

Isonipecotinoylisonipectic acid, N'-(3-fluoro-4-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)
DUQWLBLWWIJHJW-UHFFFAOYSA-N

Formula: C24H30F4N2O4

SMILES: CCCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(C(F)(F)F)c(F)c3)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
rinpole	3501.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361486&Units=SI>

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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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