# L-Proline, N-(3-trifluoromethylbenzoyl)-, heptyl ester

**Inchi:** InChI=1S/C20H26F3NO3/c1-2-3-4-5-6-13-27-19(26)17-11-8-12-24(17)18(25)15-9-7-10-1

**InchiKey:** FXAKEAVXWUQIME-UHFFFAOYSA-N

**Formula:** C20H26F3NO3

**SMILES:** CCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1

**Mol. weight [g/mol]:** 385.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.77 | | Crippen Method |
| logp | 4.824 | | Crippen Method |
| mcvol | 282.340 | ml/mol | McGowan Method |
| rinpol | 2429.00 | | NIST Webbook |
| rinpol | 2429.00 | | 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=U346344&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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