Pyridine, 5-ethyl-2-methyl-

Other names:	2,5-Aldehydine
	2-Methyl-5-ethylpyridine
	2-Picoline, 5-ethyl-
	3-Ethyl-6-methylpyridine
	5-ETHYL-2-PICOLINE
	5-Ethyl-2-methylpyridine
	5-Ethyl-«alpha»-picoline
	5-Ethyl-Â«alphaÂ»-picoline
	5-ethyl-.alpha.-picoline
	6-Methyl-3-ethylpyridine
	ALDEHYDECOLLIDINE
	Aldehydine
	Aldehydkollidin
	Collidine, aldehydecollidine
	MEP
	NSC 1984
	Pyridine, 2-methyl-5-ethyl
	UN 2300
	pyridine, 3-ethyl-6-methyl-
Inchi:	InChI=1S/C8H11N/c1-3-8-5-4-7(2)9-6-8/h4-6H,3H2,1-2H3
InchiKey:	NTSLROIKFLNUIJ-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCc1ccc(C)nc1
Mol. weight [g/mol]:	121.18
CAS:	104-90-5

Physical Properties

Property code	Value	Unit	Source
af	0.3930		KDB
chl	-4708.70 ± 1.90	kJ/mol	NIST Webbook
hf	34.90 ± 2.00	kJ/mol	NIST Webbook
hfl	-11.40 ± 1.90	kJ/mol	NIST Webbook
hvap	46.30	kJ/mol	NIST Webbook
hvap	46.30 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.52		Crippen Method
logp	1.952		Crippen Method
mcvol	109.800	ml/mol	McGowan Method

nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=3)		KDB
pc	3046.00	kPa	KDB
rinpol	1000.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1019.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1411.00		NIST Webbook
tb	451.35	K	NIST Webbook
tb	451.50	K	KDB
tb	451.50	K	NIST Webbook
tb	449.15 ± 2.00	K	NIST Webbook
tc	656.00	K	Critical point measurements of four pyridines
tc	662.00	K	KDB
tf	203.00	K	KDB
tf	202.85	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	45.40	kJ/mol	399.50	NIST Webbook
hvapt	51.60	kJ/mol	264.50	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47377e+01
Coeff. B	-3.89439e+03
Coeff. C	-6.66530e+01
Temperature range (K), min.	336.16
Temperature range (K), max.	479.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.53580e+02
Coeff. B	-2.51131e+04
Coeff. C	-6.60315e+01
Coeff. D	5.02700e-05
Temperature range (K), min.	325.15
Temperature range (K), max.	450.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104905&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=1360

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Critical point measurements of four pyridines: https://www.doi.org/10.1016/j.fluid.2017.05.010

KDB: https://www.cheric.org/files/research/kdb/mol/mol1360.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point