L-Proline, N-pentafluoropropionyl-, undecyl ester

Inchi: InChI=1S/C19H30F5NO3/c1-2-3-4-5-6-7-8-9-10-14-28-16(26)15-12-11-13-25(15)17(27)1

InchiKey: JHWFDPKZIVZHHY-UHFFFAOYSA-N

Formula: C19H30F5NO3

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

Mol. weight [g/mol]: 415.44

Physical Properties

Property code	Value	Unit	Source
logp	5.249		Crippen Method
mcvol	295.550	ml/mol	McGowan Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
tb	596.29	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321072&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

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

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