Pyrrolidine, 1-methyl-

Other names:	1-METHYLPYRROLIDINE
	METHYLPYRROLIDINE
	N-METHYLTETRAHYDROPYRROLE
	N-Methylpyrrolidine
	Pyrrolidine, N-methyl
	Pyrrolidine,l-methyl-
	pyrrolidine, N-methyl-
Inchi:	InChI=1S/C5H11N/c1-6-4-2-3-5-6/h2-5H2,1H3
InchiKey:	AVFZOVWCLRSYKC-UHFFFAOYSA-N
Formula:	C5H11N
SMILES:	CN1CCCC1
Mol. weight [g/mol]:	85.15
CAS:	120-94-5

Physical Properties

Property code	Value	Unit	Source
affp	965.60	kJ/mol	NIST Webbook
basg	934.80	kJ/mol	NIST Webbook
hvap	34.20 ± 0.70	kJ/mol	NIST Webbook
ie	8.41 ± 0.02	eV	NIST Webbook
ie	8.41 ± 0.02	eV	NIST Webbook
ie	8.41 ± 0.05	eV	NIST Webbook
ie	8.41 ± 0.02	eV	NIST Webbook
log10ws	-0.38		Crippen Method
logp	0.712		Crippen Method
mcvol	80.430	ml/mol	McGowan Method
rinpol	674.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	673.00		NIST Webbook

ripol	861.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	865.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	849.00		NIST Webbook
ripol	865.00		NIST Webbook
ripol	870.00		NIST Webbook
ripol	847.00		NIST Webbook
ripol	844.00		NIST Webbook
tb	352.45 ± 0.50	K	NIST Webbook
tb	352.50 ± 0.15	K	NIST Webbook
tb	353.70	K	NIST Webbook
tf	179.15 ± 0.40	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	161.10	J/mol×K	298.00	NIST Webbook
hvapt	33.70	kJ/mol	294.00	NIST Webbook
hvapt	35.00 ± 0.70	kJ/mol	284.00	NIST Webbook
pvap	16.80	kPa	302.94	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	11.80	kPa	295.08	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	13.47	kPa	298.19	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	15.29	kPa	300.74	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	10.82	kPa	293.36	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	20.80	kPa	307.88	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	23.69	kPa	311.12	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	27.46	kPa	314.75	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	8.62	kPa	288.56	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	6.61	kPa	283.23	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	3.90	kPa	273.17	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41909e+01
Coeff. B	-3.05442e+03

Coeff. C	-3.46200e+01
Temperature range (K), min.	254.31
Temperature range (K), max.	378.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.59271e+01
Coeff. B	-5.61155e+03
Coeff. C	-6.11939e+00
Coeff. D	4.02154e-06
Temperature range (K), min.	183.15
Temperature range (K), max.	550.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1341

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

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

Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols: https://www.doi.org/10.1021/acs.jced.6b00576

KDB: https://www.cheric.org/files/research/kdb/mol/mol1341.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120945&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp: Proton affinity
basg: Gas basicity
cpl: Liquid phase heat capacity
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
pvap: Vapor pressure

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