

# Pyrrole, 4-ethyl-2-methyl-

<b>Other names:</b>	4-Ethyl-2-methylpyrrole
<b>Inchi:</b>	InChI=1S/C7H11N/c1-3-7-4-6(2)8-5-7/h4-5,8H,3H2,1-2H3
<b>InchiKey:</b>	HWXJSNSZAOSLAS-UHFFFAOYSA-N
<b>Formula:</b>	C7H11N
<b>SMILES:</b>	CCc1c[nH]c(C)c1
<b>Mol. weight [g/mol]:</b>	109.17
<b>CAS:</b>	5690-96-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.404		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rinsol	951.00		NIST Webbook
rinsol	902.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5690960&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5690960&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>rinsol:</b>	Non-polar retention indices

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