

# 2-Pyrazoline, 1,4,5-trimethyl-

**Other names:** 1,4,5-Trimethyl-«DELTA»[2]-pyrazoline  
**Inchi:** InChI=1S/C6H12N2/c1-5-4-7-8(3)6(5)2/h4-6H,1-3H3  
**InchiKey:** QZXPNIFFNBFPOML-UHFFFAOYSA-N  
**Formula:** C6H12N2  
**SMILES:** CC1C=NN(C)C1C  
**Mol. weight [g/mol]:** 112.17  
**CAS:** 7423-11-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	0.942		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
rinpol	837.00		NIST Webbook
rinpol	837.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7423112&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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