

Pyridine, 3-ethyl-

Other names:	3-(C ₂ H ₅)-Pyridine 3-Ethylpyridine 5-Ethylpyridine BETA-LUTIDINE
Inchi:	InChI=1S/C ₇ H ₉ N/c1-2-7-4-3-5-8-6-7/h3-6H,2H ₂ ,1H ₃
InchiKey:	MFEIKQPHQINPRI-UHFFFAOYSA-N
Formula:	C ₇ H ₉ N
SMILES:	CCc1cccnc1
Mol. weight [g/mol]:	107.15
CAS:	536-78-7

Physical Properties

Property code	Value	Unit	Source
af	0.3420		KDB
affp	947.40	kJ/mol	NIST Webbook
basg	915.50	kJ/mol	NIST Webbook
log10ws	-2.04		Crippen Method
logp	1.644		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	4000.00	kPa	KDB
rinpol	964.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	937.10		NIST Webbook
rinpol	932.00		NIST Webbook

ripol	974.00		NIST Webbook
ripol	938.60		NIST Webbook
ripol	938.60		NIST Webbook
ripol	929.00		NIST Webbook
ripol	932.00		NIST Webbook
ripol	918.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	964.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	928.90		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1380.00		NIST Webbook
tb	438.20	K	NIST Webbook
tb	439.15 ± 0.50	K	NIST Webbook
tb	438.90 ± 0.50	K	NIST Webbook
tb	438.90	K	KDB
tc	651.00	K	Critical point measurements of four pyridines
tc	661.00	K	KDB
tf	196.30 ± 0.50	K	NIST Webbook
tf	196.00	K	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	44.60	kJ/mol	353.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48958e+01
Coeff. B	-3.85083e+03
Coeff. C	-6.35120e+01
Temperature range (K), min.	327.12
Temperature range (K), max.	465.30

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.37340e+02
Coeff. B	-1.05512e+04
Coeff. C	-1.83146e+01
Coeff. D	1.41840e-05
Temperature range (K), min.	334.15
Temperature range (K), max.	373.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C536787&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=1352
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/37-016-3/Pyridine-3-ethyl.pdf>

Generated by Cheméo on 2024-04-28 00:15:05.58768458 +0000 UTC m=+16552554.508261895.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.