L-Proline, N-(3-fluorobenzoyl)-, ethyl ester

Inchi: InChI=1S/C14H16FNO3/c1-2-19-14(18)12-7-4-8-16(12)13(17)10-5-3-6-11(15)9-10/h3,5-
InchiKey: IFVJEOSINLJOSC-UHFFFAOYSA-N
Formula: C14H16FNO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 265.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	1.993		Crippen Method
mcvol	194.260	ml/mol	McGowan Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346277&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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