

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
rinpola	2863.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpola: Non-polar retention indices

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