

Pyridine, 2-methyl-

Other names:	.alpha.-picoline 2-Methylpyridine 2-PICOLINE ALPA-PICOLINE NSC 3409 Picoline, «alpha» Picoline, Â«alphaÂ» Rcra waste number U191 o-Methylpyridine o-Picoline «alpha»-Methylpyridine «alpha»-Picoline Â«alphaÂ»-Methylpyridine Â«alphaÂ»-Picoline
Inchi:	InChI=1S/C6H7N/c1-6-4-2-3-5-7-6/h2-5H,1H3
InchiKey:	BSKHPKMHTQYZBB-UHFFFAOYSA-N
Formula:	C6H7N
SMILES:	Cc1ccccn1
Mol. weight [g/mol]:	93.13
CAS:	109-06-8

Physical Properties

Property code	Value	Unit	Source
af	0.2990		KDB
affp	949.10	kJ/mol	NIST Webbook
basg	917.30	kJ/mol	NIST Webbook
chl	-3292.40	kJ/mol	NIST Webbook
chl	-3415.00	kJ/mol	NIST Webbook
chl	-3420.50 ± 1.30	kJ/mol	NIST Webbook
chl	-3418.00 ± 0.67	kJ/mol	NIST Webbook
dm	1.90	debye	KDB
gf	177.20	kJ/mol	KDB
hf	-26.50	kJ/mol	NIST Webbook
hf	102.00 ± 1.30	kJ/mol	NIST Webbook
hf	87.70	kJ/mol	NIST Webbook
hf	99.02	kJ/mol	KDB
hf	101.90 ± 1.30	kJ/mol	NIST Webbook

hf	98.95 ± 0.88	kJ/mol	NIST Webbook
hfl	45.27	kJ/mol	NIST Webbook
hfl	59.00 ± 1.30	kJ/mol	NIST Webbook
hfl	56.48 ± 0.75	kJ/mol	NIST Webbook
hfl	-68.99	kJ/mol	NIST Webbook
hvap	43.00	kJ/mol	NIST Webbook
hvap	42.50 ± 0.10	kJ/mol	NIST Webbook
hvap	42.51	kJ/mol	NIST Webbook
hvap	42.47	kJ/mol	NIST Webbook
hvap	42.50	kJ/mol	NIST Webbook
hvap	42.92	kJ/mol	NIST Webbook
hvap	42.51	kJ/mol	NIST Webbook
hvap	43.60	kJ/mol	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.37 ± 0.05	eV	NIST Webbook
ie	9.40 ± 0.10	eV	NIST Webbook
ie	9.02 ± 0.03	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.20 ± 0.05	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.390		Crippen Method
mcvol	81.620	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	4600.00 ± 60.79	kPa	NIST Webbook
pc	4600.00	kPa	KDB
rhoc	278.45 ± 29.80	kg/m3	NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	818.00		NIST Webbook
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rinpol	816.00		NIST Webbook
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rinpol	818.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	819.00		NIST Webbook

rinpol	820.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	786.60	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	824.00	NIST Webbook
rinpol	824.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	787.00	NIST Webbook
rinpol	805.00	NIST Webbook
rinpol	802.00	NIST Webbook
rinpol	803.00	NIST Webbook
rinpol	787.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	807.00	NIST Webbook
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rinpol	820.00	NIST Webbook
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rinpol	816.00	NIST Webbook
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rinpol	797.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	121.17	NIST Webbook
rinpol	130.12	NIST Webbook
rinpol	125.11	NIST Webbook

rinpol	821.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	803.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	819.00	NIST Webbook
rinpol	819.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	799.00	NIST Webbook
rinpol	802.20	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	802.30	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	818.00	NIST Webbook
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rinpol	802.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	800.00	NIST Webbook
ripol	1240.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1218.00	NIST Webbook
ripol	1225.00	NIST Webbook
ripol	1210.00	NIST Webbook
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ripol	1222.00	NIST Webbook
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ripol	1209.00	NIST Webbook
ripol	1211.00	NIST Webbook
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ripol	1200.00	NIST Webbook
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ripol	1215.68	NIST Webbook
ripol	1190.00	NIST Webbook
ripol	1205.00	NIST Webbook
ripol	1240.00	NIST Webbook
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ripol	1239.00	NIST Webbook
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ripol	1214.00	NIST Webbook
ripol	1219.00	NIST Webbook
ripol	1182.00	NIST Webbook
ripol	1216.00	NIST Webbook
ripol	1220.00	NIST Webbook
ripol	1210.00	NIST Webbook
ripol	1229.00	NIST Webbook

