

Isonipecotinoylisonipecotic acid, N'-pentafluorobenzoyl-, ethyl ester

Inchi: InChI=1S/C21H23F5N2O4/c1-2-32-21(31)12-5-9-27(10-6-12)19(29)11-3-7-28(8-4-11)20
InchiKey: GLLMVTGPYLCOJK-UHFFFAOYSA-N
Formula: C21H23F5N2O4
SMILES: CCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3c(F)c(F)c(F)c(F)c3F)CC2)CC1
Mol. weight [g/mol]: 462.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	3.036		Crippen Method
mcvol	300.660	ml/mol	McGowan Method
rmpol	3142.00		NIST Webbook
rmpol	3142.00		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=U361233&Units=SI>

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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