

# Isonipectic acid, N-(2,4-difluorobenzoyl)-, decyl ester

**Inchi:** InChI=1S/C23H33F2NO3/c1-2-3-4-5-6-7-8-9-16-29-23(28)18-12-14-26(15-13-18)22(27)2  
**InchiKey:** AEZFRGYKLPDQQD-UHFFFAOYSA-N  
**Formula:** C23H33F2NO3  
**SMILES:** CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2F)CC1  
**Mol. weight [g/mol]:** 409.51

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	5.501		Crippen Method
mcvol	322.840	ml/mol	McGowan Method
rinsol	2994.00		NIST Webbook
rinsol	2994.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361373&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  
**rinsol:** Non-polar retention indices

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