

# 1H-Pyrrole, 2,3,5-trimethyl-

<b>Other names:</b>	2,3,5-Trimethylpyrrole 2,3,5-Trimethyl-1H-pyrrole
<b>Inchi:</b>	InChI=1S/C7H11N/c1-5-4-6(2)8-7(5)3/h4,8H,1-3H3
<b>InchiKey:</b>	VIDOWPWTFHJVID-UHFFFAOYSA-N
<b>Formula:</b>	C7H11N
<b>SMILES:</b>	Cc1cc(C)c(C)[nH]1
<b>Mol. weight [g/mol]:</b>	109.17
<b>CAS:</b>	2199-41-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.458		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rinpol	995.00		NIST Webbook
rinpol	991.00		NIST Webbook

## 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=C2199419&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2199419&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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