

# 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-

<b>Other names:</b>	2-Pyrazolin-5-one, 3-methyl- 3-Methyl-5-pyrazolone 3-Methyl-2-pyrazolin-5-one 3-Methyl-pyrazolon-(5) 2,4-dihydro-5-methyl-3H-pyrazol-3-one
<b>Inchi:</b>	InChI=1S/C4H6N2O/c1-3-2-4(7)6-5-3/h2H2,1H3,(H,6,7)
<b>InchiKey:</b>	NHLAPJMCARJFOG-UHFFFAOYSA-N
<b>Formula:</b>	C4H6N2O
<b>SMILES:</b>	CC1=NN=C(O)C1
<b>Mol. weight [g/mol]:</b>	98.10
<b>CAS:</b>	108-26-9

## Physical Properties

Property code	Value	Unit	Source
gf	164.46	kJ/mol	Joback Method
hf	37.26	kJ/mol	Joback Method
hfus	15.01	kJ/mol	Joback Method
hvap	56.07	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.723		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	6369.39	kPa	Joback Method
tb	518.73	K	Joback Method
tc	738.84	K	Joback Method
tf	380.44	K	Joback Method
vc	0.290	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.82	J/molxK	518.73	Joback Method
cpg	186.54	J/molxK	555.41	Joback Method
cpg	195.77	J/molxK	592.10	Joback Method
cpg	204.51	J/molxK	628.78	Joback Method

cpg	212.74	J/mol×K	665.47	Joback Method
cpg	220.43	J/mol×K	702.15	Joback Method
cpg	227.59	J/mol×K	738.84	Joback Method

## 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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=C108269&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C108269&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<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>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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