

# 5-Hydroxytryptophan, methyl, 3-PFP

**Inchi:** InChI=1S/C22H13F15N2O6/c1-38(14(41)17(23,24)20(29,30)31)12(13(40)44-2)5-8-7-39(  
**InchiKey:** ZTTOCQZOJUSWSK-UHFFFAOYSA-N  
**Formula:** C22H13F15N2O6  
**SMILES:** COC(=O)C(Cc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccc(OC(=O)C(F)(F)C(F)(F)F)cc12)N(C)C(=O)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 686.32

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.11		Crippen Method
logp	5.322		Crippen Method
mcvol	346.450	ml/mol	McGowan Method
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580037&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](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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