

# Isonipecotic acid, N-(2-fluoro-3-chlorobenzoyl)-, isobutyl ester

**Inchi:** InChI=1S/C17H21ClFNO3/c1-11(2)10-23-17(22)12-6-8-20(9-7-12)16(21)13-4-3-5-14(18)  
**InchiKey:** BUUMBEHUDJUHEZ-UHFFFAOYSA-N  
**Formula:** C17H21ClFNO3  
**SMILES:** CC(C)COC(=O)C1CCN(C(=O)c2cccc(Cl)c2F)CC1  
**Mol. weight [g/mol]:** 341.81

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	3.531		Crippen Method
mcvol	248.770	ml/mol	McGowan Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361432&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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