

L-Proline, N-(5-fluoro-2-trifluoromethylbenzoyl)-, heptyl

Inchi:
ester

InChI=1S/C20H25F4NO3/c1-2-3-4-5-6-12-28-19(27)17-8-7-11-25(17)18(26)15-13-14(21)

InchiKey: YFCHWRLKPILYQO-UHFFFAOYSA-N

Formula: C20H25F4NO3

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

Mol. weight [g/mol]: 403.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	4.963		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook

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=U346009&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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