# L-Proline, N-(2,6-difluorobenzoyl)-, undecyl ester

**Inchi:** InChI=1S/C23H33F2NO3/c1-2-3-4-5-6-7-8-9-10-17-29-23(28)20-15-12-16-26(20)22(27)2

**InchiKey:** MKQQARFJXMUTHS-UHFFFAOYSA-N

**Formula:** C23H33F2NO3

**SMILES:** CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)cccc1F

**Mol. weight [g/mol]:** 409.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.01 | | Crippen Method |
| logp | 5.643 | | Crippen Method |
| mcvol | 322.840 | ml/mol | McGowan Method |
| rinpol | 2897.00 | | NIST Webbook |
| rinpol | 2897.00 | | 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=U346400&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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