

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

Inchi:	InChI=1S/C17H31NO3/c1-4-5-6-7-12-21-17(20)15-8-10-18(11-9-15)16(19)13-14(2)3/h14
InchiKey:	CXFRSNDQHBQSMU-UHFFFAOYSA-N
Formula:	C17H31NO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]:	297.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	3.395		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/42-081-5/Isonipecotic-acid-N-3-methylbutyryl-hexyl-ester.pdf>

Generated by Cheméo on 2025-12-05 15:13:48.161079869 +0000 UTC m=+4695825.691120524.

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