

L-Proline, N-pentafluoropropionyl-, tetradecyl ester

Inchi:	InChI=1S/C22H36F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-31-19(29)18-15-14-16-28(1
InchiKey:	BCKPMVAXDWSJNB-UHFFFAOYSA-N
Formula:	C22H36F5NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	457.52

Physical Properties

Property code	Value	Unit	Source
logp	6.419		Crippen Method
mcvol	337.820	ml/mol	McGowan Method
rinpol	2464.00		NIST Webbook
tb	623.12	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321074&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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<https://www.chemeo.com/cid/77-447-1/L-Proline-N-pentafluoropropionyl-tetradecyl-ester.pdf>

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