L-Proline, N-(2-fluorobenzoyl)-, pentyl ester

Inchi: InChI=1S/C17H22FNO3/c1-2-3-6-12-22-17(21)15-10-7-11-19(15)16(20)13-8-4-5-9-14(13
InchiKey: CNKILWPAVZLTEG-UHFFFAOYSA-N
Formula: C17H22FNO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1ccccc1F
Mol. weight [g/mol]: 307.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.164		Crippen Method
mcvol	236.530	ml/mol	McGowan Method
rinpol	2299.00		NIST Webbook
rinpol	2299.00		NIST Webbook

Sources

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=U346095&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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