

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

Inchi: InChI=1S/C24H35F2NO3/c1-3-4-5-6-7-8-9-10-11-17-30-24(29)20-13-12-16-27(20)23(28)
InchiKey: YHGXMQSWVPZPKI-UHFFFAOYSA-N
Formula: C24H35F2NO3
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 423.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.48		Crippen Method
logp	5.952		Crippen Method
mcvol	336.930	ml/mol	McGowan Method
rinpol	3014.00		NIST Webbook
rinpol	3014.00		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=U345895&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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