L-Proline, N-(2-trifluoromethylbenzoyl)-, methyl ester

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

InchiKey: TWHMHMAXBGTGGF-UHFFFAOYSA-N

Formula: C14H14F3NO3

SMILES: COC(=O)C1CCCN1C(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 301.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Cheméo Relay (1.0)
logp	2.483		Crippen Method
mcvol	197.800	ml/mol	McGowan Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
tf	337.71	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299686&Units=SI

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

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point