

# Tryptophan, 6-fluoro-

<b>Other names:</b>	6-fluoro-DL-tryptophan
<b>Inchi:</b>	InChI=1S/C11H11FN2O2/c12-7-1-2-8-6(3-9(13)11(15)16)5-14-10(8)4-7/h1-2,4-5,9,14H,3
<b>InchiKey:</b>	YMEXGEAJNZRQEH-UHFFFAOYSA-N
<b>Formula:</b>	C11H11FN2O2
<b>SMILES:</b>	[NH3+]C(Cc1c[nH]c2cc(F)ccc12)C(=O)[O-]
<b>Mol. weight [g/mol]:</b>	222.22
<b>CAS:</b>	7730-20-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	-1.272		Crippen Method
mcvol	156.100	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7730203&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7730203&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

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