Isonipecotic acid, N-pentafluorobenzoyl-, butyl ester

Inchi: InChI=1S/C17H18F5NO3/c1-2-3-8-26-17(25)9-4-6-23(7-5-9)16(24)10-11(18)13(20)15(22

InchiKey: RLMWFNPVFNEAMF-UHFFFAOYSA-N

Formula: C17H18F5NO3

SMILES: CCCCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1

Mol. weight [g/mol]: 379.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	3.578		Crippen Method
mcvol	243.610	ml/mol	McGowan Method
rinpol	2205.00		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=U361223&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