

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/ci990307I>
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

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