

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

**Inchi:**  
**ester**

InChI=1S/C20H25F4NO3/c1-2-3-4-5-6-10-28-19(27)17-8-7-9-25(17)18(26)14-11-15(20(2

**InchiKey:** SMZBJWGMEWDDER-UHFFFAOYSA-N

**Formula:** C20H25F4NO3

**SMILES:** CCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)cc(C(F)(F)F)c1

**Mol. weight [g/mol]:** 403.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	4.963		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpol	2336.00		NIST Webbook
rinpol	2336.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345951&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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