# Cyclopropanecarbonitrile, 1,2-diphenyl-

**Inchi:** InChI=1S/C16H13N/c17-12-16(14-9-5-2-6-10-14)11-15(16)13-7-3-1-4-8-13/h1-10,15H,11
**InchiKey:** MIVVDTYTHSYGAF-UHFFFAOYSA-N
**Formula:** C16H13N
**SMILES:** N#CC1(c2ccccc2)CC1c1ccccc1
**Mol. weight [g/mol]:** 219.28
**CAS:** 10224-14-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 489.39 | kJ/mol | Joback Method |
| hf | 332.07 | kJ/mol | Joback Method |
| hfus | 19.69 | kJ/mol | Joback Method |
| hvap | 64.69 | kJ/mol | Joback Method |
| ie | 8.80 ± 0.08 | eV | NIST Webbook |
| log10ws | -4.12 | | Crippen Method |
| logp | 3.635 | | Crippen Method |
| mcvol | 179.300 | ml/mol | McGowan Method |
| pc | 2563.69 | kPa | Joback Method |
| tb | 723.23 | K | Joback Method |
| tc | 991.75 | K | Joback Method |
| tf | 425.51 | K | Joback Method |
| vc | 0.696 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 485.40 | J/mol×K | 723.23 | Joback Method |
| cpg | 501.38 | J/mol×K | 767.98 | Joback Method |
| cpg | 516.52 | J/mol×K | 812.74 | Joback Method |
| cpg | 531.15 | J/mol×K | 857.49 | Joback Method |
| cpg | 545.58 | J/mol×K | 902.24 | Joback Method |
| cpg | 560.12 | J/mol×K | 946.99 | Joback Method |
| cpg | 575.10 | J/mol×K | 991.75 | 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=C10224143&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 |
| **ie:** | Ionization energy |
| **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 |