L-Proline, N-(3-trifluoromethylbenzoyl)-, pentyl ester

Inchi: InChI=1S/C18H22F3NO3/c1-2-3-4-11-25-17(24)15-9-6-10-22(15)16(23)13-7-5-8-14(12-1

InchiKey: XMNJUYZMZRKYOG-UHFFFAOYSA-N

Formula: C18H22F3NO3

SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 357.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	4.043		Crippen Method
mcvol	254.160	ml/mol	McGowan Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346341&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.