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

Inchi: InChI=1S/C15H15F4NO3/c1-2-23-14(22)12-4-3-7-20(12)13(21)9-5-6-10(11(16)8-9)15(17
InchiKey: WPGRGZPIPRCHNQ-UHFFFAOYSA-N
Formula: C15H15F4NO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 333.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	3.012		Crippen Method
mcvol	213.660	ml/mol	McGowan Method
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345962&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.