l-Proline, N-(3-trifluoromethylbenzoyl)-, methyl ester

Inchi: InChI=1S/C14H14F3NO3/c1-21-13(20)11-6-3-7-18(11)12(19)9-4-2-5-10(8-9)14(15,16)17

InchiKey: MSGPECJKIWFUQD-UHFFFAOYSA-N

Formula: C14H14F3NO3

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

Mol. weight [g/mol]: 301.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.483		Crippen Method
mcvol	197.800	ml/mol	McGowan Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299700&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.