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

Inchi: InChI=1S/C22H31F2NO3/c1-3-4-5-6-7-8-9-15-28-22(27)18-11-10-14-25(18)21(26)19-17(

InchiKey: OYVKWXKHXOEFHU-UHFFFAOYSA-N

Formula: C22H31F2NO3

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

Mol. weight [g/mol]: 395.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	5.172		Crippen Method
mcvol	308.750	ml/mol	McGowan Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345893&Units=SI

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

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.