L-Proline, N-(3,4-difluorobenzoyl)-, undecyl ester

Inchi: InChI=1S/C23H33F2NO3/c1-2-3-4-5-6-7-8-9-10-16-29-23(28)21-12-11-15-26(21)22(27)1
InchiKey: MFGHKNTXYOROPW-UHFFFAOYSA-N
Formula: C23H33F2NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 409.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	5.643		Crippen Method
mcvol	322.840	ml/mol	McGowan Method
rinpol	2884.00		NIST Webbook
rinpol	2884.00		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=U345911&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.