# Cinnamonitrile, 2-chloro, cis

**Inchi:** InChI=1S/C9H6ClN/c10-9-6-2-1-4-8(9)5-3-7-11/h1-6H/b5-3-
**InchiKey:** PWWUUGALKZGDSD-HYXAFXHYSA-N
**Formula:** C9H6ClN
**SMILES:** N#CC=Cc1ccccc1Cl
**Mol. weight [g/mol]:** 163.60

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 329.15 | kJ/mol | Joback Method |
| hf | 262.33 | kJ/mol | Joback Method |
| hfus | 18.62 | kJ/mol | Joback Method |
| hvap | 53.39 | kJ/mol | Joback Method |
| log10ws | -3.27 | | Crippen Method |
| logp | 2.877 | | Crippen Method |
| mcvol | 123.230 | ml/mol | McGowan Method |
| pc | 3170.40 | kPa | Joback Method |
| rinpol | 1355.00 | | NIST Webbook |
| tb | 580.65 | K | Joback Method |
| tc | 824.26 | K | Joback Method |
| tf | 319.96 | K | Joback Method |
| vc | 0.486 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 245.87 | J/mol×K | 580.65 | Joback Method |
| cpg | 255.46 | J/mol×K | 621.25 | Joback Method |
| cpg | 264.29 | J/mol×K | 661.85 | Joback Method |
| cpg | 272.42 | J/mol×K | 702.46 | Joback Method |
| cpg | 279.91 | J/mol×K | 743.06 | Joback Method |
| cpg | 286.82 | J/mol×K | 783.66 | Joback Method |
| cpg | 293.20 | J/mol×K | 824.26 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R503743&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

| | |
|---|---|
| **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 |