

Isonipecotic acid, N-(2-fluoro-6-trifluoromethylbenzoyl)-, pentyl ester

Inchi:
InchiKey:

InChI=1S/C19H23F4NO3/c1-2-3-4-12-27-18(26)13-8-10-24(11-9-13)17(25)16-14(19(21,22)23)/n1
XPORWFKQISKKAH-UHFFFAOYSA-N

Formula:

C19H23F4NO3

SMILES:

CCCCCOC(=O)C1CCN(C(=O)c2c(F)cccc2C(F)(F)F)CC1

Mol. weight [g/mol]:

389.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	4.430		Crippen Method
mcvol	270.020	ml/mol	McGowan Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		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=U361287&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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