

# 2-Pyrazoline

<b>Other names:</b>	4,5-dihydro-1H-pyrazole
<b>Inchi:</b>	InChI=1S/C3H6N2/c1-2-4-5-3-1/h2,5H,1,3H2
<b>InchiKey:</b>	MCGBIXXDQFWVDW-UHFFFAOYSA-N
<b>Formula:</b>	C3H6N2
<b>SMILES:</b>	C1=NNCC1
<b>Mol. weight [g/mol]:</b>	70.09
<b>CAS:</b>	109-98-8

## Physical Properties

Property code	Value	Unit	Source
gf	253.09	kJ/mol	Joback Method
hf	142.13	kJ/mol	Joback Method
hfus	12.34	kJ/mol	Joback Method
hvap	36.10	kJ/mol	Joback Method
log10ws	-0.32		Crippen Method
logp	-0.035		Crippen Method
mcvol	57.930	ml/mol	McGowan Method
pc	6599.09	kPa	Joback Method
rinpol	771.00		NIST Webbook
rinpol	771.00		NIST Webbook
tb	389.40	K	Joback Method
tc	618.60	K	Joback Method
tf	316.04	K	Joback Method
vc	0.217	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	99.25	J/molxK	389.40	Joback Method
cpg	109.58	J/molxK	427.60	Joback Method
cpg	119.42	J/molxK	465.80	Joback Method
cpg	128.76	J/molxK	504.00	Joback Method
cpg	137.60	J/molxK	542.20	Joback Method
cpg	145.95	J/molxK	580.40	Joback 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>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=C109988&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109988&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>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>rinpol:</b>	Non-polar retention indices
<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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