# 2,5-DIMETHYLPYRIDINE

**Other names:** 2,5-Lutidine
5-methyl-2-methylpyridine
**Inchi:** InChI=1S/C7H9N/c1-6-3-4-7(2)8-5-6/h3-5H,1-2H3
**InchiKey:** XWKFPIODWVPXLX-UHFFFAOYSA-N
**Formula:** C7H9N
**SMILES:** Cc1ccc(C)nc1
**Mol. weight [g/mol]:** 107.16
**CAS:** 589-93-5

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3411 | | Cheméo Relay (1.0) |
| affp | 958.80 | kJ/mol | NIST Webbook |
| basg | 926.90 | kJ/mol | NIST Webbook |
| chl | -4059.40 | kJ/mol | NIST Webbook |
| dm | 2.20 | debye | KDB |
| gf | 166.21 | kJ/mol | Cheméo Relay (1.0, beta) |
| hf | 66.44 | kJ/mol | KDB |
| hf | 66.40 | kJ/mol | NIST Webbook |
| hfl | 18.60 | kJ/mol | NIST Webbook |
| hvap | 47.82 | kJ/mol | NIST Webbook |
| ie | 8.80 ± 0.05 | eV | NIST Webbook |
| log10ws | 0.40 | | Aqueous Solubility Prediction Method |
| logp | 1.698 | | Crippen Method |
| mcvol | 95.710 | ml/mol | McGowan Method |
| pc | 4313.13 | kPa | Cheméo Relay (1.0, beta) |
| rinpol | 909.20 | | NIST Webbook |
| rinpol | 915.00 | | NIST Webbook |
| rinpol | 936.00 | | NIST Webbook |
| rinpol | 913.00 | | NIST Webbook |
| rinpol | 926.00 | | NIST Webbook |
| rinpol | 919.10 | | NIST Webbook |
| rinpol | 928.00 | | NIST Webbook |
| rinpol | 936.00 | | NIST Webbook |
| rinpol | 926.00 | | NIST Webbook |
| rinpol | 928.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 916.00 | | NIST Webbook |
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| rinpol | 917.00 | | NIST Webbook |
| rinpol | 909.20 | | NIST Webbook |
| rinpol | 915.00 | | NIST Webbook |
| rinpol | 919.00 | | NIST Webbook |
| rinpol | 930.00 | | NIST Webbook |
| rinpol | 903.20 | | NIST Webbook |
| rinpol | 919.10 | | NIST Webbook |
| rinpol | 920.00 | | NIST Webbook |
| rinpol | 921.00 | | NIST Webbook |
| rinpol | 917.00 | | NIST Webbook |
| rinpol | 912.00 | | NIST Webbook |
| rinpol | 926.00 | | NIST Webbook |
| rinpol | 913.00 | | NIST Webbook |
| rinpol | 911.00 | | NIST Webbook |
| rinpol | 912.00 | | NIST Webbook |
| rinpol | 912.00 | | NIST Webbook |
| rinpol | 913.00 | | NIST Webbook |
| rinpol | 946.00 | | NIST Webbook |
| ripol | 1330.00 | | NIST Webbook |
| ripol | 1371.00 | | NIST Webbook |
| ripol | 1326.00 | | NIST Webbook |
| ripol | 1412.00 | | NIST Webbook |
| ripol | 1325.00 | | NIST Webbook |
| ripol | 1330.00 | | NIST Webbook |
| ripol | 1335.00 | | NIST Webbook |
| ripol | 1332.00 | | NIST Webbook |
| ripol | 1329.00 | | NIST Webbook |
| ripol | 1415.00 | | NIST Webbook |
| ripol | 1373.00 | | NIST Webbook |
| ripol | 1372.00 | | NIST Webbook |
| ripol | 1325.00 | | NIST Webbook |
| ripol | 1395.00 | | NIST Webbook |
| ripol | 1370.00 | | NIST Webbook |
| ripol | 1371.00 | | NIST Webbook |
| ripol | 1329.00 | | NIST Webbook |
| sl | 248.81 | J/mol×K | NIST Webbook |
| tb | 426.25 ± 1.50 | K | NIST Webbook |
| tb | 429.15 ± 2.00 | K | NIST Webbook |
| tb | 430.16 | K | KDB |
| tb | 431.20 | K | NIST Webbook |
| tb | 429.90 ± 0.30 | K | NIST Webbook |
| tb | 426.65 ± 3.00 | K | NIST Webbook |

| | | | |
|---|---|---|---|
| tc | 644.15 ± 1.00 | K | NIST Webbook |
| tc | 644.16 ± 0.30 | K | NIST Webbook |
| tc | 644.20 | K | KDB |
| tf | 257.15 ± 0.50 | K | NIST Webbook |
| tf | 257.61 ± 0.03 | K | NIST Webbook |
| tf | 259.07 | K | NIST Webbook |
| tf | 257.00 | K | KDB |
| tt | 259.07 ± 0.01 | K | NIST Webbook |
| vc | 0.357 | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpl | 184.70 | J/mol×K | 298.15 | NIST Webbook |
| hfust | 14.64 | kJ/mol | 259.10 | NIST Webbook |
| hfust | 14.64 | kJ/mol | 259.10 | NIST Webbook |
| hvapt | 44.40 | kJ/mol | 400.50 | NIST Webbook |
| hvapt | 41.90 | kJ/mol | 400.50 | NIST Webbook |
| hvapt | 39.40 | kJ/mol | 400.50 | NIST Webbook |
| hvapt | 36.50 | kJ/mol | 400.50 | NIST Webbook |
| hvapt | 42.80 | kJ/mol | 394.50 | NIST Webbook |
| rhol | 938.00 | kg/m3 | 273.00 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.46024e+01 |
| Coeff. B | -3.69877e+03 |
| Coeff. C | -6.07320e+01 |
| Temperature range (K), min. | 319.12 |
| Temperature range (K), max. | 458.84 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |

| | |
|---|---|
| Coeff. A | 9.69764e+01 |
| Coeff. B | -8.86176e+03 |
| Coeff. C | -1.20654e+01 |
| Coeff. D | 7.61858e-06 |
| Temperature range (K), min. | 350.00 |
| Temperature range (K), max. | 435.00 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C589935&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Cheméo Relay (1.0, beta):** | |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1356 |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1356.mol |
| **Cheméo Relay (1.0):** | |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpl:** | Liquid phase heat capacity |
| **dm:** | Dipole Moment |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |