l-Proline, n-pentafluoropropionyl-, pentyl ester

Inchi: InChI=1S/C13H18F5NO3/c1-2-3-4-8-22-10(20)9-6-5-7-19(9)11(21)12(14,15)13(16,17)18
InchiKey: ODIMTPWSPZZDJV-UHFFFAOYSA-N
Formula: C13H18F5NO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 331.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.908		Crippen Method
mcvol	211.010	ml/mol	McGowan Method
rinpol	1573.00		NIST Webbook
rinpol	1573.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321065&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.