# 2-Pyrazoline, 5-ethyl-5-methyl

**Inchi:** InChI=1S/C6H12N2/c1-3-6(2)4-5-7-8-6/h5,8H,3-4H2,1-2H3
**InchiKey:** PYMHAFLRPRPQQA-UHFFFAOYSA-N
**Formula:** C6H12N2
**SMILES:** CCC1(C)CC=NN1
**Mol. weight [g/mol]:** 112.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 265.15 | kJ/mol | Joback Method |
| hf | 75.11 | kJ/mol | Joback Method |
| hfus | 14.88 | kJ/mol | Joback Method |
| hvap | 41.32 | kJ/mol | Joback Method |
| log10ws | -1.68 | | Crippen Method |
| logp | 1.134 | | Crippen Method |
| mcvol | 100.200 | ml/mol | McGowan Method |
| pc | 4403.25 | kPa | Joback Method |
| rinpol | 905.00 | | NIST Webbook |
| rinpol | 905.00 | | NIST Webbook |
| tb | 453.61 | K | Joback Method |
| tc | 683.63 | K | Joback Method |
| tf | 369.51 | K | Joback Method |
| vc | 0.383 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 215.98 | J/mol×K | 453.61 | Joback Method |
| cpg | 231.26 | J/mol×K | 491.95 | Joback Method |
| cpg | 245.48 | J/mol×K | 530.28 | Joback Method |
| cpg | 258.74 | J/mol×K | 568.62 | Joback Method |
| cpg | 271.16 | J/mol×K | 606.95 | Joback Method |
| cpg | 282.83 | J/mol×K | 645.29 | Joback Method |
| cpg | 293.87 | J/mol×K | 683.63 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R511190&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |