

# L-Proline, N-(2-fluorobenzoyl)-, heptadecyl ester

**Inchi:** InChI=1S/C29H46FNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-24-34-29(33)27-22-19  
**InchiKey:** XTCDWSLLOPXBJS-UHFFFAOYSA-N  
**Formula:** C29H46FNO3  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1F  
**Mol. weight [g/mol]:** 475.68

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -9.19   |        | Crippen Method |
| logp          | 7.845   |        | Crippen Method |
| mcvol         | 405.610 | ml/mol | McGowan Method |
| rinpol        | 3572.00 |        | NIST Webbook   |
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## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346106&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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