# 3-tert-Butyl-2-pyrazolin-5-one

**Inchi:** InChI=1S/C7H12N2O/c1-7(2,3)5-4-6(10)9-8-5/h4H2,1-3H3,(H,9,10)
**InchiKey:** VDNOHRWEOSDGQX-UHFFFAOYSA-N
**Formula:** C7H12N2O
**SMILES:** CC(C)(C)C1=NNC(=O)C1
**Mol. weight [g/mol]:** 140.18
**CAS:** 29211-68-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 157.39 | kJ/mol | Joback Method |
| hf | -98.35 | kJ/mol | Joback Method |
| hfus | 14.41 | kJ/mol | Joback Method |
| hvap | 48.62 | kJ/mol | Joback Method |
| log10ws | -1.52 | | Crippen Method |
| logp | 0.908 | | Crippen Method |
| mcvol | 115.860 | ml/mol | McGowan Method |
| pc | 4026.13 | kPa | Joback Method |
| tb | 550.49 | K | Joback Method |
| tc | 800.47 | K | Joback Method |
| tf | 444.28 | K | Joback Method |
| vc | 0.438 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 288.33 | J/mol×K | 550.49 | Joback Method |
| cpg | 304.39 | J/mol×K | 592.15 | Joback Method |
| cpg | 319.49 | J/mol×K | 633.82 | Joback Method |
| cpg | 333.60 | J/mol×K | 675.48 | Joback Method |
| cpg | 346.73 | J/mol×K | 717.14 | Joback Method |
| cpg | 358.86 | J/mol×K | 758.81 | Joback Method |
| cpg | 369.99 | J/mol×K | 800.47 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C29211685&Units=SI |

# Legend

| | |
|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |