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

Inchi: InChI=1S/C15H16F3NO3/c1-2-22-14(21)12-8-5-9-19(12)13(20)10-6-3-4-7-11(10)15(16,1

InchiKey: FPJALEMHARAFHK-UHFFFAOYSA-N

Formula: C15H16F3NO3

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

Mol. weight [g/mol]: 315.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.873		Crippen Method
mcvol	211.890	ml/mol	McGowan Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346202&Units=SI

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

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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