Isonipecotic acid, N-(3-trifluoromethylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C16H18F3NO3/c1-2-23-15(22)11-6-8-20(9-7-11)14(21)12-4-3-5-13(10-12)16(1

InchiKey: QBHCDRNQQRHVRH-UHFFFAOYSA-N

Formula: C16H18F3NO3

SMILES: CCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]: 329.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	3.121		Crippen Method
mcvol	225.980	ml/mol	McGowan Method
rinpol	2129.00		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=U361540&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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