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

Inchi: InChI=1S/C20H27F2NO3/c1-3-4-5-6-7-13-26-20(25)16-9-8-12-23(16)19(24)17-15(21)11-

InchiKey: ZOOBRVNXKVTBFW-UHFFFAOYSA-N

Formula: C20H27F2NO3

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

Mol. weight [g/mol]: 367.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.81		Crippen Method
logp	4.391		Crippen Method
mcvol	280.570	ml/mol	McGowan Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		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=U345891&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.