

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

Inchi: InChI=1S/C27H51NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-31-27(30)25-18-20-2
InchiKey: OBOFWDUNCIRFIH-UHFFFAOYSA-N
Formula: C27H51NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]: 437.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.74		Crippen Method
logp	7.296		Crippen Method
mcvol	399.420	ml/mol	McGowan Method
rmpol	3328.00		NIST Webbook
rmpol	3328.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U361000&Units=SI>

Legend

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

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