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
log10ws	-2.20		Crippen Method
logp	1.738		Crippen Method
mcvol	168.740	ml/mol	McGowan Method
rinpol	1323.00		NIST Webbook

Sources

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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