L-Proline, N-(2-fluoro-3-trifluoromethylbenzoyl)-, pentyl ester

Inchi: InChI=1S/C18H21F4NO3/c1-2-3-4-11-26-17(25)14-9-6-10-23(14)16(24)12-7-5-8-13(15(1

InchiKey: SCMROPLYOMVEHM-UHFFFAOYSA-N

Formula: C18H21F4NO3

SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 375.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.27		Crippen Method
logp	4.183		Crippen Method
mcvol	255.930	ml/mol	McGowan Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345993&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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