l-Proline, n-pentafluoropropionyl-, decyl ester

Inchi:	InChI=1S/C18H28F5NO3/c1-2-3-4-5-6-7-8-9-13-27-15(25)14-11-10-12-24(14)16(26)17(1
InchiKey:	VFMZYZJBMXRPJX-UHFFFAOYSA-N
Formula:	C18H28F5NO3
SMILES:	CCCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	401.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.55		Crippen Method
logp	4.859		Crippen Method
mcvol	281.460	ml/mol	McGowan Method
rinpol	2067.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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