Isonipecotic acid, N-pentafluorobenzoyl-, hexyl ester

Inchi: InChI=1S/C19H22F5NO3/c1-2-3-4-5-10-28-19(27)11-6-8-25(9-7-11)18(26)12-13(20)15(2
InchiKey: OHFMITAJUSHHNL-UHFFFAOYSA-N
Formula: C19H22F5NO3
SMILES: CCCCCCOC(=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	-5.98		Crippen Method
logp	4.358		Crippen Method
mcvol	271.790	ml/mol	McGowan Method
rinpol	2404.00		NIST Webbook
rinpol	2404.00		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=U361226&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.