Isonipecotic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C16H17F4NO3/c1-2-24-15(23)10-3-5-21(6-4-10)14(22)11-7-12(16(18,19)20)9-

InchiKey: IVVFALYTBPUUEP-UHFFFAOYSA-N

Formula: C16H17F4NO3

SMILES: CCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]: 347.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.260		Crippen Method
mcvol	227.750	ml/mol	McGowan Method
rinpol	2039.00		NIST Webbook
rinpol	2039.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361444&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.