Isonipecotic acid, N-(2-fluoro-5-trifluoromethylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C16H17F4NO3/c1-2-24-15(23)10-5-7-21(8-6-10)14(22)12-9-11(16(18,19)20)3-
InchiKey: WSAMUGCGGBHODW-UHFFFAOYSA-N
Formula: C16H17F4NO3
SMILES: CCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2F)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	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361385&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

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