

# Tryptophan, methyl, 1-PFP

**Inchi:** InChI=1S/C14H11F5N2O3/c1-24-11(22)10(21-12(23)13(15,16)14(17,18)19)8-6-20-9-5-3  
**InchiKey:** VDBGHQVUWWIZJQ-UHFFFAOYSA-N  
**Formula:** C14H11F5N2O3  
**SMILES:** COC(=O)C(NC(=O)C(F)(F)C(F)(F)F)c1c[nH]c2ccccc12  
**Mol. weight [g/mol]:** 350.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	2.214		Crippen Method
mcvol	207.020	ml/mol	McGowan Method
rinpol	2004.00		NIST Webbook
rinpol	2004.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580082&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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