

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

InChI: InChI=1S/C23H28F4N2O4/c1-2-13-33-22(32)16-7-11-28(12-8-16)20(30)15-5-9-29(10-6-31)3
InChIKey: CBZTYTAEAJTTDB-UHFFFAOYSA-N
Formula: C23H28F4N2O4
SMILES: CCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(F)cc3C(F)(F)F)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	3338.00		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=U361260&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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