

Isonipecotic acid, N-(3-fluoro-4-trifluoromethylbenzoyl)-, hexyl

Inchi:
ester

InChI=1S/C20H25F4NO3/c1-2-3-4-5-12-28-19(27)14-8-10-25(11-9-14)18(26)15-6-7-16(1

InchiKey: IZZAPHMABOWYLR-UHFFFAOYSA-N

Formula: C20H25F4NO3

SMILES: CCCCCOC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(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	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.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=U361470&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

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