

I-Proline, n-pentafluoropropionyl-, isobutyl ester

Inchi:	InChI=1S/C12H16F5NO3/c1-7(2)6-21-9(19)8-4-3-5-18(8)10(20)11(13,14)12(15,16)17/h7
InchiKey:	MAFHRCHNNUDHHP-UHFFFAOYSA-N
Formula:	C12H16F5NO3
SMILES:	CC(C)COC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	317.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	2.374		Crippen Method
mcvol	196.920	ml/mol	McGowan Method
rinpole	1448.00		NIST Webbook
rinpole	1448.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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