ripol	1239.00		NIST Webbook
ripol	1216.00		NIST Webbook
sl	217.86	J/molxK	NIST Webbook
tb	402.59 ± 0.08	K	NIST Webbook
tb	402.57 ± 0.10	K	NIST Webbook
tb	401.65 ± 2.00	K	NIST Webbook
tb	402.58 ± 0.08	K	NIST Webbook
tb	402.65 ± 2.00	K	NIST Webbook
tb	403.85 ± 0.50	K	NIST Webbook
tb	400.15 ± 1.50	K	NIST Webbook
tb	402.55 ± 0.30	K	NIST Webbook
tb	402.25 ± 0.30	K	NIST Webbook
tb	401.45 ± 0.50	K	NIST Webbook
tb	402.54 ± 0.20	K	NIST Webbook
tb	401.20 ± 1.50	K	NIST Webbook
tb	401.15 ± 1.50	K	NIST Webbook
tb	401.95 ± 0.30	K	NIST Webbook
tb	401.15 ± 1.00	K	NIST Webbook
tb	401.15 ± 1.00	K	NIST Webbook
tb	402.53	K	KDB
tb	402.20	K	Isobaric Vapor Liquid Equilibrium Data for the Binary System of Water + 2-Methylpyridine at 101.3, 60.0, and 20.0 kPa
tb	402.00	K	NIST Webbook
tb	402.60	K	NIST Webbook
tb	401.95	K	NIST Webbook
tb	402.40 ± 0.30	K	NIST Webbook
tb	402.65 ± 1.00	K	NIST Webbook
tb	399.35 ± 2.00	K	NIST Webbook
tb	402.41 ± 0.20	K	NIST Webbook
tb	402.45 ± 0.30	K	NIST Webbook
tb	401.15 ± 1.50	K	NIST Webbook
tb	401.15 ± 2.00	K	NIST Webbook
tb	401.00 ± 1.00	K	NIST Webbook
tb	402.59 ± 0.20	K	NIST Webbook
tb	402.62 ± 0.05	K	NIST Webbook
tb	402.59 ± 0.06	K	NIST Webbook
tb	402.55 ± 0.15	K	NIST Webbook
tb	402.25 ± 0.50	K	NIST Webbook
tb	402.45 ± 0.25	K	NIST Webbook
tb	402.95 ± 0.40	K	NIST Webbook
tb	402.35 ± 0.20	K	NIST Webbook
tb	402.15 ± 1.50	K	NIST Webbook
tb	402.80 ± 0.20	K	NIST Webbook

tc	621.00	K	NIST Webbook
tc	621.00	K	KDB
tc	621.10 ± 1.00	K	NIST Webbook
tf	206.29 ± 0.15	K	NIST Webbook
tf	206.47	K	KDB
tf	203.25	K	NIST Webbook
tf	204.35 ± 0.50	K	NIST Webbook
tf	206.29 ± 0.20	K	NIST Webbook
tf	206.29 ± 0.15	K	NIST Webbook
tf	207.15 ± 1.00	K	NIST Webbook
tf	203.40 ± 0.20	K	NIST Webbook
tf	206.41 ± 0.06	K	NIST Webbook
tf	206.60 ± 0.10	K	NIST Webbook
tf	208.95 ± 0.30	K	NIST Webbook
tf	206.55 ± 0.50	K	NIST Webbook
tf	203.25 ± 0.30	K	NIST Webbook
tf	206.29 ± 0.15	K	NIST Webbook
tt	206.45	K	KDB
tt	206.46 ± 0.05	K	NIST Webbook
tt	206.44 ± 0.03	K	NIST Webbook
vc	0.292	m ³ /kmol	KDB
zc	0.2601430		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	157.07	J/mol×K	293.15	Excess heat capacities of 1-methyl pyrrolidin-2-one and pyridine orpicolines mixtures
cpl	158.41	J/mol×K	298.15	NIST Webbook
cpl	160.14	J/mol×K	303.15	Excess heat capacities of 1-methyl pyrrolidin-2-one and pyridine orpicolines mixtures

