

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

Inchi: InChI=1S/C29H53NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-25-33-29(32)27-21-23-30(31)22-24-26-28-30
InchiKey: FJHRGPVJHOPOCF-UHFFFAOYSA-N
Formula: C29H53NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]: 463.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.48		Crippen Method
logp	7.830		Crippen Method
mcvol	416.740	ml/mol	McGowan Method
rinpola	3091.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361039&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpola: Non-polar retention indices

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