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

Inchi: InChI=1S/C25H35F4NO3/c1-2-3-4-5-6-7-8-9-10-11-17-33-24(32)22-13-12-16-30(22)23(3

InchiKey: GKVWMWBTVBYJSP-UHFFFAOYSA-N

Formula: C25H35F4NO3

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

Mol. weight [g/mol]: 473.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.20		Crippen Method
logp	6.913		Crippen Method
mcvol	354.560	ml/mol	McGowan Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345928&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.