Pyridine, 3,4-dimethyl-

Other names:	3,4-Dimethylpyridine
	3,4-LUTIDINE
	3,4-Lutidene
Inchi:	InChI=1S/C7H9N/c1-6-3-4-8-5-7(6)2/h3-5H,1-2H3
InchiKey:	NURQLCJSMXZBPC-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	Cc1ccncc1C
Mol. weight [g/mol]:	107.15
CAS:	583-58-4

Physical Properties

Property code	Value	Unit	Source
affp	957.30	kJ/mol	NIST Webbook
basg	925.50	kJ/mol	NIST Webbook
chl	-4059.10	kJ/mol	NIST Webbook
dm	1.90	debye	KDB
hf	70.05	kJ/mol	KDB
hf	70.00	kJ/mol	NIST Webbook
hfl	18.20	kJ/mol	NIST Webbook
hvap	50.54	kJ/mol	NIST Webbook
hvap	51.80	kJ/mol	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
log10ws	0.36		Estimated Solubility Method
log10ws	0.36		Aqueous Solubility Prediction Method
logp	1.698		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
rinpol	161.12		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1001.30		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	999.00		NIST Webbook

rinpol	1001.30		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	986.20		NIST Webbook
rinpol	982.80		NIST Webbook
rinpol	986.20		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1040.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1471.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1473.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1441.00		NIST Webbook
sl	240.72	J/mol×K	NIST Webbook
tb	452.30	K	NIST Webbook
tb	436.70	K	NIST Webbook
tb	452.28	K	KDB
tc	683.80	K	NIST Webbook
tc	683.80	K	KDB
tc	683.71 ± 0.40	K	NIST Webbook
tc	683.75 ± 1.00	K	NIST Webbook
tf	260.65	K	NIST Webbook
tf	262.03	K	KDB
tf	262.11 ± 0.05	K	NIST Webbook
tt	262.70 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	191.84	J/mol×K	298.15	NIST Webbook

cpl	196.00	J/mol×K	298.00	NIST Webbook
hfust	14.70	kJ/mol	262.70	NIST Webbook
hfust	14.70	kJ/mol	262.70	NIST Webbook
hvapt	45.90	kJ/mol	368.00	NIST Webbook
hvapt	39.99	kJ/mol	452.30	NIST Webbook
hvapt	47.60	kJ/mol	355.00	NIST Webbook
hvapt	46.60	kJ/mol	418.00	NIST Webbook
hvapt	44.20	kJ/mol	418.00	NIST Webbook
hvapt	41.70	kJ/mol	418.00	NIST Webbook
hvapt	39.00	kJ/mol	418.00	NIST Webbook
hvapt	44.80	kJ/mol	419.50	NIST Webbook
hvapt	48.80	kJ/mol	328.00	NIST Webbook
hvapt	47.60	kJ/mol	343.00	NIST Webbook
rhol	954.00	kg/m3	298.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63197e+01
Coeff. B	-4.32747e+03
Coeff. C	-6.68750e+01
Temperature range (K), min.	336.80
Temperature range (K), max.	459.99

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.13976e+02
Coeff. B	-1.00446e+04
Coeff. C	-1.45520e+01
Coeff. D	8.92937e-06
Temperature range (K), min.	274.15
Temperature range (K), max.	494.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C583584&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=1358
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1358.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

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

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