Pyridine, 3,5-dimethyl-

Other names:	3,5-Dimethylpyridine
	3,5-LUTIDINE
Inchi:	InChI=1S/C7H9N/c1-6-3-7(2)5-8-4-6/h3-5H,1-2H3
InchiKey:	HWWYDZCSSYKIAD-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	Cc1cncc(C)c1
Mol. weight [g/mol]:	107.15
CAS:	591-22-0

Physical Properties

Property code	Value	Unit	Source
affp	955.40	kJ/mol	NIST Webbook
basg	923.50	kJ/mol	NIST Webbook
chl	-4063.20	kJ/mol	NIST Webbook
dm	2.60	debye	KDB
hf	72.80	kJ/mol	NIST Webbook
hf	72.81	kJ/mol	KDB
hfl	22.40	kJ/mol	NIST Webbook
hvap	50.38	kJ/mol	NIST Webbook
hvap	48.70	kJ/mol	NIST Webbook
hvap	48.50	kJ/mol	NIST Webbook
hvap	49.49	kJ/mol	NIST Webbook
ie	9.25	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	957.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	155.01		NIST Webbook

rinpol	917.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	961.40		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	980.50		NIST Webbook
rinpol	978.90		NIST Webbook
rinpol	947.40		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	957.70		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	957.70		NIST Webbook
rinpol	963.50		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1415.00		NIST Webbook
sl	241.72	J/mol×K	NIST Webbook
tb	445.10	K	NIST Webbook
tb	444.60 ± 0.50	K	NIST Webbook
tb	445.00	K	KDB
tb	442.70	K	NIST Webbook
tb	444.80	K	NIST Webbook
tc	667.25 ± 1.00	K	NIST Webbook
tc	667.25 ± 0.30	K	NIST Webbook
tc	667.20	K	NIST Webbook
tc	667.20	K	KDB
tf	266.82	K	NIST Webbook
tf	265.35	K	Aqueous Solubility Prediction Method
tf	266.50	K	KDB
tf	266.85 ± 0.30	K	NIST Webbook
tf	266.65 ± 0.02	K	NIST Webbook

tt	266.81 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	184.55	J/mol×K	298.15	NIST Webbook
hfust	13.11	kJ/mol	266.90	NIST Webbook
hfust	13.11	kJ/mol	266.90	NIST Webbook
hvapt	41.80	kJ/mol	411.00	NIST Webbook
hvapt	47.00	kJ/mol	340.00	NIST Webbook
hvapt	46.70	kJ/mol	411.00	NIST Webbook
hvapt	44.30	kJ/mol	411.00	NIST Webbook
hvapt	39.46	kJ/mol	445.10	NIST Webbook
hvapt	39.20	kJ/mol	411.00	NIST Webbook
hvapt	44.30	kJ/mol	409.50	NIST Webbook
hvapt	49.10	kJ/mol	315.50	NIST Webbook
hvapt	49.60	kJ/mol	313.00	NIST Webbook
hvapt	46.50	kJ/mol	343.00	NIST Webbook
hvapt	44.80	kJ/mol	368.00	NIST Webbook
pvap	0.17	kPa	293.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction
pvap	0.04	kPa	273.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction
pvap	0.08	kPa	283.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction

pvap	0.02	kPa	263.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction
pvap	0.33	kPa	303.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction
pvap	0.60	kPa	313.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction
pvap	1.05	kPa	323.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction
pvap	1.77	kPa	333.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction
pvap	2.90	kPa	343.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction
pvap	4.60	kPa	353.15	Isothermal vapour pressures and excess functions of 3,5- and 2,6-dimethylpyridine with toluene measurement and prediction

pvap	0.04	kPa	273.50	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction
pvap	0.09	kPa	283.45	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction
pvap	0.17	kPa	293.47	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction
pvap	0.33	kPa	303.54	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction
pvap	0.61	kPa	313.56	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction

pvap	1.08	kPa	323.59	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction
pvap	1.82	kPa	333.66	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction
pvap	2.97	kPa	343.62	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction
pvap	4.69	kPa	353.63	Isothermal vapour pressures and thermodynamic excess properties of 3,5- and 2,6-dimethylpyridine with cyclohexane. Measurements and prediction
rhol	939.00	kg/m3	298.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49416e+01
Coeff. B	-3.90039e+03
Coeff. C	-6.48740e+01
Temperature range (K), min.	331.04

Temperature range (K), max.	469.89

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.57116e+01
Coeff. B	-7.85524e+03
Coeff. C	-7.19996e+00
Coeff. D	2.34668e-06
Temperature range (K), min.	273.15
Temperature range (K), max.	487.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591220&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1359
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1359.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapour pressures and excess functions of (3,5; 2,6)dimethylpyridine + n-hexane, + n-heptane and + n-octane measurement and prediction:	https://www.doi.org/10.1016/j.fluid.2005.03.028
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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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https://www.chemeo.com/cid/46-353-9/Pyridine-3-5-dimethyl.pdf
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