# 1,4-Benzenediacetonitrile

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|---|---|
| **Other names:** | p-Benzenediacetonitrile |
| | p-(Cyanomethyl)benzyl cyanide |
| | p-Bis(cyanomethyl)benzene |
| | p-Phenylenediacetonitrile |
| | p-Xylylene dicyanide |
| | 1,4-Bis(cyanomethyl)benzene |
| | 1,4-Phenylenediacetonitrile |
| **Inchi:** | InChI=1S/C10H8N2/c11-7-5-9-1-2-10(4-3-9)6-8-12/h1-4H,5-6H2 |
| **InchiKey:** | FUQCKESKNZBNOG-UHFFFAOYSA-N |
| **Formula:** | C10H8N2 |
| **SMILES:** | N#CCc1ccc(CC#N)cc1 |
| **Mol. weight [g/mol]:** | 156.18 |
| **CAS:** | 622-75-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 402.46 | kJ/mol | Joback Method |
| hf | 305.09 | kJ/mol | Joback Method |
| hfus | 18.32 | kJ/mol | Joback Method |
| hvap | 61.75 | kJ/mol | Joback Method |
| log10ws | -2.81 | | Crippen Method |
| logp | 1.819 | | Crippen Method |
| mcvol | 130.760 | ml/mol | McGowan Method |
| pc | 2735.42 | kPa | Joback Method |
| tb | 664.02 | K | Joback Method |
| tc | 902.09 | K | Joback Method |
| tf | 371.38 | K | Joback Method |
| vc | 0.539 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 304.87 | J/mol×K | 664.02 | Joback Method |
| cpg | 314.46 | J/mol×K | 703.70 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 323.36 | J/mol×K | 743.38 | Joback Method |
| cpg | 331.60 | J/mol×K | 783.05 | Joback Method |
| cpg | 339.22 | J/mol×K | 822.73 | Joback Method |
| cpg | 346.26 | J/mol×K | 862.41 | Joback Method |
| cpg | 352.75 | J/mol×K | 902.09 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C622753&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 |

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