Pyridine, 2,4-dimethyl-

Other names:	2,4-Dimethylpyridine
	2,4-LUTIDINE
	2,4-Lutidene
	«alpha»,«gamma»-Dimethylpyridine
	Â«alphaÂ»,Â«gammaÂ»-Dimethylpyridine
Inchi:	InChI=1S/C7H9N/c1-6-3-4-8-7(2)5-6/h3-5H,1-2H3
InchiKey:	JYYNAJVZFGKDEQ-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	Cc1ccnc(C)c1
Mol. weight [g/mol]:	107.15
CAS:	108-47-4

Physical Properties

Property code	Value	Unit	Source
affp	962.90	kJ/mol	NIST Webbook
basg	930.80	kJ/mol	NIST Webbook
chl	-4056.90	kJ/mol	NIST Webbook
dm	2.30	debye	KDB
hf	63.90	kJ/mol	NIST Webbook
hfl	16.10	kJ/mol	NIST Webbook
hvap	47.49	kJ/mol	NIST Webbook
hvap	47.50	kJ/mol	NIST Webbook
hvap	47.78	kJ/mol	NIST Webbook
ie	8.85 ± 0.03	eV	NIST Webbook
log10ws	0.38		Estimated Solubility Method
log10ws	0.38		Aqueous Solubility Prediction Method
logp	1.698		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
rinpol	919.50		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	903.90		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	916.00		NIST Webbook

rinpol	903.40		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	941.30		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	918.70		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	145.96		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	917.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1342.00		NIST Webbook
sl	248.50	J/mol×K	NIST Webbook
tb	431.60	K	KDB

tc	647.00	K	NIST Webbook
tc	647.15 ± 1.50	K	NIST Webbook
tc	647.00	K	KDB
tf	209.19 ± 0.03	K	NIST Webbook
tf	205.25 ± 0.50	K	NIST Webbook
tf	209.15	K	KDB
tf	209.41	K	NIST Webbook
tf	205.20 ± 1.00	K	NIST Webbook
tt	209.35 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	184.76	J/mol×K	298.15	NIST Webbook
hfust	8.82	kJ/mol	209.40	NIST Webbook
hfust	8.82	kJ/mol	209.40	NIST Webbook
hvapt	37.00	kJ/mol	402.00	NIST Webbook
hvapt	45.50	kJ/mol	330.50	NIST Webbook
hvapt	44.80	kJ/mol	402.00	NIST Webbook
hvapt	42.30	kJ/mol	402.00	NIST Webbook
hvapt	39.80	kJ/mol	402.00	NIST Webbook
hvapt	38.53	kJ/mol	431.60	NIST Webbook
hvapt	47.10	kJ/mol	364.50	NIST Webbook
hvapt	43.50	kJ/mol	391.00	NIST Webbook
hvapt	47.50	kJ/mol	312.50	NIST Webbook
hvapt	46.50	kJ/mol	313.00	NIST Webbook
hvapt	44.60	kJ/mol	343.00	NIST Webbook
hvapt	43.90	kJ/mol	368.00	NIST Webbook
rhol	949.00	kg/m3	273.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47499e+01
Coeff. B	-3.74747e+03
Coeff. C	-6.11210e+01

Temperature range (K), min.	320.24
Temperature range (K), max.	458.16

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.42387e-01
Coeff. B	-4.91659e+03
Coeff. C	2.70817e+00
Coeff. D	-7.32161e-06
Temperature range (K), min.	418.00
Temperature range (K), max.	438.00

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1355.mol

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C108474&Units=SI

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1355

Legend

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