

Isonipecotic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, butyl

Inchi:
ester

InChI=1S/C18H21F4NO3/c1-2-3-8-26-17(25)12-4-6-23(7-5-12)16(24)13-9-14(18(20,21)2

InchiKey:

VPRRMMMLNRRELE-UHFFFAOYSA-N

Formula:

C18H21F4NO3

SMILES:

CCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]:

375.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	4.040		Crippen Method
mcvol	255.930	ml/mol	McGowan Method
rinpol	2241.00		NIST Webbook
rinpol	2241.00		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=U361447&Units=SI>

Crippen Method:

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

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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