# 2,6-Lutidine

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|---|---|
| **Other names:** | 2,6-Dimethylpyridine |
| | 2,6-Dimethypyridine |
| | NSC 2155 |
| | Pyridine, 2,6-dimethyl- |
| | «alpha»,«alpha»'-Dimethylpyridine |
| | «alpha»,«alpha»'-Lutidin |
| | «alpha»,«alpha»'-Lutidine |
| | Â«alphaÂ»,Â«alphaÂ»'-Dimethylpyridine |
| | Â«alphaÂ»,Â«alphaÂ»'-Lutidin |
| | Â«alphaÂ»,Â«alphaÂ»'-Lutidine |
| **Inchi:** | InChI=1S/C7H9N/c1-6-4-3-5-7(2)8-6/h3-5H,1-2H3 |
| **InchiKey:** | OISVCGZHLKNMSJ-UHFFFAOYSA-N |
| **Formula:** | C7H9N |
| **SMILES:** | Cc1cccc(C)n1 |
| **Mol. weight [g/mol]:** | 107.15 |
| **CAS:** | 108-48-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 963.00 | kJ/mol | NIST Webbook |
| basg | 931.10 | kJ/mol | NIST Webbook |
| chl | -4053.50 | kJ/mol | NIST Webbook |
| dm | 1.70 | debye | KDB |
| hf | 56.10 ± 1.50 | kJ/mol | NIST Webbook |
| hf | 58.70 | kJ/mol | NIST Webbook |
| hfl | 12.60 | kJ/mol | NIST Webbook |
| hvap | 45.38 | kJ/mol | NIST Webbook |
| hvap | 46.06 | kJ/mol | NIST Webbook |
| hvap | 45.30 | kJ/mol | NIST Webbook |
| hvap | 45.90 ± 2.40 | kJ/mol | NIST Webbook |
| hvap | 46.40 | kJ/mol | NIST Webbook |
| ie | 8.86 ± 0.03 | eV | NIST Webbook |
| ie | 9.23 ± 0.05 | eV | NIST Webbook |
| ie | 9.23 | eV | NIST Webbook |
| ie | 8.87 | eV | NIST Webbook |
| ie | 8.90 ± 0.05 | eV | NIST Webbook |
| ie | 8.85 ± 0.02 | eV | NIST Webbook |

