

Pyridine, 4-ethyl-

Other names:	.gamma.-ethylpyridine 4-(C2H5)-Pyridine 4-Ethylpyridine GAMMA-ETHYLPYRIDINE «gamma»-Ethylpyridine Â«gammaÂ»-Ethylpyridine
Inchi:	InChI=1S/C7H9N/c1-2-7-3-5-8-6-4-7/h3-6H,2H2,1H3
InchiKey:	VJXRKZJMGVSPX-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	CCc1ccncc1
Mol. weight [g/mol]:	107.15
CAS:	536-75-4

Physical Properties

Property code	Value	Unit	Source
af	0.3530		KDB
affp	951.10	kJ/mol	NIST Webbook
basg	919.20	kJ/mol	NIST Webbook
hvap	46.30 ± 0.70	kJ/mol	NIST Webbook
log10ws	-2.04		Crippen Method
logp	1.644		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	4100.00	kPa	KDB
rinpol	941.10		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	151.78		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	934.30		NIST Webbook
rinpol	943.50		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	941.10		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	921.40		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	943.00		NIST Webbook

ripol	958.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1389.00		NIST Webbook
ripol	1390.00		NIST Webbook
tb	438.15 ± 1.50	K	NIST Webbook
tb	438.40 ± 0.30	K	NIST Webbook
tb	441.40 ± 0.30	K	NIST Webbook
tb	441.50	K	NIST Webbook
tb	410.10	K	KDB
tc	653.00	K	Critical point measurements of four pyridines
tc	663.00	K	KDB
tf	183.00	K	KDB
tf	182.65 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	45.30	kJ/mol	352.50	NIST Webbook
rhol	942.96	kg/m ³	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47994e+01
Coeff. B	-3.84209e+03

Coeff. C	-6.41230e+01
Temperature range (K), min.	328.88
Temperature range (K), max.	469.07

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.47803e+02
Coeff. B	-1.10550e+04
Coeff. C	-1.98968e+01
Coeff. D	1.55614e-05
Temperature range (K), min.	333.15
Temperature range (K), max.	373.15

Sources

Critical point measurements of four pyridines:
KDB:

<https://www.doi.org/10.1016/j.fluid.2017.05.010>

<https://www.thermochimica.org/files/research/kdb/mol/mol1353.mol>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C536754&Units=SI>

The Yaws Handbook of Vapor Pressure:
KDB Vapor Pressure Data:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.thermochimica.org/research/kdb/hcprop/showprop.php?cmpid=1353>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemedoc.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
pc:	Critical Pressure
pvap:	Vapor pressure

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

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