Pyridine, 2,6-dimethyl-

Other names:	2,6-Dimethypyridine
	2,6-dimethylpyridine
	2,6-lutidine
	NSC 2155
	«alpha»,«alpha»'-Dimethylpyridine
	«alpha»,«alpha»'-Lutidin
	«alpha»,«alpha»'-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]:	107.16
CAS:	108-48-5

Physical Properties

Property code	Value	Unit	Source
af	0.3321		Cheméo Relay (1.0)
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
gf	157.52	kJ/mol	Cheméo Relay (1.0, beta)
hf	58.70	kJ/mol	NIST Webbook
hf	56.10 ± 1.50	kJ/mol	NIST Webbook
hfl	12.60	kJ/mol	NIST Webbook
hvap	46.40	kJ/mol	NIST Webbook
hvap	46.06	kJ/mol	NIST Webbook
hvap	45.38	kJ/mol	NIST Webbook
hvap	45.90 ± 2.40	kJ/mol	NIST Webbook
hvap	45.30	kJ/mol	NIST Webbook
ie	8.85 ± 0.02	eV	NIST Webbook
ie	8.86 ± 0.03	eV	NIST Webbook
ie	8.90 ± 0.05	eV	NIST Webbook
ie	8.87	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.23 ± 0.05	eV	NIST Webbook

log10ws	0.45		Estimated Solubility Method
log10ws	0.45		Aqueous Solubility Prediction Method
logp	1.698		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	4344.63	kPa	Cheméo Relay (1.0, beta)
rinpol	868.30		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	136.27		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	887.20		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	869.00		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	868.00		NIST Webbook
rinpol	866.00		NIST Webbook
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rinpol	876.00		NIST Webbook

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rinpol	869.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	870.10		NIST Webbook
ripol	1245.00		NIST Webbook
ripol	1258.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1243.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1271.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1245.00		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	1245.00		NIST Webbook
ripol	1245.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1241.00		NIST Webbook
sl	244.24	J/mol×K	NIST Webbook
tb	417.15 ± 0.60	K	NIST Webbook
tb	417.19 ± 0.09	K	NIST Webbook
tb	417.20	K	KDB
tb	417.15 ± 0.20	K	NIST Webbook
tb	417.30 ± 0.30	K	NIST Webbook
tb	417.15 ± 0.20	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	417.20	K	NIST Webbook
tb	417.30	K	NIST Webbook
tb	417.15 ± 0.40	K	NIST Webbook
tb	417.85 ± 0.60	K	NIST Webbook
tb	415.65 ± 1.00	K	NIST Webbook
tb	417.25 ± 0.30	K	NIST Webbook
tb	417.23 ± 0.25	K	NIST Webbook
tb	446.15 ± 1.00	K	NIST Webbook
tb	416.35 ± 0.80	K	NIST Webbook
tb	410.70 ± 0.60	K	NIST Webbook
tb	413.65 ± 1.50	K	NIST Webbook
tb	417.15 ± 0.40	K	NIST Webbook
tc	623.75 ± 0.20	K	NIST Webbook
tc	623.80	K	KDB
tc	623.80	K	NIST Webbook
tf	266.41 ± 0.35	K	NIST Webbook
tf	267.05 ± 0.06	K	NIST Webbook
tf	267.00	K	KDB
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	267.25 ± 0.30	K	NIST Webbook
tf	267.08 ± 0.10	K	NIST Webbook
tf	267.65 ± 0.20	K	NIST Webbook
tf	267.15 ± 0.20	K	NIST Webbook
tf	266.65 ± 0.50	K	NIST Webbook
tt	267.03 ± 0.01	K	NIST Webbook
vc	0.352	m3/kmol	Cheméo Relay (1.0)

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	42.50	kJ/mol	343.00	NIST Webbook
hvapt	44.40	kJ/mol	313.00	NIST Webbook

hvapt	46.10	kJ/mol	312.50	NIST Webbook
hvapt	41.60	kJ/mol	385.00	NIST Webbook
hvapt	45.00	kJ/mol	356.00	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
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	0.07	kPa	263.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement 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	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	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	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	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

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

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1357
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Viscosity of Associated Mixtures Approximated by the Grunberg-Nissan Model:	https://www.doi.org/10.1007/s10765-011-1100-1
Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane: Measurements and prediction:	https://www.doi.org/10.1016/j.fluid.2014.04.004
Mesoscale solubilization and critical phenomena in binary and quasi binary [bmim][PF6] ionic liquid mixtures:	https://www.doi.org/10.1016/j.fluid.2015.06.030
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108485&Units=SI
Chemeo Relay (1.0):	
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1357.mol
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
Chemeo Relay (1.0, beta):	
Vapour pressures and excess functions of (3,5- 2,6-dimethylpyridine + n-hexane, n-heptane and n-octane:	https://www.doi.org/10.1016/j.fluid.2005.03.028
Thermodynamic interactions of hydrogen bonding of amines in methanol: head space analysis and solution calorimetry:	https://www.doi.org/10.1016/j.tca.2012.02.005
Critical Point and Acentric Factor Prediction:	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.tca.2017.08.007
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Association in Dilute Aqueous Solution of Pyridine and Its Methyl Derivatives Studied by Cryoscopic Method:	https://www.doi.org/10.1007/s10765-010-0792-y
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurements of heat capacities and turbidities for binary mixtures {water + 2,6-dimethylpyridine} and {water, or heavy water + 2,6-dimethylpiperidine} in the critical regions:	https://www.doi.org/10.1016/j.fluid.2015.10.027

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