# L-Proline, N-(3-fluoro-5-trifluoromethylbenzoyl)-, decyl ester

**Inchi:** InChI=1S/C23H31F4NO3/c1-2-3-4-5-6-7-8-9-13-31-22(30)20-11-10-12-28(20)21(29)17-1
**InchiKey:** CABQGYAMEIVEEY-UHFFFAOYSA-N
**Formula:** C23H31F4NO3
**SMILES:** CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)cc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 445.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.36 | | Crippen Method |
| logp | 6.133 | | Crippen Method |
| mcvol | 326.380 | ml/mol | McGowan Method |
| rinpol | 2632.00 | | NIST Webbook |
| rinpol | 2632.00 | | NIST Webbook |

## Sources

**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=U345954&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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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