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

Inchi: InChI=1S/C27H41F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-33-27(32)25-16-15-19-3

InchiKey: ISILURSJGCKVGV-UHFFFAOYSA-N

Formula: C27H41F2NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1

Mol. weight [g/mol]: 465.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.68		Crippen Method
logp	7.204		Crippen Method
mcvol	379.200	ml/mol	McGowan Method
rinpol	3326.00		NIST Webbook
rinpol	3326.00		NIST Webbook

Sources

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=U345914&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.