L-Proline, N-(3-fluoro-4-trifluoromethylbenzoyl)-, octyl ester

Inchi: InChI=1S/C21H27F4NO3/c1-2-3-4-5-6-7-13-29-20(28)18-9-8-12-26(18)19(27)15-10-11-1

InchiKey: MFTURZIIDAKVBY-UHFFFAOYSA-N

Formula: C21H27F4NO3

SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 417.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Crippen Method
logp	5.353		Crippen Method
mcvol	298.200	ml/mol	McGowan Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345967&Units=SI

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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