| | | | |
|---|---|---|---|
| log10ws | 0.45 | | Aqueous Solubility Prediction Method |
| log10ws | 0.45 | | Estimated Solubility Method |
| logp | 1.698 | | Crippen Method |
| mcvol | 95.710 | ml/mol | McGowan Method |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 846.00 | | NIST Webbook |
| rinpol | 870.10 | | NIST Webbook |
| rinpol | 857.00 | | NIST Webbook |
| rinpol | 857.00 | | NIST Webbook |
| rinpol | 882.00 | | NIST Webbook |
| rinpol | 869.00 | | NIST Webbook |
| rinpol | 869.00 | | NIST Webbook |
| rinpol | 136.27 | | NIST Webbook |
| rinpol | 865.80 | | NIST Webbook |
| rinpol | 876.00 | | NIST Webbook |
| rinpol | 868.00 | | NIST Webbook |
| rinpol | 844.00 | | NIST Webbook |
| rinpol | 868.30 | | NIST Webbook |
| rinpol | 887.20 | | NIST Webbook |
| rinpol | 890.00 | | NIST Webbook |
| rinpol | 874.00 | | NIST Webbook |
| rinpol | 884.00 | | NIST Webbook |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 859.20 | | NIST Webbook |
| rinpol | 884.95 | | NIST Webbook |
| rinpol | 865.80 | | NIST Webbook |
| rinpol | 850.00 | | NIST Webbook |
| rinpol | 852.00 | | NIST Webbook |
| rinpol | 868.00 | | NIST Webbook |
| rinpol | 880.00 | | NIST Webbook |
| rinpol | 863.80 | | NIST Webbook |
| rinpol | 903.00 | | NIST Webbook |
| rinpol | 866.00 | | NIST Webbook |
| rinpol | 868.00 | | NIST Webbook |
| rinpol | 866.00 | | NIST Webbook |
| rinpol | 866.00 | | NIST Webbook |
| rinpol | 866.00 | | NIST Webbook |
| rinpol | 866.00 | | NIST Webbook |
| rinpol | 876.00 | | NIST Webbook |
| rinpol | 852.00 | | NIST Webbook |
| rinpol | 869.00 | | NIST Webbook |
| rinpol | 874.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 887.20 | | NIST Webbook |
| rinpol | 857.00 | | NIST Webbook |
| rinpol | 872.00 | | NIST Webbook |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 872.00 | | NIST Webbook |
| ripol | 1276.00 | | NIST Webbook |
| ripol | 1282.00 | | NIST Webbook |
| ripol | 1300.00 | | NIST Webbook |
| ripol | 1280.00 | | NIST Webbook |
| ripol | 1285.00 | | NIST Webbook |
| ripol | 1257.00 | | NIST Webbook |
| ripol | 1288.00 | | NIST Webbook |
| ripol | 1243.00 | | NIST Webbook |
| ripol | 1253.00 | | NIST Webbook |
| ripol | 1258.00 | | NIST Webbook |
| ripol | 1255.00 | | NIST Webbook |
| ripol | 1243.00 | | NIST Webbook |
| ripol | 1241.00 | | NIST Webbook |
| ripol | 1243.00 | | NIST Webbook |
| ripol | 1245.00 | | NIST Webbook |
| ripol | 1266.00 | | NIST Webbook |
| ripol | 1271.00 | | NIST Webbook |
| ripol | 1245.00 | | NIST Webbook |
| ripol | 1245.00 | | NIST Webbook |
| ripol | 1245.00 | | NIST Webbook |
| ripol | 1246.00 | | NIST Webbook |
| ripol | 1246.00 | | NIST Webbook |
| ripol | 1241.00 | | NIST Webbook |
| ripol | 1245.00 | | NIST Webbook |
| sl | 244.24 | J/mol×K | NIST Webbook |
| tb | 417.30 ± 0.30 | K | NIST Webbook |
| tb | 417.20 | K | NIST Webbook |
| tb | 417.30 | K | NIST Webbook |
| tb | 417.23 ± 0.25 | K | NIST Webbook |
| tb | 417.25 ± 0.30 | K | NIST Webbook |
| tb | 417.15 ± 0.20 | K | NIST Webbook |
| tb | 417.20 | K | KDB |
| tb | 417.15 ± 0.20 | K | NIST Webbook |
| tb | 417.19 ± 0.09 | K | NIST Webbook |
| tb | 415.15 ± 2.00 | K | NIST Webbook |
| tb | 417.65 ± 0.30 | K | NIST Webbook |
| tb | 414.40 ± 1.00 | K | NIST Webbook |
| tb | 417.21 ± 0.10 | K | NIST Webbook |
| tb | 417.21 ± 0.10 | K | NIST Webbook |

| | | | |
|---|---|---|---|
| tb | 417.17 ± 0.06 | K | NIST Webbook |
| tb | 415.90 ± 0.30 | K | NIST Webbook |
| tb | 417.15 ± 0.30 | K | NIST Webbook |
| tb | 416.56 ± 0.30 | K | NIST Webbook |
| tb | 417.15 ± 0.40 | K | NIST Webbook |
| tb | 417.85 ± 0.60 | K | NIST Webbook |
| tb | 417.15 ± 0.60 | K | NIST Webbook |
| tb | 417.15 ± 0.40 | K | NIST Webbook |
| tb | 413.65 ± 1.50 | K | NIST Webbook |
| tb | 410.70 ± 0.60 | K | NIST Webbook |
| tb | 416.35 ± 0.80 | K | NIST Webbook |
| tb | 415.65 ± 1.00 | K | NIST Webbook |
| tb | 446.15 ± 1.00 | K | NIST Webbook |
| tc | 623.80 | K | NIST Webbook |
| tc | 623.80 | K | KDB |
| tc | 623.75 ± 0.20 | K | NIST Webbook |
| tf | 267.08 ± 0.10 | K | NIST Webbook |
| tf | 266.78 | K | Aqueous Solubility Prediction Method |
| tf | 266.45 ± 0.30 | K | NIST Webbook |
| tf | 278.90 ± 0.30 | K | NIST Webbook |
| tf | 267.05 ± 0.06 | K | NIST Webbook |
| tf | 267.00 | K | KDB |
| tf | 266.41 ± 0.35 | K | NIST Webbook |
| tf | 267.15 ± 0.20 | K | NIST Webbook |
| tf | 266.65 ± 0.50 | K | NIST Webbook |
| tf | 267.65 ± 0.20 | K | NIST Webbook |
| tf | 267.25 ± 0.30 | K | NIST Webbook |
| tf | 267.05 ± 0.06 | K | NIST Webbook |
| tt | 267.03 ± 0.01 | K | NIST Webbook |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpl | 185.17 | J/mol×K | 298.15 | NIST Webbook |
| hfust | 13.04 | kJ/mol | 267.10 | NIST Webbook |
| hvapt | 40.80 | kJ/mol | 368.00 | NIST Webbook |
| hvapt | 36.00 | kJ/mol | 386.00 | NIST Webbook |
| hvapt | 38.80 | kJ/mol | 386.00 | NIST Webbook |
| hvapt | 41.40 | kJ/mol | 386.00 | NIST Webbook |
| hvapt | 43.90 | kJ/mol | 386.00 | NIST Webbook |

