

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

Inchi: InChI=1S/C25H47NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-20-29-25(28)23-16-18-26(19-1
InchiKey: DFBYZOBGFHAYAL-UHFFFAOYSA-N
Formula: C25H47NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]: 409.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	6.515		Crippen Method
mcvol	371.240	ml/mol	McGowan Method
rinpol	3123.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360998&Units=SI>
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>

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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