

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

Inchi: InChI=1S/C22H41NO3/c1-3-5-7-9-11-13-19-26-22(25)20-15-17-23(18-16-20)21(24)14-12
InchiKey: FPJCKMGOZHIBPL-UHFFFAOYSA-N
Formula: C22H41NO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)CCCCC)CC1
Mol. weight [g/mol]: 367.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.89		Crippen Method
logp	5.489		Crippen Method
mcvol	328.970	ml/mol	McGowan Method
rinpol	2863.00		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=U361574&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

Latest version available from:

<https://www.chemeo.com/cid/15-720-5/Isonipecotic-acid-N-octanoyl-octyl-ester.pdf>

Generated by Cheméo on 2024-05-24 09:27:46.146680881 +0000 UTC m=+18832115.067258196.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.