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

Inchi: InChI=1S/C18H33NO3/c1-4-5-6-7-8-9-17(20)19-12-10-16(11-13-19)18(21)22-14-15(2)3/l
InchiKey: JWESKGOLWARBFE-UHFFFAOYSA-N
Formula: C18H33NO3
SMILES: CCCCCCCC(=O)N1CCC(C(=O)OCC(C)C)CC1
Mol. weight [g/mol]: 311.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.785		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
rinpol	2413.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361568&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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