# 4-Cyanobenzyl radical

**Inchi:** InChI=1S/C8H6N/c1-7-2-4-8(6-9)5-3-7/h2-5H,1H2
**InchiKey:** SMVKJBOGSRFNKW-UHFFFAOYSA-N
**Formula:** C8H6N
**SMILES:** [CH2]c1ccc(C#N)cc1
**Mol. weight [g/mol]:** 116.14
**CAS:** 4939-73-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 304.82 | kJ/mol | Joback Method |
| hf | 237.30 | kJ/mol | Joback Method |
| hfus | 13.32 | kJ/mol | Joback Method |
| hvap | 46.67 | kJ/mol | Joback Method |
| ie | 8.40 ± 0.10 | eV | NIST Webbook |
| log10ws | -1.92 | | Crippen Method |
| logp | 1.740 | | Crippen Method |
| mcvol | 99.050 | ml/mol | McGowan Method |
| pc | 3668.65 | kPa | Joback Method |
| tb | 515.48 | K | Joback Method |
| tc | 744.40 | K | Joback Method |
| tf | 300.22 | K | Joback Method |
| vc | 0.393 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 193.45 | J/mol×K | 515.48 | Joback Method |
| cpg | 202.36 | J/mol×K | 553.63 | Joback Method |
| cpg | 210.57 | J/mol×K | 591.79 | Joback Method |
| cpg | 218.13 | J/mol×K | 629.94 | Joback Method |
| cpg | 225.11 | J/mol×K | 668.09 | Joback Method |
| cpg | 231.58 | J/mol×K | 706.24 | Joback Method |
| cpg | 237.60 | J/mol×K | 744.40 | Joback Method |

# Sources

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|---|---|
| **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=C4939735&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **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 |