

Isonipecotinoylisonipecotic acid, N'-pentafluorobenzoyl-, butyl ester

Inchi: InChI=1S/C23H27F5N2O4/c1-2-3-12-34-23(33)14-6-10-29(11-7-14)21(31)13-4-8-30(9-5)
InchiKey: FAEDPCOAZOQRTK-UHFFFAOYSA-N
Formula: C23H27F5N2O4
SMILES: CCCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3c(F)c(F)c(F)c(F)c3F)CC2)CC1
Mol. weight [g/mol]: 490.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.65		Crippen Method
logp	3.816		Crippen Method
mcvol	328.840	ml/mol	McGowan Method
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361236&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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