

# 1H-Pyrrole, 1-(4-methylphenyl)-

<b>Other names:</b>	1-(4-Methylphenyl)pyrrole 1-(4-methylphenyl)-1H-pyrrole 1-p-tolylpyrrole Pyrrole, 1-p-tolyl-
<b>Inchi:</b>	InChI=1S/C11H11N/c1-10-4-6-11(7-5-10)12-8-2-3-9-12/h2-9H,1H3
<b>InchiKey:</b>	VYUNLDVEMSMJNP-UHFFFAOYSA-N
<b>Formula:</b>	C11H11N
<b>SMILES:</b>	Cc1ccc(-n2cccc2)cc1
<b>Mol. weight [g/mol]:</b>	157.21
<b>CAS:</b>	827-60-1

## Physical Properties

Property code	Value	Unit	Source
hfus	83.70	kJ/mol	Experimental and computational thermochemistry of 1-phenylpyrrole and 1-(4-methylphenyl)pyrrole
log10ws	-3.60		Crippen Method
logp	2.786		Crippen Method
mccvol	132.610	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>Experimental and computational thermochemistry of 1-phenylpyrrole and 1-(4-methylphenyl)pyrrole:</b>	<a href="https://www.doi.org/10.1016/j.jct.2010.01.009">https://www.doi.org/10.1016/j.jct.2010.01.009</a> <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=C827601&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C827601&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

**hfus:** Enthalpy of fusion at standard conditions

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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