# 3-methylpentanenitrile

**Inchi:** InChI=1S/C6H11N/c1-3-6(2)4-5-7/h6H,3-4H2,1-2H3
**InchiKey:** MMRQLDRBAXLMRH-UHFFFAOYSA-N
**Formula:** C6H11N
**SMILES:** CCC(C)CC#N
**Mol. weight [g/mol]:** 97.16
**CAS:** 21101-88-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.4110 | | Cheméo Relay (1.0) |
| gf | 130.38 | kJ/mol | Joback Method |
| hf | -18.92 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 9.28 | kJ/mol | Joback Method |
| hvap | 43.39 | kJ/mol | Cheméo Relay (1.0) |
| ie | 10.84 | eV | Cheméo Relay (1.0) |
| log10ws | -1.96 | | Cheméo Relay (1.0) |
| logp | 1.946 | | Crippen Method |
| mcvol | 96.780 | ml/mol | McGowan Method |
| pc | 3049.04 | kPa | Joback Method |
| tb | 425.00 ± 3.00 | K | NIST Webbook |
| tc | 605.76 | K | Cheméo Relay (1.0) |
| tf | 169.64 | K | Cheméo Relay (1.0) |
| vc | 0.347 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 189.99 | J/mol×K | 438.32 | Joback Method |
| cpg | 199.58 | J/mol×K | 470.54 | Joback Method |
| cpg | 208.77 | J/mol×K | 502.76 | Joback Method |
| cpg | 217.55 | J/mol×K | 534.97 | Joback Method |
| cpg | 225.93 | J/mol×K | 567.19 | Joback Method |
| cpg | 233.94 | J/mol×K | 599.41 | Joback Method |
| cpg | 241.57 | J/mol×K | 631.63 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.45973e+01 |
| Coeff. B | -3.64611e+03 |
| Coeff. C | -5.96200e+01 |
| Temperature range (K), min. | 314.42 |
| Temperature range (K), max. | 452.27 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C21101882&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |