

# Isonipecotic acid, N-ethoxycarbonyl-, isobutyl ester

**Inchi:** InChI=1S/C13H23NO4/c1-4-17-13(16)14-7-5-11(6-8-14)12(15)18-9-10(2)3/h10-11H,4-9H  
**InchiKey:** MSOURNUAHFPUCW-UHFFFAOYSA-N  
**Formula:** C13H23NO4  
**SMILES:** CCOC(=O)N1CCC(C(=O)OCC(C)C)CC1  
**Mol. weight [g/mol]:** 257.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	2.054		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinsol	1827.00		NIST Webbook
rinsol	1827.00		NIST Webbook

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322002&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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