L-Proline, N-(2,4-difluorobenzoyl)-, isohexyl ester

Inchi: InChI=1S/C18H23F2NO3/c1-12(2)5-4-10-24-18(23)16-6-3-9-21(16)17(22)14-8-7-13(19)1

InchiKey: FFEVRPBECZKNND-UHFFFAOYSA-N

Formula: C18H23F2NO3

SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1F

Mol. weight [g/mol]: 339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	3.549		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346036&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.