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

Inchi: InChI=1S/C15H17F2NO3/c1-2-8-21-15(20)13-4-3-7-18(13)14(19)10-5-6-11(16)12(17)9-1

InchiKey: PFXLPPUORPSSCF-UHFFFAOYSA-N

Formula: C15H17F2NO3

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

Mol. weight [g/mol]: 297.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	2.523		Crippen Method
mcvol	210.120	ml/mol	McGowan Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345909&Units=SI

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

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.