L-Proline, N-pentafluoropropionyl-, ethyl ester

Inchi: InChI=1S/C10H12F5NO3/c1-2-19-7(17)6-4-3-5-16(6)8(18)9(11,12)10(13,14)15/h6H,2-5H
InchiKey: AJXXYHNJFLEKCQ-UHFFFAOYSA-N
Formula: C10H12F5NO3
SMILES: CCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 289.20

Physical Properties

Property code	Value	Unit	Source
logp	1.738		Crippen Method
mcvol	168.740	ml/mol	McGowan Method
rinpol	1323.00		NIST Webbook
tb	488.89	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321061&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature