

L-Proline, N-(pentafluorobenzoyl)-, isohexyl ester

Inchi:	InChI=1S/C18H20F5NO3/c1-9(2)5-4-8-27-18(26)10-6-3-7-24(10)17(25)11-12(19)14(21)1
InchiKey:	RWZNQKYITBGJCG-UHFFFAOYSA-N
Formula:	C18H20F5NO3
SMILES:	CC(C)CCCOC(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	393.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.67		Crippen Method
logp	3.966		Crippen Method
mcvol	257.700	ml/mol	McGowan Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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