

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)18
InchiKey: JHWFDPKZIVZHYY-UHFFFAOYSA-N
Formula: C19H30F5NO3
SMILES: CCCCCCCCCCOC(=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
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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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<https://www.cheméo.com/cid/78-303-9/L-Proline-N-pentafluoropropionyl-undecyl-ester.pdf>

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