

# 3,4,5-Trimethylpyrazole

<b>Other names:</b>	1H-Pyrazole, 3,4,5-trimethyl-
<b>Inchi:</b>	InChI=1S/C6H10N2/c1-4-5(2)7-8-6(4)3/h1-3H3,(H,7,8)
<b>InchiKey:</b>	HUVAAOZUPLEYBH-UHFFFAOYSA-N
<b>Formula:</b>	C6H10N2
<b>SMILES:</b>	Cc1n[nH]c(C)c1C
<b>Mol. weight [g/mol]:</b>	110.16
<b>CAS:</b>	5519-42-6

## Physical Properties

Property code	Value	Unit	Source
affp	949.30	kJ/mol	NIST Webbook
basg	916.00	kJ/mol	NIST Webbook
log10ws	-1.88		Crippen Method
logp	0.853		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
ripol	2194.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5519426&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5519426&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>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

**ripol:** Polar retention indices

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