

L-Proline, N-(4-fluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C21H30FNO3/c1-2-3-4-5-6-7-8-16-26-21(25)19-10-9-15-23(19)20(24)17-11-13
InchiKey: NXEUFMMQFXGDHN-UHFFFAOYSA-N
Formula: C21H30FNO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 363.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	4.724		Crippen Method
mcvol	292.890	ml/mol	McGowan Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		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=U346129&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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<https://www.chemeo.com/cid/119-381-7/L-Proline-N-4-fluorobenzoyl-nonyl-ester.pdf>

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