l-Proline, n-heptafluorobutyryl-, ethyl ester

Inchi: InChI=1S/C11H12F7NO3/c1-2-22-7(20)6-4-3-5-19(6)8(21)9(12,13)10(14,15)11(16,17)18
InchiKey: FDCZUNMXHDNQHK-UHFFFAOYSA-N
Formula: C11H12F7NO3
SMILES: CCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 339.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	2.373		Crippen Method
mcvol	186.370	ml/mol	McGowan Method
rinpol	1344.00		NIST Webbook
rinpol	1344.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321096&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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