

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

Inchi: InChI=1S/C14H15F2NO3/c1-2-20-14(19)12-4-3-7-17(12)13(18)10-6-5-9(15)8-11(10)16/h
InchiKey: CMRFGLGLVNAIHY-UHFFFAOYSA-N
Formula: C14H15F2NO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 283.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.132		Crippen Method
mcvol	196.030	ml/mol	McGowan Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		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=U346033&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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