l-Proline, n-heptafluorobutyryl-, isohexyl ester

Inchi: InChI=1S/C15H20F7NO3/c1-9(2)5-4-8-26-11(24)10-6-3-7-23(10)12(25)13(16,17)14(18,1
InchiKey: IHQXSPLYNGYVCE-UHFFFAOYSA-N
Formula: C15H20F7NO3
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 395.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	3.790		Crippen Method
mcvol	242.730	ml/mol	McGowan Method
rinpol	1639.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321101&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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