

L-Proline, N-pentafluoropropionyl-, propyl ester

Inchi:	InChI=1S/C11H14F5NO3/c1-2-6-20-8(18)7-4-3-5-17(7)9(19)10(12,13)11(14,15)16/h7H,2
InchiKey:	WGKSCFPPYPEBDI-UHFFFAOYSA-N
Formula:	C11H14F5NO3
SMILES:	CCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	303.23

Physical Properties

Property code	Value	Unit	Source
logp	2.128		Crippen Method
mcvol	182.830	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321062&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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