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

Inchi: InChI=1S/C18H23F2NO3/c1-2-3-4-5-11-24-18(23)16-7-6-10-21(16)17(22)14-9-8-13(19)1
InchiKey: LKJOFXOAHZWVJW-UHFFFAOYSA-N
Formula: C18H23F2NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	3.693		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		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=U346037&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.