

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

Inchi:	InChI=1S/C16H16F5NO3/c1-7(2)6-25-16(24)8-4-3-5-22(8)15(23)9-10(17)12(19)14(21)13
InchiKey:	ZZADLLWSKPQLSV-UHFFFAOYSA-N
Formula:	C16H16F5NO3
SMILES:	CC(C)COC(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	365.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.186		Crippen Method
mcvol	229.520	ml/mol	McGowan Method
rinpol	1958.00		NIST Webbook
rinpol	1958.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U346292&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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