

Isonipecotic acid, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, butyl

Inchi:
ester

InChI=1S/C18H22F3NO4/c1-3-4-9-26-18(24)11-5-7-22(8-6-11)17(23)12-10-13(19)15(21)

InchiKey:

LXANBVOEMPKETI-UHFFFAOYSA-N

Formula:

C18H22F3NO4

SMILES:

CCCCOC(=O)C1CCN(C(=O)c2cc(F)c(F)c(OC)c2F)CC1

Mol. weight [g/mol]:

373.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.308		Crippen Method
mcvol	260.030	ml/mol	McGowan Method
rinpole	2531.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361350&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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