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

Inchi: InChI=1S/C18H21F4NO3/c1-11(2)10-26-17(25)12-5-7-23(8-6-12)16(24)14-4-3-13(19)9-1
InchiKey: KCTHANMBLKDCKT-UHFFFAOYSA-N
Formula: C18H21F4NO3
SMILES: CC(C)COC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)CC1
Mol. weight [g/mol]: 375.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	3.896		Crippen Method
mcvol	255.930	ml/mol	McGowan Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook

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=U361242&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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