

# Isonipecotic acid, N-(3-methylbutyryl)-, isoheyl ester

**Inchi:** InChI=1S/C17H31NO3/c1-13(2)6-5-11-21-17(20)15-7-9-18(10-8-15)16(19)12-14(3)4/h13  
**InchiKey:** KCDYBGSABUBEKX-UHFFFAOYSA-N  
**Formula:** C17H31NO3  
**SMILES:** CC(C)CCCOC(=O)C1CCN(C(=O)CC(C)C)CC1  
**Mol. weight [g/mol]:** 297.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	3.250		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
rinpola	2247.00		NIST Webbook
rinpola	2247.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360989&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](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  
**rinpola:** Non-polar retention indices

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