

L-Proline, N-(3-fluoro-5-trifluoromethylbenzoyl)-, isohexyl ester

InChI: InChI=1S/C19H23F4NO3/c1-12(2)5-4-8-27-18(26)16-6-3-7-24(16)17(25)13-9-14(19(21,22)20)/q1
InChIKey: NHAVKWKDPRSDKB-UHFFFAOYSA-N

Formula: C₁₉H₂₃F₄NO₃
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 389.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	4.428		Crippen Method
mcvol	270.020	ml/mol	McGowan Method
rinsol	2186.00		NIST Webbook
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Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345949&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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