

# Pyrazole, 1,4-dimethyl-

<b>Other names:</b>	1,4-Dimethylpyrazole 1H-Pyrazole, 1,4-dimethyl-
<b>Inchi:</b>	InChI=1S/C5H8N2/c1-5-3-6-7(2)4-5/h3-4H,1-2H3
<b>InchiKey:</b>	SZQCPRPWDXLMM-UHFFFAOYSA-N
<b>Formula:</b>	C5H8N2
<b>SMILES:</b>	Cc1cnn(C)c1
<b>Mol. weight [g/mol]:</b>	96.13
<b>CAS:</b>	1072-68-0

## Physical Properties

Property code	Value	Unit	Source
affp	928.40	kJ/mol	NIST Webbook
basg	896.80	kJ/mol	NIST Webbook
log10ws	-3.00		Crippen Method
logp	0.729		Crippen Method
mcvol	81.810	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>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=C1072680&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072680&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

<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
<b>mcvol:</b>	McGowan's characteristic volume

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