

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

Inchi: InChI=1S/C22H31F2NO3/c1-2-3-4-5-6-7-8-9-15-28-22(27)20-11-10-14-25(20)21(26)18-1
InchiKey: SJWDOPAGCQQTLD-UHFFFAOYSA-N
Formula: C22H31F2NO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 395.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.59		Crippen Method
logp	5.253		Crippen Method
mcvol	308.750	ml/mol	McGowan Method
rinpola	2735.00		NIST Webbook
rinpola	2735.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U346041&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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