

Isonipecotinoylisonipecotic acid, N'-(2-fluoro-5-trifluoromethylbenzoyl)-, isobutyl ester

InChI: InChI=1S/C24H30F4N2O4/c1-15(2)14-34-23(33)17-7-11-29(12-8-17)21(31)16-5-9-30(10)
InChIKey: UMIQYSGQSAQQLL-UHFFFAOYSA-N

Formula: C24H30F4N2O4

SMILES: CC(C)COC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cc(C(F)(F)F)ccc3F)CC2)CC1

Mol. weight [g/mol]: 486.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	4.135		Crippen Method
mcvol	341.160	ml/mol	McGowan Method
rinpol	3383.00		NIST Webbook
rinpol	3383.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361406&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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