

5-Hydroxytryptophan, methyl, 2-PFP

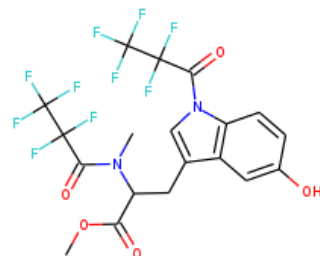
InChI: InChI=1S/C19H14F10N2O5/c1-30(14(34)16(20,21)18(24,25)26)12(13(33)36-2)5-8-7-31(11-4-3-9(32)6-10(8)11)15(35)17(22,23)19(27,28)29/h3-4,6-7,12,32H,5H2,1-2H3

InChI Key: ZDHDCRAOTJITHN-UHFFFAOYSA-N

Formula: C19H14F10N2O5

SMILES: COC(=O)C(Cc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccc(O)cc12)N(C)C(=O)C(F)(F)C(F)(F)F

Molecular Weight: 540.31



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	3.925		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H14F10N2O5/c1-30\(14\(34\)16\(20,21\)18\(24,25\)26\)12\(13\(33\)36-2\)5-8-7-31\(11-4-3-9\(32\)6-10\(8\)11\)15\(35\)17\(22,23\)19\(27,28\)29/h3-4,6-7,12,32H,5H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H14F10N2O5/c1-30(14(34)16(20,21)18(24,25)26)12(13(33)36-2)5-8-7-31(11-4-3-9(32)6-10(8)11)15(35)17(22,23)19(27,28)29/h3-4,6-7,12,32H,5H2,1-2H3)

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

Legend

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

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