# 1,2-Cyclobutanedicarbonitrile, trans-

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|---|---|
| **Other names:** | trans-1,2-Cyclobutanedicarbonitrile |
| | trans-1,2-Dicyanocyclobutane |
| | USAF st-1 |
| | 1,2-Cyclobutanedicarbonitrile, (E)- |
| **Inchi:** | InChI=1S/C6H6N2/c7-3-5-1-2-6(5)4-8/h5-6H,1-2H2/t5-,6-/m1/s1 |
| **InchiKey:** | CZPLUOCTUPJSIZ-PHDIDXHHSA-N |
| **Formula:** | C6H6N2 |
| **SMILES:** | N#CC1CCC1C#N |
| **Mol. weight [g/mol]:** | 106.13 |
| **CAS:** | 3211-20-9 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 306.94 | kJ/mol | Joback Method |
| hf | 208.89 | kJ/mol | Joback Method |
| hfus | 11.41 | kJ/mol | Joback Method |
| hvap | 49.68 | kJ/mol | Joback Method |
| log10ws | -1.48 | | Crippen Method |
| logp | 1.060 | | Crippen Method |
| mcvol | 87.300 | ml/mol | McGowan Method |
| pc | 3372.36 | kPa | Joback Method |
| tb | 547.18 | K | Joback Method |
| tc | 779.51 | K | Joback Method |
| tf | 297.54 | K | Joback Method |
| vc | 0.371 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 194.51 | J/mol×K | 547.18 | Joback Method |
| cpg | 203.68 | J/mol×K | 585.90 | Joback Method |
| cpg | 212.25 | J/mol×K | 624.62 | Joback Method |
| cpg | 220.24 | J/mol×K | 663.35 | Joback Method |
| cpg | 227.68 | J/mol×K | 702.07 | Joback Method |

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|---|---|---|---|---|
| cpg | 234.61 | J/mol×K | 740.79 | Joback Method |
| cpg | 241.05 | J/mol×K | 779.51 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3211209&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |