

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

Inchi:
ester

InChI=1S/C17H19F4NO3/c1-2-7-25-16(24)11-3-5-22(6-4-11)15(23)12-8-13(17(19,20)21)

InchiKey:

SOEKVIGICNPDRN-UHFFFAOYSA-N

Formula:

C17H19F4NO3

SMILES:

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

Mol. weight [g/mol]:

361.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	3.650		Crippen Method
mcvol	241.840	ml/mol	McGowan Method
rinpole	2142.00		NIST Webbook
rinpole	2142.00		NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361445&Units=SI>

Crippen Method:

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

Crippen Method:

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

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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