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

Inchi: InChI=1S/C19H23F4NO3/c1-12(2)5-4-10-27-18(26)16-6-3-9-24(16)17(25)14-11-13(20)7-
InchiKey: AUCXGTNHMVSYRL-UHFFFAOYSA-N
Formula: C19H23F4NO3
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]: 389.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	4.428		Crippen Method
mcvol	270.020	ml/mol	McGowan Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		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=U346007&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

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