

# 5-Hydroxyindoleacetic acid, methyl, 2-PFP

<b>Inchi:</b>	InChI=1S/C17H9F10NO5/c1-32-11(29)4-7-6-28(12(30)14(18,19)16(22,23)24)10-3-2-8(5-
<b>InchiKey:</b>	VHHAIUXARNGGEQ-UHFFFAOYSA-N
<b>Formula:</b>	C17H9F10NO5
<b>SMILES:</b>	COC(=O)Cc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccc(OC(=O)C(F)(F)C(F)(F)F)cc12
<b>Mol. weight [g/mol]:</b>	497.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.58		Crippen Method
logp	4.298		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
rinpole	1710.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R579998&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R579998&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpole:</b>	Non-polar retention indices

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