

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

**Inchi:** InChI=1S/C15H17ClFNO3/c1-2-21-15(20)10-6-8-18(9-7-10)14(19)11-4-3-5-12(16)13(11)  
**InchiKey:** AULHNFSSVDNKNKNN-UHFFFAOYSA-N  
**Formula:** C15H17ClFNO3  
**SMILES:** CCOC(=O)C1CCN(C(=O)c2cccc(Cl)c2F)CC1  
**Mol. weight [g/mol]:** 313.75

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	2.894		Crippen Method
mcvol	220.590	ml/mol	McGowan Method
rinpola	2393.00		NIST Webbook
rinpola	2393.00		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=U361430&Units=SI>

## 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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