

L-Proline, N-(2,4-difluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C21H29F2NO3/c1-2-3-4-5-6-7-8-14-27-21(26)19-10-9-13-24(19)20(25)17-12-1
InchiKey: OGBQRCZBIXXFAS-UHFFFAOYSA-N
Formula: C21H29F2NO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 381.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.17		Crippen Method
logp	4.863		Crippen Method
mcvol	294.660	ml/mol	McGowan Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346040&Units=SI>
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>

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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