Aniline, N-methyl-

Other names:	(Methylamino)benzene
	ANILINOMETHANE
	Benzenamine, N-methyl-
	Benzeneamine, N-methyl-
	Methylaniline
	Methylphenylamine
	Monomethylaniline
	N-METHYLBENZENAMINE
	N-Methylaminobenzene
	N-Methylaniline
	N-Methylphenylamine
	N-Monomethylaniline
	N-Phenylmethylamine
	NSC 3502
	UN 2294
	phenylmethylamine
Inchi:	InChI=1S/C7H9N/c1-8-7-5-3-2-4-6-7/h2-6,8H,1H3
InchiKey:	AFBPFSWMIHJQDM-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	CNc1ccccc1
Mol. weight [g/mol]:	107.15
CAS:	100-61-8

Physical Properties

Property code	Value	Unit	Source
af	0.4750		KDB
affp	916.60	kJ/mol	NIST Webbook
basg	890.10	kJ/mol	NIST Webbook
chl	-4073.00	kJ/mol	NIST Webbook
chl	-4077.00	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
gf	199.30	kJ/mol	KDB
hf	85.41	kJ/mol	KDB
hf	83.90 ± 6.30	kJ/mol	NIST Webbook
hf	85.40	kJ/mol	NIST Webbook
hfl	32.00	kJ/mol	NIST Webbook
hfl	33.40 ± 7.50	kJ/mol	NIST Webbook

hfus	13.03	kJ/mol	Joback Method
hvap	50.50 ± 4.20	kJ/mol	NIST Webbook
hvap	50.50	kJ/mol	NIST Webbook
hvap	53.10	kJ/mol	NIST Webbook
hvap	53.40	kJ/mol	NIST Webbook
ie	7.35 ± 0.02	eV	NIST Webbook
ie	7.38 ± 0.05	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
ie	7.30 ± 0.05	eV	NIST Webbook
ie	7.34 ± 0.02	eV	NIST Webbook
ie	7.53	eV	NIST Webbook
ie	7.32 ± 0.02	eV	NIST Webbook
ie	7.32	eV	NIST Webbook
ie	7.73	eV	NIST Webbook
log10ws	-1.28		Aqueous Solubility Prediction Method
log10ws	-1.28		Estimated Solubility Method
logp	1.728		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	5200.00	kPa	KDB
pc	5197.97 ± 70.92	kPa	NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1052.20		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1040.40		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1056.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1719.80		NIST Webbook
ripol	1717.90		NIST Webbook
ripol	1719.80		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1726.60		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1726.60		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1737.00		NIST Webbook

ripol	1746.00		NIST Webbook
ripol	1750.00		NIST Webbook
tb	467.15 ± 0.40	K	NIST Webbook
tb	468.90 ± 1.00	K	NIST Webbook
tb	465.15 ± 5.00	K	NIST Webbook
tb	468.65 ± 0.50	K	NIST Webbook
tb	464.90 ± 1.00	K	NIST Webbook
tb	469.25 ± 0.20	K	NIST Webbook
tb	467.05 ± 0.50	K	NIST Webbook
tb	469.25 ± 0.30	K	NIST Webbook
tb	467.90 ± 0.60	K	NIST Webbook
tb	469.40	K	NIST Webbook
tb	469.40	K	KDB
tb	469.40 ± 0.30	K	NIST Webbook
tb	469.40 ± 0.25	K	NIST Webbook
tb	469.40 ± 0.30	K	NIST Webbook
tc	701.00	K	KDB
tf	216.00	K	NIST Webbook
tf	216.00	K	KDB
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.91	J/mol×K	436.41	Joback Method
cpg	189.97	J/mol×K	472.29	Joback Method
cpg	201.30	J/mol×K	508.17	Joback Method
cpg	211.93	J/mol×K	544.05	Joback Method
cpg	221.89	J/mol×K	579.93	Joback Method
cpg	231.21	J/mol×K	615.81	Joback Method
cpg	239.92	J/mol×K	651.69	Joback Method
cpl	230.10	J/mol×K	290.00	NIST Webbook
cpl	210.92	J/mol×K	303.15	Thermodynamic properties and molecular interactions of [Bmim][NTf2]/[Bmim][Pf6] and N-Methylaniline binary systems from T = (298.15 to 323.15) K at 0.1 MPa

