# 2-Pyrimidinecarbamonitrile, 4,6-dihydroxy- (keto form)

**Other names:** (1,4,5,6-tetrahydro-4,6-dioxopyrimidin-2-yl)cyanamide
**Inchi:** InChI=1S/C5H4N4O2/c6-2-7-5-8-3(10)1-4(11)9-5/h1H2,(H2,7,8,9,10,11)
**InchiKey:** JCHNBNRIALLIDT-UHFFFAOYSA-N
**Formula:** C5H4N4O2
**SMILES:** N#CNC1=NC(=O)CC(=O)N1
**Mol. weight [g/mol]:** 152.11
**CAS:** 55067-10-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 225.59 | kJ/mol | Joback Method |
| hf | 26.17 | kJ/mol | Joback Method |
| hfus | 20.66 | kJ/mol | Joback Method |
| hvap | 66.79 | kJ/mol | Joback Method |
| log10ws | -0.26 | | Crippen Method |
| logp | -1.540 | | Crippen Method |
| mcvol | 100.610 | ml/mol | McGowan Method |
| pc | 5446.55 | kPa | Joback Method |
| tb | 732.30 | K | Joback Method |
| tc | 1008.23 | K | Joback Method |
| tf | 601.67 | K | Joback Method |
| vc | 0.397 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 275.84 | J/mol×K | 732.30 | Joback Method |
| cpg | 286.56 | J/mol×K | 778.29 | Joback Method |
| cpg | 296.09 | J/mol×K | 824.28 | Joback Method |
| cpg | 304.27 | J/mol×K | 870.26 | Joback Method |
| cpg | 310.96 | J/mol×K | 916.25 | Joback Method |
| cpg | 316.02 | J/mol×K | 962.24 | Joback Method |
| cpg | 319.30 | J/mol×K | 1008.23 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C55067102&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |