L-Proline, N-pentafluoropropionyl-, propyl ester

Inchi: InChI=1S/C11H14F5NO3/c1-2-6-20-8(18)7-4-3-5-17(7)9(19)10(12,13)11(14,15)16/h7H,2

InchiKey: WGKSCFPPYPEBDI-UHFFFAOYSA-N

Formula: C11H14F5NO3

SMILES: CCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 303.23

Physical Properties

Property code	Value	Unit	Source
logp	2.128		Crippen Method
mcvol	182.830	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321062&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume