Pyridine, 2,3-dimethyl-

Other names: 2,3-Dimethylpyridine
2,3-LUTIDINE
Inchi: InChI=1S/C7H9N/c1-6-4-3-5-8-7(6)2/h3-5H,1-2H3
InchiKey: HPYNZHMRTTWQTB-UHFFFAOYSA-N
Formula: C7H9N
SMILES: Cc1cccnc1C
Mol. weight [g/mol]: 107.15
CAS: 583-61-9

Physical Properties

Property code	Value	Unit	Source
affp	958.90	kJ/mol	NIST Webbook
basg	927.00	kJ/mol	NIST Webbook
chl	-4060.20	kJ/mol	NIST Webbook
dm	2.20	debye	KDB
hf	68.30	kJ/mol	NIST Webbook
hf	68.29	kJ/mol	KDB
hfl	19.30	kJ/mol	NIST Webbook
hvap	47.74	kJ/mol	NIST Webbook
hvap	48.95	kJ/mol	NIST Webbook
hvap	47.60	kJ/mol	NIST Webbook
hvap	52.00 ± 0.60	kJ/mol	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	8.85 ± 0.02	eV	NIST Webbook
log10ws	0.38		Aqueous Solubility Prediction Method
log10ws	0.38		Estimated Solubility Method
logp	1.698		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
rinpol	953.00		NIST Webbook
rinpol	933.90		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	924.00		NIST Webbook

rinpol	925.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	934.30		NIST Webbook
rinpol	923.40		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	952.20		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	933.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1407.00		NIST Webbook
sl	243.70	J/mol×K	NIST Webbook
tb	433.40 ± 0.50	K	NIST Webbook
tb	434.41	K	KDB
tb	436.70	K	NIST Webbook
tb	434.40	K	NIST Webbook
tb	433.60 ± 1.00	K	NIST Webbook
tb	430.75 ± 1.00	K	NIST Webbook
tc	655.45 ± 0.30	K	NIST Webbook
tc	655.45 ± 1.00	K	NIST Webbook
tc	655.40	K	KDB
tc	655.40	K	NIST Webbook
tf	257.93 ± 0.03	K	NIST Webbook
tf	257.88	K	KDB
tf	258.35 ± 0.30	K	NIST Webbook
tt	258.57 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	189.55	J/mol×K	298.15	NIST Webbook
hfust	13.48	kJ/mol	258.60	NIST Webbook
hfust	13.48	kJ/mol	258.60	NIST Webbook
hvapt	46.90	kJ/mol	313.00	NIST Webbook
hvapt	37.40	kJ/mol	402.00	NIST Webbook
hvapt	43.00	kJ/mol	404.00	NIST Webbook
hvapt	40.20	kJ/mol	402.00	NIST Webbook
hvapt	45.00	kJ/mol	343.00	NIST Webbook
hvapt	43.50	kJ/mol	368.00	NIST Webbook
hvapt	42.70	kJ/mol	402.00	NIST Webbook
hvapt	45.20	kJ/mol	402.00	NIST Webbook
hvapt	39.08	kJ/mol	434.40	NIST Webbook
rhol	942.00	kg/m3	298.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44984e+01
Coeff. B	-3.70307e+03
Coeff. C	-6.18990e+01
Temperature range (K), min.	322.48
Temperature range (K), max.	464.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.39525e+01
Coeff. B	-7.61891e+03
Coeff. C	-6.94364e+00
Coeff. D	2.02753e-06
Temperature range (K), min.	372.15
Temperature range (K), max.	440.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1354
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1354.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=C583619&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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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