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

**Inchi:** InChI=1S/C29H45F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-35-29(34)26-21-1
**InchiKey:** ATMCIEOITOJLQY-UHFFFAOYSA-N
**Formula:** C29H45F2NO3
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)cccc1F
**Mol. weight [g/mol]:** 493.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -9.52 | | Crippen Method |
| logp | 7.984 | | Crippen Method |
| mcvol | 407.380 | ml/mol | McGowan Method |
| rinpol | 3581.00 | | NIST Webbook |
| rinpol | 3581.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U346405&Units=SI
**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

## 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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