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

Inchi: InChI=1S/C21H29F2NO3/c1-3-4-5-6-7-8-14-27-21(26)17-10-9-13-24(17)20(25)18-16(22)
InchiKey: LTNYQRZJHYGMHK-UHFFFAOYSA-N
Formula: C21H29F2NO3
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 381.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.23		Crippen Method
logp	4.782		Crippen Method
mcvol	294.660	ml/mol	McGowan Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		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=U345892&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.