Isonipecotic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, ethyl ester

Inchi: InChI=1S/C17H17F6NO3/c1-2-27-15(26)10-5-7-24(8-6-10)14(25)12-9-11(16(18,19)20)3-

InchiKey: HPESPIAKZWTSKW-UHFFFAOYSA-N

Formula: C17H17F6NO3

SMILES: CCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1

Mol. weight [g/mol]: 397.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	4.140		Crippen Method
mcvol	245.380	ml/mol	McGowan Method
rinpol	1983.00		NIST Webbook
rinpol	1983.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361200&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.