cpl	214.73	J/mol×K	308.15	Thermodynamic properties and molecular interactions of [Bmim][NTf2]/[Bmim][Pf6] and N-Methylaniline binary systems from T = (298.15 to 323.15) K at 0.1 MPa
cpl	218.53	J/mol×K	313.15	Density, Speed of Sound, and Dynamic Viscosity of 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide/1-Butyl-3-methylimidazolium Hexafluorophosphate and N-Methylaniline Binary Systems from T = 298.15 to 323.15 K at 0.1 MPa
cpl	222.37	J/mol×K	318.15	Thermodynamic properties and molecular interactions of [Bmim][NTf2]/[Bmim][Pf6] and N-Methylaniline binary systems from T = (298.15 to 323.15) K at 0.1 MPa
cpl	225.88	J/mol×K	323.15	Thermodynamic properties and molecular interactions of [Bmim][NTf2]/[Bmim][Pf6] and N-Methylaniline binary systems from T = (298.15 to 323.15) K at 0.1 MPa
cpl	207.12	J/mol×K	298.15	Density, Speed of Sound, and Dynamic Viscosity of 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide/1-Butyl-3-methylimidazolium Hexafluorophosphate and N-Methylaniline Binary Systems from T = 298.15 to 323.15 K at 0.1 MPa

cpl	210.92	J/mol×K	303.15	Density, Speed of Sound, and Dynamic Viscosity of 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide/1-Butyl-3-methylimidazolium Hexafluorophosphate and N-Methylaniline Binary Systems from T = 298.15 to 323.15 K at 0.1 MPa
cpl	214.73	J/mol×K	308.15	Density, Speed of Sound, and Dynamic Viscosity of 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide/1-Butyl-3-methylimidazolium Hexafluorophosphate and N-Methylaniline Binary Systems from T = 298.15 to 323.15 K at 0.1 MPa
cpl	207.12	J/mol×K	298.15	Thermodynamic properties and molecular interactions of [Bmim][NTf2]/[Bmim][Pf6] and N-Methylaniline binary systems from T = (298.15 to 323.15) K at 0.1 MPa
cpl	222.37	J/mol×K	318.15	Density, Speed of Sound, and Dynamic Viscosity of 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide/1-Butyl-3-methylimidazolium Hexafluorophosphate and N-Methylaniline Binary Systems from T = 298.15 to 323.15 K at 0.1 MPa
cpl	225.88	J/mol×K	323.15	Density, Speed of Sound, and Dynamic Viscosity of 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide/1-Butyl-3-methylimidazolium Hexafluorophosphate and N-Methylaniline Binary Systems from T = 298.15 to 323.15 K at 0.1 MPa
cpl	207.10	J/mol×K	298.00	NIST Webbook

cpl	218.53	J/mol×K	313.15	Thermodynamic properties and molecular interactions of [Bmim][NTf2]/[Bmim][Pf6] and N-Methylaniline binary systems from T = (298.15 to 323.15) K at 0.1 MPa
hvapt	53.60	kJ/mol	389.00	NIST Webbook
hvapt	45.35	kJ/mol	466.60	NIST Webbook
pvap	0.07	kPa	298.15	Thermodynamic Properties of Binary Mixtures of Tetrahydropyran with Anilines at 308.15 K
rhol	978.20	kg/m3	303.15	Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines
rhol	981.72	kg/m3	303.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method
rhol	989.00	kg/m3	293.00	KDB
rhol	970.89	kg/m3	313.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method

