

Isonipecotinoylisonipecotic acid, N'-(4-fluoro-2-trifluoromethylbenzoyl)-, butyl ester

Inchi:
InchiKey:

InChI=1S/C24H30F4N2O4/c1-2-3-14-34-23(33)17-8-12-29(13-9-17)21(31)16-6-10-30(11)
QDDHIBZQGOGWX-UHFFFAOYSA-N

Formula: C24H30F4N2O4

SMILES: CCCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(F)cc3C(F)(F)F)CC2)CC1

Mol. weight [g/mol]: 486.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.279		Crippen Method
mcvol	341.160	ml/mol	McGowan Method
rropol	3450.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rropol:	Non-polar retention indices

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