

Isonipecotinoylisonipecotic acid, N'-(4-fluoro-2-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: BICSXTWHCBQDLY-UHFFFAOYSA-N

Formula: C₂₄H₃₀F₄N₂O₄

SMILES: CC(C)COC(=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	-5.18		Crippen Method
logp	4.135		Crippen Method
mcvol	341.160	ml/mol	McGowan Method
rinpole	3396.00		NIST Webbook

Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361261&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/36-919-2/Isonipecotinoylisonipecotic-acid-N-4-fluoro-2-trifluoromethylbenzoyl-isobutyl-e>

Generated by Cheméo on 2024-04-25 14:41:24.30081178 +0000 UTC m=+16345333.221389093.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.