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

Inchi: InChI=1S/C28H43F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-21-34-28(33)24-17-16-20-

InchiKey: UPUCCGVXYKZOEV-UHFFFAOYSA-N

Formula: C28H43F2NO3

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

Mol. weight [g/mol]: 479.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.16		Crippen Method
logp	7.512		Crippen Method
mcvol	393.290	ml/mol	McGowan Method
rinpol	3440.00		NIST Webbook
rinpol	3440.00		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=U345898&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

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