Isonipecotic acid, N-(2-fluoro-3-trifluoromethylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C20H25F4NO3/c1-2-3-4-5-13-28-19(27)14-9-11-25(12-10-14)18(26)15-7-6-8-1

InchiKey: PEOBFFWGLSQBHE-UHFFFAOYSA-N

Formula: C20H25F4NO3

SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2F)CC1

Mol. weight [g/mol]: 403.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.75		Crippen Method
logp	4.820		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpol	2536.00		NIST Webbook

Sources

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

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=U361312&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices