# trans-Cyclopropanecarbonitrile, 2-methyl-2-phenyl

**Inchi:** InChI=1S/C11H11N/c1-11(7-10(11)8-12)9-5-3-2-4-6-9/h2-6,10H,7H2,1H3/t10-,11-/m0/s1
**InchiKey:** NXEGBZUVVOEMCE-QWRGUYRKSA-N
**Formula:** C11H11N
**SMILES:** CC1(c2ccccc2)CC1C#N
**Mol. weight [g/mol]:** 157.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 334.88 | kJ/mol | Joback Method |
| hf | 198.74 | kJ/mol | Joback Method |
| hfus | 12.70 | kJ/mol | Joback Method |
| hvap | 51.29 | kJ/mol | Joback Method |
| log10ws | -2.72 | | Crippen Method |
| logp | 2.488 | | Crippen Method |
| mcvol | 132.610 | ml/mol | McGowan Method |
| pc | 2999.15 | kPa | Joback Method |
| rinpol | 1330.00 | | NIST Webbook |
| rinpol | 1330.00 | | NIST Webbook |
| tb | 582.15 | K | Joback Method |
| tc | 827.89 | K | Joback Method |
| tf | 342.74 | K | Joback Method |
| vc | 0.523 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 319.80 | J/mol×K | 582.15 | Joback Method |
| cpg | 333.78 | J/mol×K | 623.11 | Joback Method |
| cpg | 346.68 | J/mol×K | 664.06 | Joback Method |
| cpg | 358.70 | J/mol×K | 705.02 | Joback Method |
| cpg | 370.07 | J/mol×K | 745.98 | Joback Method |
| cpg | 380.98 | J/mol×K | 786.94 | Joback Method |
| cpg | 391.64 | J/mol×K | 827.89 | 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=R13553&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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