

L-Proline, N-(2,5-ditrifluoromethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C21H25F6NO3/c1-2-3-4-5-6-12-31-19(30)17-8-7-11-28(17)18(29)15-13-14(20)
InchiKey: ZKSGCIAKBLYHRD-UHFFFAOYSA-N
Formula: C21H25F6NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 453.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.88		Crippen Method
logp	5.842		Crippen Method
mcvol	301.740	ml/mol	McGowan Method
rinpol	2247.00		NIST Webbook
rinpol	2247.00		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=U345979&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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