# L-Proline, N-(2,3,4-trifluorobenzoyl)-, hexyl ester

**Inchi:** InChI=1S/C18H22F3NO3/c1-2-3-4-5-11-25-18(24)14-7-6-10-22(14)17(23)12-8-9-13(19)1

**InchiKey:** OBXQQRCHVFKWPV-UHFFFAOYSA-N

**Formula:** C18H22F3NO3

**SMILES:** CCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1F

**Mol. weight [g/mol]:** 357.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.25 | | Crippen Method |
| logp | 3.832 | | Crippen Method |
| mcvol | 254.160 | ml/mol | McGowan Method |
| rinpol | 2313.00 | | NIST Webbook |
| rinpol | 2313.00 | | 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=U346327&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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