l-Proline, n-pentafluoropropionyl-, nonyl ester

Inchi:	InChI=1S/C17H26F5NO3/c1-2-3-4-5-6-7-8-12-26-14(24)13-10-9-11-23(13)15(25)16(18,1
InchiKey:	IVTPIDXTLZRVPK-UHFFFAOYSA-N
Formula:	C17H26F5NO3
SMILES:	CCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	387.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	4.469		Crippen Method
mcvol	267.370	ml/mol	McGowan Method
rinpol	1970.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321070&Units=SI

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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