

# Pyrrole, 1-ethyl-2,5-dimethyl

<b>Other names:</b>	2,5-dimethyl-1-ethylpyrrole
<b>Inchi:</b>	InChI=1S/C8H13N/c1-4-9-7(2)5-6-8(9)3/h5-6H,4H2,1-3H3
<b>InchiKey:</b>	WIXUFIYVGRNTDD-UHFFFAOYSA-N
<b>Formula:</b>	C8H13N
<b>SMILES:</b>	CCn1c(C)ccc1C
<b>Mol. weight [g/mol]:</b>	123.20

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	2.125		Crippen Method
mcvol	114.100	ml/mol	McGowan Method
rinpol	942.00		NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R2396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R2396&amp;Units=SI</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>rinpol:</b>	Non-polar retention indices

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