Cyclohexanamine, N-methyl-

Other names:	(Methylamino)cyclohexane
	1-METHYLCYCLOHEXYLAMINE
	CYCLOHEXYLMETHYLAMINE
	Cyclohexylamine, N-methyl-
	Methylcyclohexylamine
	N-Cyclohexyl-N-methylamine
	N-Cyclohexylmethylamine
	N-Methyl-N-cyclohexylamine
	N-Methylcyclohexanamine
	N-Methylcyclohexylamine
	NSC 434
Inchi:	InChI=1S/C7H15N/c1-8-7-5-3-2-4-6-7/h7-8H,2-6H2,1H3
InchiKey:	XTUVJUMINZSXGF-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CNC1CCCCC1
Mol. weight [g/mol]:	113.20
CAS:	100-60-7

Physical Properties

Property code	Value	Unit	Source
gf	121.90	kJ/mol	Joback Method
hf	-80.02	kJ/mol	Joback Method
hfus	10.82	kJ/mol	Joback Method
hvap	38.04	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.538		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	934.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	947.00		NIST Webbook
tb	422.20	K	NIST Webbook
tc	636.06	K	Joback Method
tf	228.69	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.47	J/mol×K	532.67	Joback Method
cpg	308.11	J/mol×K	636.06	Joback Method
cpg	295.33	J/mol×K	601.60	Joback Method
cpg	281.79	J/mol×K	567.13	Joback Method
cpg	219.57	J/mol×K	429.28	Joback Method
cpg	236.38	J/mol×K	463.74	Joback Method
cpg	252.34	J/mol×K	498.21	Joback Method
pvap	1.78	kPa	314.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	1.04	kPa	305.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	1.28	kPa	308.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	1.51	kPa	311.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.14	kPa	275.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.18	kPa	278.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.22	kPa	281.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.27	kPa	284.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study

pvap	0.34	kPa	287.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.42	kPa	290.40	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.49	kPa	293.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.61	kPa	296.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.74	kPa	299.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.89	kPa	302.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
rhol	838.68	kg/m3	328.15	The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K
rhol	847.67	kg/m3	318.15	The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K
rhol	856.57	kg/m3	308.15	The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K

rhol	865.20	kg/m3	298.15	The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45983e+01
Coeff. B	-3.63216e+03
Coeff. C	-5.80540e+01
Temperature range (K), min.	311.86
Temperature range (K), max.	449.16

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.26251e+02
Coeff. B	-9.94278e+03
Coeff. C	-1.65629e+01
Coeff. D	1.15695e-05
Temperature range (K), min.	264.65
Temperature range (K), max.	622.00

Sources

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1331

KDB: https://www.cheric.org/files/research/kdb/mol/mol1331.mol

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100607&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of cyclohexanamines: Experimental and theoretical study:	https://www.doi.org/10.1016/j.tca.2015.03.016
The study of physico-chemical properties of binary systems consisting of N-Methylcyclohexylamine with 2-alkanols at T = (298.15-328.15) K:	https://www.doi.org/10.1016/j.jct.2017.02.023
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume