

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

Inchi:	InChI=1S/C24H45NO3/c1-4-5-6-7-8-9-10-11-12-13-14-19-28-24(27)22-15-17-25(18-16-2
InchiKey:	SSYBAGRYTYPFIP-UHFFFAOYSA-N
Formula:	C24H45NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]:	395.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	6.125		Crippen Method
mcvol	357.150	ml/mol	McGowan Method
rmpol	3018.00		NIST Webbook
rmpol	3018.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360997&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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