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

Inchi: InChI=1S/C26H49NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-21-30-26(29)24-17-19-27(2

InchiKey: UCUDFBXTMGZFEA-UHFFFAOYSA-N

Formula: C26H49NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1

Mol. weight [g/mol]: 423.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.33		Crippen Method
logp	6.905		Crippen Method
mcvol	385.330	ml/mol	McGowan Method
rinpol	3226.00		NIST Webbook
rinpol	3226.00		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=U360999&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.