Isonipecotic acid, N-(octanoyl)-, tridecyl ester

Inchi: InChI=1S/C27H51NO3/c1-3-5-7-9-10-11-12-13-14-16-18-24-31-27(30)25-20-22-28(23-21
InchiKey: KFEQDDJOYTZJJV-UHFFFAOYSA-N
Formula: C27H51NO3
SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CCCCCCC)CC1
Mol. weight [g/mol]: 437.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.99		Crippen Method
logp	7.440		Crippen Method
mcvol	399.420	ml/mol	McGowan Method
rinpol	3388.00		NIST Webbook
rinpol	3388.00		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=U361579&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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