

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

**Inchi:** InChI=1S/C18H23ClFNO3/c1-2-3-4-12-24-18(23)13-8-10-21(11-9-13)17(22)14-6-5-7-15(20)  
**InchiKey:** NWEGLQWDEFPCAB-UHFFFAOYSA-N  
**Formula:** C18H23ClFNO3  
**SMILES:** CCCCCOC(=O)C1CCN(C(=O)c2cccc(Cl)c2F)CC1  
**Mol. weight [g/mol]:** 355.83

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	4.065		Crippen Method
mcvol	262.860	ml/mol	McGowan Method
rinpole	2710.00		NIST Webbook
rinpole	2710.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361434&Units=SI>  
**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)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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