l-Proline, n-heptafluorobutyryl-, pentyl ester

Inchi: InChI=1S/C14H18F7NO3/c1-2-3-4-8-25-10(23)9-6-5-7-22(9)11(24)12(15,16)13(17,18)14
InchiKey: ZCUBABLTMDYRGX-UHFFFAOYSA-N
Formula: C14H18F7NO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 381.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	3.544		Crippen Method
mcvol	228.640	ml/mol	McGowan Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		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=U321100&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.