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

Inchi: InChI=1S/C19H23F4NO3/c1-2-3-4-5-11-27-18(26)16-7-6-10-24(16)17(25)14-12-13(19(21
InchiKey: RQLBDCYFVIISFG-UHFFFAOYSA-N
Formula: C19H23F4NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 389.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	4.573		Crippen Method
mcvol	270.020	ml/mol	McGowan Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		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=U345922&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

Latest version available from:
https://www.chemeo.com/cid/122-149-1/L-Proline-N-2-fluoro-5-trifluoromethylbenzoyl-hexyl-ester.pdf
Generated by Cheméo on 2024-04-29 21:13:00.230333763 +0000 UTC m=+16714429.150911075.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.