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

Inchi: InChI=1S/C16H17F4NO3/c1-2-8-24-15(23)13-4-3-7-21(13)14(22)11-9-10(16(18,19)20)5-

InchiKey: DUYSAQOMJBJDHW-UHFFFAOYSA-N

Formula: C16H17F4NO3

SMILES: CCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]: 347.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	3.402		Crippen Method
mcvol	227.750	ml/mol	McGowan Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		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=U345918&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.