

Isonipecotic acid, N-(3-fluoro-4-trifluoromethylbenzoyl)-, isobutyl ester

InChI: InChI=1S/C18H21F4NO3/c1-11(2)10-26-17(25)12-5-7-23(8-6-12)16(24)13-3-4-14(15(19)
InChIKey: VQGDKKPNRPEXSS-UHFFFAOYSA-N

Formula: C18H21F4NO3

SMILES: CC(C)COC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(F)c2)CC1

Mol. weight [g/mol]: 375.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	3.896		Crippen Method
mcvol	255.930	ml/mol	McGowan Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpol:	Non-polar retention indices

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