rhol	965.81	kg/m3	318.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method
rhol	961.13	kg/m3	323.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method
rhol	982.24	kg/m3	298.15	Thermodynamics of mixtures containing amines. XI. Liquid + liquid equilibria and molar excess enthalpies at 298.15 K for N-methylaniline + hydrocarbon systems. Characterization in terms of DISQUAC and ERAS models
rhol	978.20	kg/m3	303.15	Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures
rhol	973.53	kg/m3	308.15	Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures

rhol	969.92	kg/m3	313.15	Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures	
rhol	964.90	kg/m3	318.15	Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures	
rhol	982.40	kg/m3	298.15	Thermodynamic properties of liquid mixtures containing 1,3-dioxolane and anilines: Excess molar volumes, excess molar enthalpies, excess Gibb's free energy and isentropic compressibilities changes of mixing	
rhol	982.24	kg/m3	298.15	Thermodynamics of Ketone + Amine Mixtures. Part VIII. Molar Excess Enthalpies at 298.15 K for n-Alkanone + Aniline or + N-Methylaniline Systems	
rhol	986.44	kg/m3	293.15	Thermodynamics of Mixtures Containing Amines. XII. Volumetric and Speed of Sound Data at (293.15, 298.15, and 303.15) K for N-Methylaniline + Hydrocarbon Systems	

rhol	982.49	kg/m3	298.15	Thermodynamics of Mixtures Containing Amines. XII. Volumetric and Speed of Sound Data at (293.15, 298.15, and 303.15) K for N-Methylaniline + Hydrocarbon Systems
rhol	978.54	kg/m3	303.15	Thermodynamics of Mixtures Containing Amines. XII. Volumetric and Speed of Sound Data at (293.15, 298.15, and 303.15) K for N-Methylaniline + Hydrocarbon Systems
rhol	986.20	kg/m3	293.15	Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines
rhol	982.20	kg/m3	298.15	Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines
rhol	976.04	kg/m3	308.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method
rhol	974.20	kg/m3	308.15	Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines

speedsl	1548.00	m/s	303.15	Thermodynamic and acoustic properties of binary mixtures of oxolane with aniline and substituted anilines at 303.15, 313.15 and 323.15 K	
speedsl	1512.00	m/s	313.15	Thermodynamic and acoustic properties of binary mixtures of oxolane with aniline and substituted anilines at 303.15, 313.15 and 323.15 K	
speedsl	1477.00	m/s	323.15	Thermodynamic and Acoustic Properties of Binary Mixtures of Ethers. 2. Diisopropyl Ether with Arylamines at (303.15, 313.15, and 323.15) K and Application of ERAS Model to Aniline Mixtures with Diisopropyl Ether and Oxolane	
speedsl	1582.50	m/s	293.15	Thermodynamics of Ketone + Amine Mixtures. Part III. Volumetric and Speed of Sound Data at (293.15, 298.15, and 303.15) K for 2-Butanone + Aniline, + N-Methylaniline, or + Pyridine Systems	
speedsl	1563.90	m/s	298.15	Thermodynamics of Ketone + Amine Mixtures. Part III. Volumetric and Speed of Sound Data at (293.15, 298.15, and 303.15) K for 2-Butanone + Aniline, + N-Methylaniline, or + Pyridine Systems	