cpl	158.86	J/mol×K	298.15	Excess heat capacities of 1-methyl pyrrolidin-2-one and pyridine orpicolines mixtures
hfust	9.72	kJ/mol	206.50	NIST Webbook
hfust	9.72	kJ/mol	206.50	NIST Webbook
hfust	9.72	kJ/mol	206.45	NIST Webbook
hvapt	41.60 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	39.80 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	36.20 ± 0.10	kJ/mol	402.00	NIST Webbook
hvapt	40.70 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	38.30 ± 0.10	kJ/mol	368.00	NIST Webbook
hvapt	39.80	kJ/mol	370.00	NIST Webbook
hvapt	38.80 ± 0.10	kJ/mol	359.00	NIST Webbook
hvapt	37.70 ± 0.10	kJ/mol	379.00	NIST Webbook
hvapt	36.17	kJ/mol	402.60	NIST Webbook
hvapt	41.20 ± 0.10	kJ/mol	374.50	NIST Webbook
hvapt	38.80 ± 0.10	kJ/mol	374.50	NIST Webbook
hvapt	36.40 ± 0.10	kJ/mol	374.50	NIST Webbook
hvapt	33.70 ± 0.30	kJ/mol	374.50	NIST Webbook
hvapt	42.00	kJ/mol	347.50	NIST Webbook
hvapt	46.90	kJ/mol	227.00	NIST Webbook
hvapt	36.50	kJ/mol	483.00	NIST Webbook
hvapt	35.40	kJ/mol	571.00	NIST Webbook
hvapt	39.10	kJ/mol	398.50	NIST Webbook
hvapt	39.10	kJ/mol	397.00	NIST Webbook
rfi	1.49840		298.15	Bubble Temperature Measurements on Binary Mixtures Formed by Cyclohexane at 94.7 kPa
rfi	1.49840		298.15	Bubble temperature measurements on seven binary mixtures formed by ethylbenzene at 94.7 kPa
rhoI	950.00	kg/m3	288.00	KDB

rho1	939.80	kg/m3	298.15	Thermodynamic and topological investigations of ternary mixtures with o-toluidine, tetrahydropyran, and picolines: Excess molar volume and excess isentropic compressibility
rho1	944.40	kg/m3	293.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquid and Organic Liquids: Excess Molar Volume and Excess Isentropic Compressibility
rho1	939.80	kg/m3	298.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquid and Organic Liquids: Excess Molar Volume and Excess Isentropic Compressibility
rho1	935.12	kg/m3	303.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquid and Organic Liquids: Excess Molar Volume and Excess Isentropic Compressibility
rho1	930.41	kg/m3	308.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquid and Organic Liquids: Excess Molar Volume and Excess Isentropic Compressibility
rho1	943.34	kg/m3	293.15	Viscosity of Associated Mixtures Approximated by the Grunberg-Nissan Model

rhoI	939.80	kg/m ³	298.15	Thermodynamic studies of molecular interactions in mixtures of o-toulidine with pyridine and picolines: Excess molar volumes, excess molar enthalpies, and excess isentropic compressibilities
sfust	47.10	J/mol×K	206.45	NIST Webbook
speedsl	1380.12	m/s	298.15	Thermodynamic properties of binary mixtures of tetrahydropyran with pyridine and isomeric picolines: Excess molar volumes, excess molar enthalpies and excess isentropic compressibilities
speedsl	1361.02	m/s	303.15	Thermodynamic properties of binary mixtures of tetrahydropyran with pyridine and isomeric picolines: Excess molar volumes, excess molar enthalpies and excess isentropic compressibilities
speedsl	1339.89	m/s	308.15	Topological investigations of binary mixtures containing ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate and pyridine or isomeric picolines
speedsl	1361.02	m/s	303.15	Topological investigations of binary mixtures containing ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate and pyridine or isomeric picolines

speedsl	1380.12	m/s	298.15	Topological investigations of binary mixtures containing ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate and pyridine or isomeric picolines
speedsl	1400.54	m/s	293.15	Topological investigations of binary mixtures containing ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate and pyridine or isomeric picolines
speedsl	1339.89	m/s	308.15	Thermodynamic properties of binary mixtures of tetrahydropyran with pyridine and isomeric picolines: Excess molar volumes, excess molar enthalpies and excess isentropic compressibilities

