

# Isonipecotic acid, N-(3,4-difluorobenzoyl)-, ethyl ester

**Inchi:** InChI=1S/C15H17F2NO3/c1-2-21-15(20)10-5-7-18(8-6-10)14(19)11-3-4-12(16)13(17)9-1  
**InchiKey:** IFVIIAILMHDVSH-UHFFFAOYSA-N  
**Formula:** C15H17F2NO3  
**SMILES:** CCOC(=O)C1CCN(C(=O)c2ccc(F)c(F)c2)CC1  
**Mol. weight [g/mol]:** 297.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.380		Crippen Method
mcvol	210.120	ml/mol	McGowan Method
rinpole	2183.00		NIST Webbook
rinpole	2183.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361263&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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