

L-Proline, N-(5-fluoro-2-trifluoromethylbenzoyl)-, nonyl ester

InChI: InChI=1S/C22H29F4NO3/c1-2-3-4-5-6-7-8-14-30-21(29)19-10-9-13-27(19)20(28)17-15-16
InChIKey: QJTJUWYQXGZORK-UHFFFAOYSA-N

Formula: C22H29F4NO3

SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]: 431.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.94		Crippen Method
logp	5.743		Crippen Method
mcvol	312.290	ml/mol	McGowan Method
rinpol	2553.00		NIST Webbook
rinpol	2553.00		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=U346011&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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