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45105e+01
Coeff. B	-3.48004e+03
Coeff. C	-5.02010e+01
Temperature range (K), min.	294.88
Temperature range (K), max.	428.51

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.64716e+01
Coeff. B	-7.53285e+03

Coeff. C	-8.99076e+00
Coeff. D	4.84390e-06
Temperature range (K), min.	206.44
Temperature range (K), max.	621.00

Sources

Excess molar enthalpies of ternary mixtures
 Isothermic Vapor-Liquid Equilibrium Data for the Binary System of Ionic Solvents: 2-Methylpyridine at 101.3, 60.0, and 20.0 kPa:
 Topological investigations of binary mixtures containing ionic liquid KDB (1-methyl-3-methylimidazolium tetrafluoroborate and pyridine or isomeric pyridines)
 Approximated by the Grunberg-Nissan-Mooney Method:
<https://www.doi.org/10.1016/j.tca.2013.07.006>

KDB Pure (Korean Thermophysical Properties Databank):
 Bubble temperature measurements on seven binary mixtures formed by tetrahydrofuran, diethyl ether, and ethyl acetate:
 Thermodynamic studies of molecular interactions in mixtures of o-toluidine with diethyl ether, methyl acetate, and ethyl acetate:
 Binary Mixtures Formed by Chloroform and Ethyl Chloride Vapor Pressure and Excess Entropic Capacities:
<https://www.doi.org/10.1021/acs.jced.6b00713>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C109068&Units=SI>
<https://www.doi.org/10.1016/j.jct.2012.07.007>
<https://www.thermochimica.org/files/research/kdb/mol/mol1346.mol>
<https://www.doi.org/10.1007/s10765-011-1100-1>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

KDB Pure (Korean Thermophysical Properties Databank):
 Bubble temperature measurements on seven binary mixtures formed by tetrahydrofuran, diethyl ether, and ethyl acetate:
 Thermodynamic studies of molecular interactions in mixtures of o-toluidine with diethyl ether, methyl acetate, and ethyl acetate:
 Binary Mixtures Formed by Chloroform and Ethyl Chloride Vapor Pressure and Excess Entropic Capacities:
 McGowan Method:
<https://www.thermochimica.org/research/kdb/hcprop/showprop.php?cmpid=1346>
<https://www.doi.org/10.1016/j.jct.2004.11.015>
<https://www.doi.org/10.1016/j.jct.2010.12.028>
<https://www.doi.org/10.1021/je020148t>
<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://link.springer.com/article/10.1007/BF02311772>

Thermodynamic properties of binary mixtures of tetrahydrofuran with KDB Pure and diethyl ether:
 KDB Pure and diethyl ether:
 Excess molar volumes, excess molar enthalpies and excess entropic capacities of binary mixtures of organic liquids and tetrahydrofuran:
 Investigations of ternary mixtures with diethyl ether, tetrahydrofuran, and picolines:
 Excess molar volume and excess molar enthalpies of binary mixtures containing o-toluidine + tetrahydrofuran and o-toluidine + tetrahydrofuran + picoline or diethyl ether mixtures:
<https://www.doi.org/10.1016/j.tca.2011.02.002>
<https://www.thermochimica.org/research/kdb/hcprop/showprop.php?cmpid=1346>
<https://www.doi.org/10.1021/je4004965>
<https://www.doi.org/10.1016/j.jct.2011.10.002>
https://www.chemeo.com/doc/models/crippen_log10ws
<https://www.doi.org/10.1016/j.tca.2011.12.023>
<https://www.doi.org/10.1016/j.tca.2013.06.033>

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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