

Isonipecotic acid, N-(2-fluoro-3-trifluoromethylbenzoyl)-, isobutyl ester

InChI: InChI=1S/C18H21F4NO3/c1-11(2)10-26-17(25)12-6-8-23(9-7-12)16(24)13-4-3-5-14(15(16)17)21-22
InChIKey: BBUZIUXTFZBEPC-UHFFFAOYSA-N

Formula: C18H21F4NO3
SMILES: CC(C)COC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2F)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	2289.00		NIST Webbook
rinpol	2289.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361308&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
rinpol: Non-polar retention indices

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