

L-Proline, N-(2-trifluoromethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C20H26F3NO3/c1-2-3-4-5-8-14-27-19(26)17-12-9-13-24(17)18(25)15-10-6-7-1
InchiKey: BBWPBWPDOIKFDB-UHFFFAOYSA-N
Formula: C20H26F3NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 385.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	4.824		Crippen Method
mcvol	282.340	ml/mol	McGowan Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346208&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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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