

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

Inchi:	InChI=1S/C13H23NO3/c1-4-17-13(16)11-5-7-14(8-6-11)12(15)9-10(2)3/h10-11H,4-9H2,1
InchiKey:	LHMXIRVZMGWCLY-UHFFFAOYSA-N
Formula:	C13H23NO3
SMILES:	CCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]:	241.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	1.834		Crippen Method
mcvol	202.160	ml/mol	McGowan Method
rinsol	1867.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U360985&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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