# 1-Pyrroline, 2-butanoyl

**Inchi:** InChI=1S/C8H13NO/c1-2-4-8(10)7-5-3-6-9-7/h2-6H2,1H3
**InchiKey:** HKVIHNPWRLQVTI-UHFFFAOYSA-N
**Formula:** C8H13NO
**SMILES:** CCCC(=O)C1=NCCC1
**Mol. weight [g/mol]:** 139.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 68.93 | kJ/mol | Joback Method |
| hf | -122.93 | kJ/mol | Joback Method |
| hfus | 16.91 | kJ/mol | Joback Method |
| hvap | 47.88 | kJ/mol | Joback Method |
| log10ws | -1.51 | | Crippen Method |
| logp | 1.590 | | Crippen Method |
| mcvol | 119.970 | ml/mol | McGowan Method |
| pc | 3509.58 | kPa | Joback Method |
| rinpol | 1118.00 | | NIST Webbook |
| tb | 514.10 | K | Joback Method |
| tc | 733.02 | K | Joback Method |
| tf | 329.81 | K | Joback Method |
| vc | 0.467 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 280.15 | J/mol×K | 514.10 | Joback Method |
| cpg | 295.33 | J/mol×K | 550.59 | Joback Method |
| cpg | 309.66 | J/mol×K | 587.07 | Joback Method |
| cpg | 323.16 | J/mol×K | 623.56 | Joback Method |
| cpg | 335.84 | J/mol×K | 660.05 | Joback Method |
| cpg | 347.73 | J/mol×K | 696.54 | Joback Method |
| cpg | 358.83 | J/mol×K | 733.02 | Joback Method |

# Sources

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|---|---|
| **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=R66219&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |