L-Proline, N-(2-fluoro-5-trifluoromethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C20H25F4NO3/c1-2-3-4-5-6-12-28-19(27)17-8-7-11-25(17)18(26)15-13-14(20(
InchiKey: NPKRWMJWNDXSCM-UHFFFAOYSA-N
Formula: C20H25F4NO3
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 403.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	4.963		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345923&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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