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

Inchi: InChI=1S/C20H25F4NO3/c1-13(2)4-3-11-28-19(27)14-7-9-25(10-8-14)18(26)16-12-15(20

InchiKey: RWVFXANBPLCCRO-UHFFFAOYSA-N

Formula: C20H25F4NO3

SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2F)CC1

Mol. weight [g/mol]: 403.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.51		Crippen Method
logp	4.676		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpol	2447.00		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=U361390&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