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

Inchi: InChI=1S/C20H37NO3/c1-4-5-6-7-8-11-19(22)21-14-12-18(13-15-21)20(23)24-16-9-10-1
InchiKey: YXTNHCYADQRFNN-UHFFFAOYSA-N
Formula: C20H37NO3
SMILES: CCCCCCCC(=O)N1CCC(C(=O)OCCCC(C)C)CC1
Mol. weight [g/mol]: 339.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	4.565		Crippen Method
mcvol	300.790	ml/mol	McGowan Method
rinpol	2624.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361571&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices