

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

Inchi:	InChI=1S/C16H29NO3/c1-4-5-6-11-20-16(19)14-7-9-17(10-8-14)15(18)12-13(2)3/h13-14
InchiKey:	JITFTNMMCHAEJB-UHFFFAOYSA-N
Formula:	C16H29NO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]:	283.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	3.004		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
rinpol	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook

Sources

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=U360988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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