

# Isonipecotic acid, N-(2,6-difluoro-3-methylbenzoyl)-, butyl ester

**Inchi:** InChI=1S/C18H23F2NO3/c1-3-4-11-24-18(23)13-7-9-21(10-8-13)17(22)15-14(19)6-5-12  
**InchiKey:** HXNBOMPQJWHOSX-UHFFFAOYSA-N  
**Formula:** C18H23F2NO3  
**SMILES:** CCCCOC(=O)C1CCN(C(=O)c2c(F)ccc(C)c2F)CC1  
**Mol. weight [g/mol]:** 339.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	3.469		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		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=U361300&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  
**rinpol:** Non-polar retention indices

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