

Isonipecotinoylisonipecotic acid, N'-(2-fluoro-3-trifluoromethylbenzoyl)-, propyl ester

Inchi:
InchiKey:

InChI=1S/C23H28F4N2O4/c1-2-14-33-22(32)16-8-12-28(13-9-16)20(30)15-6-10-29(11-7)UOANNASGLLQXDZ-UHFFFAOYSA-N

Formula: C23H28F4N2O4

SMILES: CCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cccc(C(F)(F)F)c3F)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	3387.00		NIST Webbook
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Sources

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=U361324&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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