Isonipecotic acid, N-(4-fluoro-2-trifluoromethylbenzoyl)-, nonyl ester

Inchi: InChI=1S/C23H31F4NO3/c1-2-3-4-5-6-7-8-15-31-22(30)17-11-13-28(14-12-17)21(29)19-
InchiKey: STQNLOCARREUGR-UHFFFAOYSA-N
Formula: C23H31F4NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)CC1
Mol. weight [g/mol]: 445.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	5.991		Crippen Method
mcvol	326.380	ml/mol	McGowan Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U361249&Units=SI

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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