

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

Inchi: InChI=1S/C25H37F2NO3/c1-3-4-5-6-7-8-9-10-11-12-18-31-25(30)21-14-13-17-28(21)24
InchiKey: LCVYKTMWTFIFPD-UHFFFAOYSA-N
Formula: C25H37F2NO3
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 437.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.90		Crippen Method
logp	6.342		Crippen Method
mcvol	351.020	ml/mol	McGowan Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U345896&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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