

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

Inchi:	InChI=1S/C15H27NO3/c1-4-5-10-19-15(18)13-6-8-16(9-7-13)14(17)11-12(2)3/h12-13H,4
InchiKey:	AIJODJFJPWKUDR-UHFFFAOYSA-N
Formula:	C15H27NO3
SMILES:	CCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]:	269.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	2.614		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
rinpol	2081.00		NIST Webbook
rinpol	2081.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360987&Units=SI

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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