| | | | | |
|---|---|---|---|---|
| hvapt | 43.70 | kJ/mol | 330.50 | NIST Webbook |
| hvapt | 37.46 | kJ/mol | 417.30 | NIST Webbook |
| hvapt | 45.00 | kJ/mol | 356.00 | NIST Webbook |
| hvapt | 41.60 | kJ/mol | 385.00 | NIST Webbook |
| hvapt | 46.10 | kJ/mol | 312.50 | NIST Webbook |
| hvapt | 44.40 | kJ/mol | 313.00 | NIST Webbook |
| hvapt | 42.50 | kJ/mol | 343.00 | NIST Webbook |
| pvap | 8.10 | kPa | 343.20 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |
| pvap | 1.88 | kPa | 313.27 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |
| pvap | 3.16 | kPa | 323.24 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |
| pvap | 5.14 | kPa | 333.21 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |

| | | | | |
|---|---|---|---|---|
| pvap | 1.07 | kPa | 303.27 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |
| pvap | 12.23 | kPa | 353.14 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |
| pvap | 0.79 | kPa | 298.30 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |
| pvap | 0.58 | kPa | 293.30 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |
| pvap | 0.42 | kPa | 288.33 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |

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|---|---|---|---|---|
| pvap | 0.30 | kPa | 283.37 | Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction |
| pvap | 12.31 | kPa | 353.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| pvap | 8.07 | kPa | 343.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| pvap | 5.13 | kPa | 333.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| pvap | 3.15 | kPa | 323.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| pvap | 1.87 | kPa | 313.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |

| | | | | |
|---|---|---|---|---|
| pvap | 1.06 | kPa | 303.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| pvap | 0.57 | kPa | 293.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| pvap | 0.30 | kPa | 283.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| pvap | 0.14 | kPa | 273.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| pvap | 0.07 | kPa | 263.15 | Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction |
| rhol | 918.19 | kg/m3 | 298.15 | Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating-Tube Densimetry |

| | | | | |
|---|---|---|---|---|
| rhol | 922.44 | kg/m3 | 293.15 | Viscosity of Associated Mixtures Approximated by the Grunberg-Nissan Model |
| rhol | 923.00 | kg/m3 | 298.00 | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.46861e+01 |
| Coeff. B | -3.62307e+03 |
| Coeff. C | -5.71320e+01 |
| Temperature range (K), min. | 308.76 |
| Temperature range (K), max. | 443.61 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 1.02873e+02 |
| Coeff. B | -9.01515e+03 |
| Coeff. C | -1.29258e+01 |
| Coeff. D | 7.73468e-06 |
| Temperature range (K), min. | 267.00 |
| Temperature range (K), max. | 623.75 |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C108485&Units=SI

**KDB Vapor Pressure Data:** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1357

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol1357.mol

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**KDB Pure (Korean Thermophysical Properties Databank):** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1357

| | |
|---|---|
| **Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating Tube Densimetry.** | https://www.doi.org/10.1021/je200093f |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction:** | https://www.doi.org/10.1016/j.fluid.2005.11.016 |
| **Mesoscale solubilization and critical phenomena in binary and quasi-binary solutions of hydrotropes:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Toward an inherently safer alternative for operating N-oxidation of alkylpyridines. Effect of N-oxide on lutidine–water phase separation:** | https://www.doi.org/10.1016/j.fluid.2015.06.030 |
| **Vapour pressures and excess functions of (3,5- 2,6-dimethylpyridine + n-hexane, n-heptane and n-octane measurement and prediction:** | https://www.doi.org/10.1016/j.tca.2017.08.007 |
| **Viscosity of Associated Mixtures. Approximated by the Grunberg-Nissan Model:** | https://www.doi.org/10.1016/j.fluid.2005.03.028 |
| **Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction:** | https://www.doi.org/10.1007/s10765-011-1100-1 |
| | https://www.doi.org/10.1016/j.fluid.2014.04.004 |

# Legend

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|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpl:** | Liquid phase heat capacity |
| **dm:** | Dipole Moment |
| **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 |
| **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 |

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