# 4-Pyridinecarbonitrile

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|---|---|
| **Other names:** | .gamma.-cyanopyridine |
| | 4-azabenzonitrile |
| | 4-cyanopyridine |
| | 4-pyridinenitrile |
| | 4-pyridyl cyanide |
| | isonicotinic acid nitrile |
| | isonicotinonitrile |
| | «gamma»-Cyanopyridine |
| **Inchi:** | InChI=1S/C6H4N2/c7-5-6-1-3-8-4-2-6/h1-4H |
| **InchiKey:** | GPHQHTOMRSGBNZ-UHFFFAOYSA-N |
| **Formula:** | C6H4N2 |
| **SMILES:** | N#Cc1ccncc1 |
| **Mol. weight [g/mol]:** | 104.11 |
| **CAS:** | 100-48-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 880.60 | kJ/mol | NIST Webbook |
| basg | 848.80 | kJ/mol | NIST Webbook |
| chs | -3143.00 ± 0.50 | kJ/mol | NIST Webbook |
| hf | 283.50 ± 1.10 | kJ/mol | NIST Webbook |
| hfs | 210.30 ± 0.90 | kJ/mol | NIST Webbook |
| hsub | 73.20 | kJ/mol | NIST Webbook |
| hsub | 73.20 ± 0.60 | kJ/mol | NIST Webbook |
| hsub | 73.20 ± 0.60 | kJ/mol | NIST Webbook |
| ie | 10.70 | eV | NIST Webbook |
| ie | 10.40 ± 0.10 | eV | NIST Webbook |
| ie | 10.30 | eV | NIST Webbook |
| log10ws | -1.59 | | Crippen Method |
| logp | 0.953 | | Crippen Method |
| mcvol | 83.000 | ml/mol | McGowan Method |
| rinpol | 955.00 | | NIST Webbook |
| rinpol | 978.00 | | NIST Webbook |
| rinpol | 955.00 | | NIST Webbook |
| ripol | 1665.00 | | NIST Webbook |
| tb | 352.00 ± 1.00 | K | NIST Webbook |
| tf | 352.40 ± 1.00 | K | NIST Webbook |

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|---|---|---|---|
| tf | 353.55 | K | Measurement and Correlation of Solubility of Two Isomers of Cyanopyridine in Eight Pure Solvents from 268.15 K to 318.15 K |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C100481&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Measurement and Correlation of Solubility of Two Isomers of Cyanopyridine in Eight Pure Solvents from 268.15 K to 318.15 K:** | https://www.doi.org/10.1021/acs.jced.7b00301 |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chs:** | Standard solid enthalpy of combustion |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |

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