Pyridine, 2,5-dimethyl-

Other names:	2,5-Dimethylpyridine
	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]:	107.15
CAS:	589-93-5

Physical Properties

Property code	Value	Unit	Source
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
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
rinpol	926.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	919.10		NIST Webbook
rinpol	909.20		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	903.20		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook

rinpol	909.20		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	912.00		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	917.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	926.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1325.00		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	1370.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1330.00		NIST Webbook
sl	248.81	J/mol×K	NIST Webbook
tb	430.16	K	KDB
tb	429.90 ± 0.30	K	NIST Webbook
tb	426.25 ± 1.50	K	NIST Webbook
tb	429.15 ± 2.00	K	NIST Webbook
tb	426.65 ± 3.00	K	NIST Webbook
tb	431.20	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	257.61 ± 0.03	K	NIST Webbook
tf	257.00	K	KDB
tf	259.07	K	NIST Webbook
tf	257.15 ± 0.50	K	NIST Webbook
tt	259.07 ± 0.01	K	NIST Webbook

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
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=1356
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1356.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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