

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

Inchi: InChI=1S/C18H24FNO3/c1-13(2)5-4-12-23-18(22)16-6-3-11-20(16)17(21)14-7-9-15(19)1
InchiKey: ZMALDJAEXXKPCC-UHFFFAOYSA-N
Formula: C18H24FNO3
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 321.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.410		Crippen Method
mcvol	250.620	ml/mol	McGowan Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346125&Units=SI>
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>

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.cheméo.com/cid/122-542-4/L-Proline-N-4-fluorobenzoyl-isohexyl-ester.pdf>

Generated by Cheméo on 2024-05-15 18:23:20.493676103 +0000 UTC m=+18086649.414253418.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.