

# 4-P-methoxyanilino-6-methyl-1,3,3a,7-tetrazainden

<b>Inchi:</b>	InChI=1S/C13H13N5O/c1-9-7-12(18-13(16-9)14-8-15-18)17-10-3-5-11(19-2)6-4-10/h3-8
<b>InchiKey:</b>	DLVXCEBZMMWMQK-UHFFFAOYSA-N
<b>Formula:</b>	C13H13N5O
<b>SMILES:</b>	COc1ccc(Nc2cc(C)nc3ncnn23)cc1
<b>Mol. weight [g/mol]:</b>	255.28
<b>CAS:</b>	91769-08-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	2.185		Crippen Method
mcvol	187.120	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C91769083&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C91769083&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>

## 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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