Isonipecotic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C20H25F4NO3/c1-2-3-4-5-10-28-19(27)14-6-8-25(9-7-14)18(26)15-11-16(20(2

InchiKey: NKJJHSPRMNNERH-UHFFFAOYSA-N

Formula: C20H25F4NO3

SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)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	2441.00		NIST Webbook
rinpol	2441.00		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=U361450&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.