L-Proline, N-(2,6-difluoro-3-methylbenzoyl)-, pentyl ester

Inchi: InChI=1S/C18H23F2NO3/c1-3-4-5-11-24-18(23)14-7-6-10-21(14)17(22)15-13(19)9-8-12(

InchiKey: AOQJMGCQVFXMMJ-UHFFFAOYSA-N

Formula: C18H23F2NO3

SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	3.611		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpol	2383.00		NIST Webbook
rinpol	2383.00		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=U345888&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.