

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

Inchi: InChI=1S/C26H49NO3/c1-3-5-7-9-10-11-12-13-15-17-23-30-26(29)24-19-21-27(22-20-25)
InchiKey: BRDSVAUNJDZTAL-UHFFFAOYSA-N
Formula: C26H49NO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)CCCCCCC)CC1
Mol. weight [g/mol]: 423.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	7.050		Crippen Method
mcvol	385.330	ml/mol	McGowan Method
rinpol	3287.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U361578&Units=SI>

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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