

I-Proline, n-pentafluoropropionyl-, hexyl ester

Inchi: InChI=1S/C14H20F5NO3/c1-2-3-4-5-9-23-11(21)10-7-6-8-20(10)12(22)13(15,16)14(17,18)
InchiKey: XHYLNQKDMYJSDZ-UHFFFAOYSA-N
Formula: C14H20F5NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 345.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	3.298		Crippen Method
mcvol	225.100	ml/mol	McGowan Method
rinpola	1663.00		NIST Webbook
rinpola	1663.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U321067&Units=SI>

Legend

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

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