# L-Proline, N-(2-fluoro-6-trifluoromethylbenzoyl)-, dodecyl ester

**Inchi:** InChI=1S/C25H35F4NO3/c1-2-3-4-5-6-7-8-9-10-11-18-33-24(32)21-16-13-17-30(21)23(3
**InchiKey:** ZTZOWJXDFZCMAI-UHFFFAOYSA-N
**Formula:** C25H35F4NO3
**SMILES:** CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)cccc1C(F)(F)F
**Mol. weight [g/mol]:** 473.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -8.20 | | Crippen Method |
| logp | 6.913 | | Crippen Method |
| mcvol | 354.560 | ml/mol | McGowan Method |
| rinpol | 2950.00 | | NIST Webbook |
| rinpol | 2950.00 | | 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=U345904&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.