

# 5-Hydroxytryptamine, 3-PFP

**Inchi:** InChI=1S/C19H9F15N2O4/c20-14(21,17(26,27)28)11(37)35-4-3-7-6-36(12(38)15(22,23)  
**InchiKey:** DINKCIWMIVSBAF-UHFFFAOYSA-N  
**Formula:** C19H9F15N2O4  
**SMILES:** O=C(NCCc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccc(OC(=O)C(F)(F)C(F)(F)F)cc12)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 614.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.50		Crippen Method
logp	5.438		Crippen Method
mcvol	296.740	ml/mol	McGowan Method
rinpol	1835.00		NIST Webbook
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## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580002&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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