L-Proline, N-(2,5-ditrifluoromethylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C20H23F6NO3/c1-2-3-4-5-11-30-18(29)16-7-6-10-27(16)17(28)14-12-13(19(21
InchiKey: TUNNMHBDKFRLEX-UHFFFAOYSA-N
Formula: C20H23F6NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 439.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.46		Crippen Method
logp	5.452		Crippen Method
mcvol	287.650	ml/mol	McGowan Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		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=U345978&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.