Isonipecotinoylisonipecotic acid, N'-(3-fluoro-4-trifluoromethylbenzoyl)-, propyl ester

Inchi: InChI=1S/C23H28F4N2O4/c1-2-13-33-22(32)16-7-11-28(12-8-16)20(30)15-5-9-29(10-6-1

InchiKey: NTEOZUAFHHAIAD-UHFFFAOYSA-N

Formula: C23H28F4N2O4

SMILES: CCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(C(F)(F)F)c(F)c3)CC2)CC1

Mol. weight [g/mol]: 472.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	3.889		Crippen Method
mcvol	327.070	ml/mol	McGowan Method
rinpol	3378.00		NIST Webbook
rinpol	3378.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361485&Units=SI

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

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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