

# 1H-Pyrazole, 3,4-dimethyl-

<b>Other names:</b>	3(5),4-Dimethylpyrazole Pyrazole, 3,4-dimethyl-
<b>Inchi:</b>	InChI=1S/C5H8N2/c1-4-3-6-7-5(4)2/h3H,1-2H3,(H,6,7)
<b>InchiKey:</b>	VQTVFIMEENGCSJA-UHFFFAOYSA-N
<b>Formula:</b>	C5H8N2
<b>SMILES:</b>	Cc1c[nH]nc1C
<b>Mol. weight [g/mol]:</b>	96.13
<b>CAS:</b>	2820-37-3

## Physical Properties

Property code	Value	Unit	Source
affp	927.30	kJ/mol	NIST Webbook
basg	895.40	kJ/mol	NIST Webbook
log10ws	-1.41		Crippen Method
logp	0.545		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
tf	331.15 ± 1.50	K	NIST Webbook

## Sources

<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=C2820373&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2820373&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>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**tf:** Normal melting (fusion) point

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