

Isonipectic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, isobutyl ester

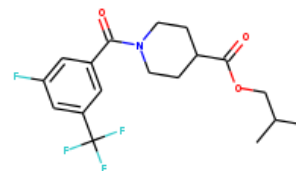
InChI: InChI=1S/C18H21F4NO3/c1-11(2)10-26-17(25)12-3-5-23(6-4-12)16(24)13-7-14(18(20,21)22)9-15(19)8-13/h7-9,11-12H,3-6,10H2,1-2H3

InChI Key: JVUMNZDZWPIFOT-UHFFFAOYSA-N

Formula: C18H21F4NO3

SMILES: CC(C)COC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1

Molecular Weight: 375.36



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	3.90		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H21F4NO3/c1-11\(2\)10-26-17\(25\)12-3-5-23\(6-4-12\)16\(24\)13-7-14\(18\(20,21\)22\)9-15\(19\)8-13/h7-9,11-12H,3-6,10H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H21F4NO3/c1-11(2)10-26-17(25)12-3-5-23(6-4-12)16(24)13-7-14(18(20,21)22)9-15(19)8-13/h7-9,11-12H,3-6,10H2,1-2H3)

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

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

Latest version available from:

<https://www.cheméo.com/cid/60-357-9/Isonipectic%20acid%2C%20N-%283-fluoro-5-trifluoromethylbenzoyl%29-%2C%20isobutyl%20ester>

Generated by Cheméo on Fri, 20 Sep 2019 07:57:34 +0000.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.