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

Inchi: InChI=1S/C19H24F3NO3/c1-13(2)6-5-11-26-18(25)16-9-4-10-23(16)17(24)14-7-3-8-15(1

InchiKey: VJNBKZGLZGQDFP-UHFFFAOYSA-N

Formula: C19H24F3NO3

SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 371.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.11		Crippen Method
logp	4.289		Crippen Method
mcvol	268.250	ml/mol	McGowan Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346342&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.