.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.55		Crippen Method
logp	5.099		Crippen Method
mcvol	318.110	ml/mol	McGowan Method
rinpol	2972.00		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=U361032&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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