

# Isonipecotinoylisonipecotic acid, N'-pentafluorobenzoyl-, isobutyl ester

**Inchi:** InChI=1S/C23H27F5N2O4/c1-12(2)11-34-23(33)14-5-9-29(10-6-14)21(31)13-3-7-30(8-4)  
**InchiKey:** CAHVHOKNOWSMMJ-UHFFFAOYSA-N  
**Formula:** C23H27F5N2O4  
**SMILES:** CC(C)COC(=O)C1CCN(C(=O)C2CCN(C(=O)c3c(F)c(F)c(F)c(F)c3F)CC2)CC1  
**Mol. weight [g/mol]:** 490.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.41		Crippen Method
logp	3.672		Crippen Method
mcvol	328.840	ml/mol	McGowan Method
rinpol	3305.00		NIST Webbook
rinpol	3305.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361235&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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>

## 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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