

# Isonipecotic acid, N-(3-chloropropionyl)-, isobutyl ester

**Inchi:** InChI=1S/C13H22ClNO3/c1-10(2)9-18-13(17)11-4-7-15(8-5-11)12(16)3-6-14/h10-11H,3-  
**InchiKey:** SWGVFU YCDUTROE-UHFFFAOYSA-N  
**Formula:** C13H22ClNO3  
**SMILES:** CC(C)COC(=O)C1CCN(C(=O)CCCI)CC1  
**Mol. weight [g/mol]:** 275.77

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	2.053		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360942&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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

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