

# Pyridine, 2-ethyl-

<b>Other names:</b>	2-Ethylpyridine 2-ethyl pyridine ALPHA-ETHYLPYRIDINE «alpha»-Ethylpyridine Â«alphaÂ»-Ethylpyridine
<b>Inchi:</b>	InChI=1S/C7H9N/c1-2-7-5-3-4-6-8-7/h3-6H,2H2,1H3
<b>InchiKey:</b>	NRGGMCIBEHEAIL-UHFFFAOYSA-N
<b>Formula:</b>	C7H9N
<b>SMILES:</b>	CCc1ccccn1
<b>Mol. weight [g/mol]:</b>	107.15
<b>CAS:</b>	100-71-0

## Physical Properties

Property code	Value	Unit	Source
af	0.3630		KDB
affp	952.40	kJ/mol	NIST Webbook
basg	920.60	kJ/mol	NIST Webbook
chl	-4042.30	kJ/mol	NIST Webbook
hfl	1.50	kJ/mol	NIST Webbook
hvap	44.70 ± 0.80	kJ/mol	NIST Webbook
log10ws	0.51		Aqueous Solubility Prediction Method
log10ws	0.51		Estimated Solubility Method
logp	1.644		Crippen Method
mvol	95.710	ml/mol	McGowan Method
pc	4100.00	kPa	KDB
rinpol	863.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	140.78		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	866.00		NIST Webbook

rinpol	905.00	NIST Webbook
rinpol	904.00	NIST Webbook
rinpol	905.70	NIST Webbook
rinpol	910.00	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	886.90	NIST Webbook
rinpol	886.90	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	914.00	NIST Webbook
rinpol	871.80	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	908.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	884.40	NIST Webbook
rinpol	919.00	NIST Webbook
rinpol	919.00	NIST Webbook
rinpol	879.40	NIST Webbook
rinpol	951.00	NIST Webbook
rinpol	906.00	NIST Webbook
ripol	1290.00	NIST Webbook
ripol	1282.00	NIST Webbook
ripol	1275.00	NIST Webbook
ripol	1275.00	NIST Webbook
ripol	1275.00	NIST Webbook
ripol	1274.00	NIST Webbook
ripol	1274.00	NIST Webbook
ripol	1273.00	NIST Webbook
ripol	1272.00	NIST Webbook
ripol	1282.00	NIST Webbook
ripol	1267.00	NIST Webbook
ripol	1284.00	NIST Webbook
ripol	1279.00	NIST Webbook
ripol	1288.00	NIST Webbook
ripol	1279.00	NIST Webbook
ripol	1286.00	NIST Webbook
ripol	1277.00	NIST Webbook
ripol	1311.00	NIST Webbook
ripol	1284.00	NIST Webbook
ripol	1275.00	NIST Webbook
ripol	1282.00	NIST Webbook

tb	421.80	K	NIST Webbook
tb	421.80	K	KDB
tb	423.15 ± 1.50	K	NIST Webbook
tb	422.05 ± 0.40	K	NIST Webbook
tb	417.00 ± 4.00	K	NIST Webbook
tb	422.00 ± 3.00	K	NIST Webbook
tc	628.00	K	Critical point measurements of four pyridines
tc	634.00	K	KDB
tf	210.00	K	KDB
tf	210.10	K	Aqueous Solubility Prediction Method
tf	210.05 ± 0.50	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	43.70	kJ/mol	348.00	NIST Webbook
rho1	932.25	kg/m <sup>3</sup>	293.10	KDB

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47492e+01
Coeff. B	-3.67933e+03
Coeff. C	-5.86190e+01
Temperature range (K), min.	313.04
Temperature range (K), max.	448.47

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.84456e+01
Coeff. B	-7.49816e+03
Coeff. C	-7.73720e+00

Coeff. D	4.01534e-06
Temperature range (K), min.	225.15
Temperature range (K), max.	631.15

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>KDB:</b>	<a href="https://www.chemic.org/files/research/kdb/mol/mol1351.mol">https://www.chemic.org/files/research/kdb/mol/mol1351.mol</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C100710&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C100710&amp;Units=SI</a>
<b>Critical point measurements of four pyridines:</b>	<a href="https://www.doi.org/10.1016/j.fluid.2017.05.010">https://www.doi.org/10.1016/j.fluid.2017.05.010</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>KDB Vapor Pressure Data:</b>	<a href="https://www.chemic.org/research/kdb/hcprop/showprop.php?cmpid=1351">https://www.chemic.org/research/kdb/hcprop/showprop.php?cmpid=1351</a>

## Legend

<b>af:</b>	Acentric Factor
<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rho:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

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