

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

Inchi: InChI=1S/C23H43NO3/c1-3-5-7-9-10-12-14-20-27-23(26)21-16-18-24(19-17-21)22(25)15
InchiKey: ADIGNYDSVNDYDS-UHFFFAOYSA-N
Formula: C23H43NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)CCCCCCC)CC1
Mol. weight [g/mol]: 381.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.31		Crippen Method
logp	5.879		Crippen Method
mcvol	343.060	ml/mol	McGowan Method
rmpol	2985.00		NIST Webbook
rmpol	2985.00		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=U361575&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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