

Isonipecotic acid, N-pentafluorobenzoyl-, isohexyl ester

Inchi: InChI=1S/C19H22F5NO3/c1-10(2)4-3-9-28-19(27)11-5-7-25(8-6-11)18(26)12-13(20)15(2)
InchiKey: VTNMSSWOBYEMHN-UHFFFAOYSA-N
Formula: C19H22F5NO3
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1
Mol. weight [g/mol]: 407.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.73		Crippen Method
logp	4.214		Crippen Method
mcvol	271.790	ml/mol	McGowan Method
rmpol	2368.00		NIST Webbook
rmpol	2368.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361225&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rmpol: Non-polar retention indices

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