

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

**Inchi:** InChI=1S/C16H19ClFNO3/c1-2-10-22-16(21)11-6-8-19(9-7-11)15(20)12-4-3-5-13(17)14(21)  
**InchiKey:** QQMLBCNPEDBVEH-UHFFFAOYSA-N  
**Formula:** C16H19ClFNO3  
**SMILES:** CCCOC(=O)C1CCN(C(=O)c2cccc(Cl)c2F)CC1  
**Mol. weight [g/mol]:** 327.78

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.284		Crippen Method
mcvol	234.680	ml/mol	McGowan Method
rinpola	2506.00		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=U361431&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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