

L-Proline, N-(2-fluoro-6-trifluoromethylbenzoyl)-, heptyl

Inchi:
ester

InChI=1S/C20H25F4NO3/c1-2-3-4-5-6-13-28-19(27)16-11-8-12-25(16)18(26)17-14(20(2

InchiKey:

HDUHJKPTGWPDOJ-UHFFFAOYSA-N

Formula:

C20H25F4NO3

SMILES:

CCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)cccc1C(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	2435.00		NIST Webbook
rinpol	2435.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U345901&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

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