

Isonipecotic acid, N-pentafluorobenzoyl-, isobutyl ester

Inchi:	InChI=1S/C17H18F5NO3/c1-8(2)7-26-17(25)9-3-5-23(6-4-9)16(24)10-11(18)13(20)15(22)
InchiKey:	CNTXKWUXSFBATB-UHFFFAOYSA-N
Formula:	C17H18F5NO3
SMILES:	CC(C)COC(=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	-4.90		Crippen Method
logp	3.433		Crippen Method
mcvol	243.610	ml/mol	McGowan Method
rinpol	2158.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361222&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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