# Isonipecotic acid, N-(2,4-difluorobenzoyl)-, octyl ester

**Inchi:** InChI=1S/C21H29F2NO3/c1-2-3-4-5-6-7-14-27-21(26)16-10-12-24(13-11-16)20(25)18-9-

**InchiKey:** GFCDTSFRLCKKTR-UHFFFAOYSA-N

**Formula:** C21H29F2NO3

**SMILES:** CCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2F)CC1

**Mol. weight [g/mol]:** 381.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.82 | | Crippen Method |
| logp | 4.721 | | Crippen Method |
| mcvol | 294.660 | ml/mol | McGowan Method |
| rinpol | 2760.00 | | NIST Webbook |
| rinpol | 2760.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** 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=U361371&Units=SI

## 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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