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

Inchi: InChI=1S/C23H43NO3/c1-4-5-6-7-8-9-10-11-12-13-18-27-23(26)21-14-16-24(17-15-21)2
InchiKey: OKHKBWLXFPSGNK-UHFFFAOYSA-N
Formula: C23H43NO3
SMILES: CCCCCCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]: 381.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	5.735		Crippen Method
mcvol	343.060	ml/mol	McGowan Method
rinpol	2905.00		NIST Webbook
rinpol	2905.00		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=U360996&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

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