

I-Proline, n-pentafluoropropionyl-, isohexyl ester

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	3.154		Crippen Method
mcvol	225.100	ml/mol	McGowan Method
rinpol	1622.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321066&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

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