

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

Inchi: InChI=1S/C16H20FNO3/c1-11(2)10-21-16(20)14-4-3-9-18(14)15(19)12-5-7-13(17)8-6-12
InchiKey: CINYQPFMGPUKDC-UHFFFAOYSA-N
Formula: C16H20FNO3
SMILES: CC(C)COC(=O)C1CCCN1C(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 293.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	2.629		Crippen Method
mcvol	222.440	ml/mol	McGowan Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		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=U346122&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

Latest version available from:

<https://www.chemeo.com/cid/120-059-3/L-Proline-N-4-fluorobenzoyl-isobutyl-ester.pdf>

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