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

Inchi: InChI=1S/C20H25F4NO3/c1-13(2)5-4-12-28-19(27)14-8-10-25(11-9-14)18(26)15-6-3-7-1
InchiKey: RSWQOCFIUMTSDO-UHFFFAOYSA-N
Formula: C20H25F4NO3
SMILES: CC(C)CCCOC(=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	-5.51		Crippen Method
logp	4.676		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook

Sources

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=U361311&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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