l-Proline, N-(2,3,4-trifluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C13H12F3NO3/c1-20-13(19)9-3-2-6-17(9)12(18)7-4-5-8(14)11(16)10(7)15/h4-5

InchiKey: GEGZRQZESYUFAE-UHFFFAOYSA-N

Formula: C13H12F3NO3

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

Mol. weight [g/mol]: 287.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	1.881		Crippen Method
mcvol	183.710	ml/mol	McGowan Method
rinpol	1792.00		NIST Webbook
rinpol	1792.00		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=U299631&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.