L-Proline, N-pentafluoropropionyl-, nonyl ester

Inchi: InChI=1S/C17H26F5NO3/c1-2-3-4-5-6-7-8-12-26-14(24)13-10-9-11-23(13)15(25)16(18,1
InchiKey: IVTPIDXTLZRVPK-UHFFFAOYSA-N
Formula: C17H26F5NO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 387.39

Physical Properties

Property code	Value	Unit	Source
logp	4.469		Crippen Method
mcvol	267.370	ml/mol	McGowan Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	575.69	K	Cheméo Relay (1.0)

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321070&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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