L-Proline, N-(2,6-difluorobenzoyl)-, isobutyl ester

Inchi: InChI=1S/C16H19F2NO3/c1-10(2)9-22-16(21)13-7-4-8-19(13)15(20)14-11(17)5-3-6-12(1

InchiKey: SKWBGVYUEGZICX-UHFFFAOYSA-N

Formula: C16H19F2NO3

SMILES: CC(C)COC(=O)C1CCCN1C(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 311.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.769		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
rinpol	2136.00		NIST Webbook
rinpol	2136.00		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=U346396&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.