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

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

InchiKey: UAGTTXYRWUPTPB-UHFFFAOYSA-N

Formula: C18H22F3NO3

SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 357.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	3.688		Crippen Method
mcvol	254.160	ml/mol	McGowan Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		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=U346326&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.