speedsl	1546.00	m/s	303.15	Thermodynamics of Ketone + Amine Mixtures. Part III. Volumetric and Speed of Sound Data at (293.15, 298.15, and 303.15) K for 2-Butanone + Aniline, + N-Methylaniline, or + Pyridine Systems	
speedsl	1548.00	m/s	303.15	Thermodynamic and Acoustic Properties of Binary Mixtures of Ethers. 2. Diisopropyl Ether with Arylamines at (303.15, 313.15, and 323.15) K and Application of ERAS Model to Aniline Mixtures with Diisopropyl Ether and Oxolane	
speedsl	1512.00	m/s	313.15	Thermodynamic and Acoustic Properties of Binary Mixtures of Ethers. 2. Diisopropyl Ether with Arylamines at (303.15, 313.15, and 323.15) K and Application of ERAS Model to Aniline Mixtures with Diisopropyl Ether and Oxolane	
speedsl	1477.00	m/s	323.15	Thermodynamic and acoustic properties of binary mixtures of oxolane with aniline and substituted anilines at 303.15, 313.15 and 323.15 K	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59126e+01
Coeff. B	-4.83070e+03
Coeff. C	-4.02870e+01
Temperature range (K), min.	349.45
Temperature range (K), max.	495.97

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.91078e+01
Coeff. B	-9.00734e+03
Coeff. C	-9.14371e+00
Coeff. D	4.35509e-06
Temperature range (K), min.	216.15
Temperature range (K), max.	701.55

Sources

Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures:	https://www.doi.org/10.1016/j.jct.2016.09.010
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1300.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100618&Units=SI
Spectroscopic and ultrasonic studies on the molecular interaction of certain aromatic amines with p-chloranil:	https://www.doi.org/10.1016/j.fluid.2013.09.026
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Thermodynamic properties and molecular interactions of [Bmim][NTf2]/[Bmim][PF6] and N-Methylaniline binary systems from T = (298.15 to 323.15) K at 0.1 MPa:	https://www.doi.org/10.1016/j.jct.2019.06.003
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic Properties of Binary Mixtures of Tetrahydropyran with Anilines at 308.15 K:	https://www.doi.org/10.1021/je1005196
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1300
Thermodynamic and acoustic properties of binary mixtures of oxolane with aniline and substituted anilines at 303.15, 313.15 and 323.15 K:	https://www.doi.org/10.1016/j.tca.2010.04.025
Thermodynamics of Ketone + Amine Mixtures. Part III. Volumetric and Speed of Sound Data at (293.15, 298.15, and 303.15) K for 2-Butanone + Aniline, + N-Methylaniline, or + Pyridine Systems:	https://www.doi.org/10.1021/je100472t
Thermodynamic properties of liquid mixtures containing 1,3-dioxolane and amines: Excess molar volumes, excess molar enthalpies, excess Gibb's free energy and isentropic compressibilities:	https://www.doi.org/10.1016/j.tca.2010.07.027
Thermodynamics of Mixtures Containing Amines. XII. Volumetric and [illegible] Hydrocarbon Systems:	https://www.doi.org/10.1021/je400134d
Thermodynamic and Acoustic Properties of Binary Mixtures of Ethers. [illegible]	https://www.doi.org/10.1021/je1008262
Density, Speed of Sound, and Dynamic Viscosity of [illegible] with Arylamines at (303.15, 313.15, and 323.15) K and Application of ERAS Model to Aniline [illegible]	https://www.doi.org/10.1021/acs.jced.8b01095
Excess Heat Capacities of Binary and Ternary Mixtures Containing [illegible] bis(trifluoromethylsulfonyl)imide/1-Butyl-3-methylimidazolium Hexafluorophosphate and N-Methylaniline Binary Systems from T = 298.15 to 323.15 K at 0.1 MPa:	https://www.doi.org/10.1021/je401098b
Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method:	https://www.doi.org/10.1016/j.fluid.2018.01.025

Thermodynamics of Ketone + Amine Mixtures. Part VIII. Molar Excess Enthalpies at 298.15 K for n-Alkanone + Aniline or N-Methylaniline Systems:	https://www.doi.org/10.1021/je200333p
Thermodynamics of mixtures containing amines. XI. Liquid + liquid equilibria and molar excess enthalpies at 298.15 K for N-methylaniline + hydrocarbon systems. Characterization in terms of DISQUAC and ERAS models:	https://www.doi.org/10.1016/j.jct.2012.07.006
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume