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

Inchi: InChI=1S/C17H20F3NO3/c1-2-3-4-10-24-17(23)13-6-5-9-21(13)16(22)11-7-8-12(18)15(2

InchiKey: IRRVHWOPKYZQIE-UHFFFAOYSA-N

Formula: C17H20F3NO3

SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 343.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.442		Crippen Method
mcvol	240.070	ml/mol	McGowan Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		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=U346325&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.