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

Inchi: InChI=1S/C28H53NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-32-28(31)26-19-2
InchiKey: YYCXSTIDIHYRJT-UHFFFAOYSA-N
Formula: C28H53NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]: 451.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.16		Crippen Method
logp	7.686		Crippen Method
mcvol	413.510	ml/mol	McGowan Method
rinpol	3436.00		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=U361001&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

Latest version available from:
https://www.chemeo.com/cid/19-693-2/Isonipecotic-acid-N-3-methylbutyryl-heptadecyl-ester.pdf
Generated by Cheméo on 2024-10-12 02:47:57.532041701 +0000 UTC m=+3282140.169010950.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.