Isonipecotic acid, N-(3-methylbutyryl)-, heptyl ester

Inchi: InChI=1S/C18H33NO3/c1-4-5-6-7-8-13-22-18(21)16-9-11-19(12-10-16)17(20)14-15(2)3/l

InchiKey: MBYAKLHPYOQAGV-UHFFFAOYSA-N

Formula: C18H33NO3

SMILES: CCCCCCCOC(=O)C1CCN(C(=O)CC(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	2392.00		NIST Webbook

Sources

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=U360991&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices