

Isonipecotic acid, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, isobutyl ester

InChI: InChI=1S/C18H22F3NO4/c1-10(2)9-26-18(24)11-4-6-22(7-5-11)17(23)12-8-13(19)15(21)
InChIKey: CCSMPQLHXCZHIL-UHFFFAOYSA-N

Formula: C18H22F3NO4

SMILES: COc1c(F)c(F)cc(C(=O)N2CCC(C(=O)OCC(C)C)CC2)c1F

Mol. weight [g/mol]: 373.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.164		Crippen Method
mcvol	260.030	ml/mol	McGowan Method
rinpol	2485.00		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=U361349&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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