Benzenamine, N,N-dimethyl-

Other names:	(Dimethylamino)benzene
	Aniline, N,N-dimethyl-
	DIMETHYLPHENYLAMINE
	Dimethylaniline
	Dwumetyloanilina
	N,N-(Dimethylamino)benzene
	N,N-Dimethylaniline
	N,N-Dimethylbenzenamine
	N,N-Dimethylbenzeneamine
	N,N-Dimethylphenylamine
	N,N-dimethylanilin
	NCI-C56428
	NL 63-10P
	NSC 7195
	UN 2253
	Versneller NL 63/10
Inchi:	InChI=1S/C8H11N/c1-9(2)8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey:	JLTDJTHDQAWBAV-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CN(C)c1ccccc1
Mol. weight [g/mol]:	121.18
CAS:	121-69-7

Physical Properties

Property code	Value	Unit	Source
af	0.4110		KDB
affp	941.10	kJ/mol	NIST Webbook
basg	909.20	kJ/mol	NIST Webbook
chl	-4767.80 ± 3.20	kJ/mol	NIST Webbook
chl	-4754.30	kJ/mol	NIST Webbook
dm	1.60	debye	KDB
gf	231.40	kJ/mol	KDB
hf	84.15	kJ/mol	KDB
hf	84.10	kJ/mol	NIST Webbook
hf	100.50 ± 3.40	kJ/mol	NIST Webbook
hfl	47.70 ± 3.40	kJ/mol	NIST Webbook
hfl	34.00	kJ/mol	NIST Webbook

hfus	13.54	kJ/mol	Joback Method
hvap	37.72	kJ/mol	Joback Method
ie	7.31	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
ie	7.10 ± 0.02	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
ie	7.51	eV	NIST Webbook
ie	7.11	eV	NIST Webbook
ie	7.13 ± 0.04	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
ie	7.37	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	7.35	eV	NIST Webbook
ie	7.10 ± 0.05	eV	NIST Webbook
ie	7.42	eV	NIST Webbook
ie	7.12 ± 0.02	eV	NIST Webbook
ie	7.78	eV	NIST Webbook
ie	7.14 ± 0.03	eV	NIST Webbook
log10ws	-1.92		Estimated Solubility Method
log10ws	-1.92		Aqueous Solubility Prediction Method
logp	1.753		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=3)		KDB
pc	3650.00 ± 91.19	kPa	NIST Webbook
pc	3597.04 ± 151.99	kPa	NIST Webbook
pc	3627.44 ± 151.99	kPa	NIST Webbook
pc	3637.57 ± 151.99	kPa	NIST Webbook
pc	3576.77 ± 151.99	kPa	NIST Webbook
pc	3630.00	kPa	KDB
pc	3657.83 ± 151.99	kPa	NIST Webbook
pc	3610.00 ± 91.19	kPa	NIST Webbook
rinpol	1083.90		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1083.90		NIST Webbook
rinpol	1094.50		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1100.00		NIST Webbook

rinpol	1103.00		NIST Webbook
rinpol	1065.40		NIST Webbook
rinpol	1062.37		NIST Webbook
rinpol	1062.07		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1062.71		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1086.10		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1065.40		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1569.90		NIST Webbook
ripol	1569.90		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1604.80		NIST Webbook
ripol	1603.40		NIST Webbook
ripol	1604.80		NIST Webbook
tb	467.30	K	KDB
tc	687.00	K	KDB
tf	275.60	K	KDB
tf	275.53	K	Aqueous Solubility Prediction Method
tf	275.65 ± 0.30	K	NIST Webbook
tf	272.00 ± 1.00	K	NIST Webbook
tf	275.60 ± 0.30	K	NIST Webbook
tf	275.36 ± 0.25	K	NIST Webbook
tf	275.75 ± 0.20	K	NIST Webbook
tf	275.35 ± 0.40	K	NIST Webbook
tf	274.60 ± 0.14	K	NIST Webbook
tf	274.15 ± 0.30	K	NIST Webbook
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.35	J/mol×K	456.04	Joback Method
cpg	231.52	J/mol×K	490.52	Joback Method
cpg	243.89	J/mol×K	525.00	Joback Method
cpg	255.49	J/mol×K	559.48	Joback Method
cpg	266.35	J/mol×K	593.96	Joback Method
cpg	204.33	J/mol×K	421.56	Joback Method
cpg	276.52	J/mol×K	628.44	Joback Method
cpl	212.10	J/mol×K	298.00	NIST Webbook
cpl	212.10	J/mol×K	283.00	NIST Webbook
cpl	209.60	J/mol×K	289.00	NIST Webbook
cpl	214.60	J/mol×K	302.30	NIST Webbook
cpl	214.60	J/mol×K	302.40	NIST Webbook
dvisc	0.0008410	Pa×s	343.15	Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T) (283.15 to 343.15) K
dvisc	0.0009810	Pa×s	313.15	Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T) (283.15 to 343.15) K
dvisc	0.0016960	Pa×s	283.15	Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T) (283.15 to 343.15) K
dvisc	0.0014390	Pa×s	293.15	Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T) (283.15 to 343.15) K

dvisc	0.0008259	Pa×s	323.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
dvisc	0.0009823	Pa×s	313.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
dvisc	0.0009280	Pa×s	323.15	Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T) (283.15 to 343.15) K
dvisc	0.0009110	Pa×s	333.15	Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T) (283.15 to 343.15) K
dvisc	0.0011743	Pa×s	303.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
dvisc	0.0011700	Pa×s	303.15	Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T) (283.15 to 343.15) K
hfust	11.56	kJ/mol	275.60	NIST Webbook
hfust	11.56	kJ/mol	275.60	NIST Webbook
hvapt	44.35	kJ/mol	465.70	NIST Webbook

hvapt	47.60	kJ/mol	384.50	NIST Webbook
hvapt	49.20	kJ/mol	390.50	NIST Webbook
hvapt	53.70 ± 0.50	kJ/mol	303.50	NIST Webbook
pvap	5.16	kPa	373.70	Vapor-Liquid Equilibrium for the Binary System of N,N-Dimethylaniline with 2-Amino-3-methylpyridine
pvap	8.04	kPa	384.96	Vapor-Liquid Equilibrium for the Binary System of N,N-Dimethylaniline with 2-Amino-3-methylpyridine
rhol	943.50	kg/m3	308.15	Volumetric and transport properties of binary liquid mixtures of sulfolane with aniline, N,N-dimethylaniline and N,N-diethylaniline at different temperatures and atmospheric pressure
rhol	956.50	kg/m3	293.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion
rhol	952.30	kg/m3	298.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion

rhol	948.20	kg/m3	303.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion
rhol	944.10	kg/m3	308.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion
rhol	940.00	kg/m3	313.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion
rhol	935.90	kg/m3	318.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion
rhol	931.80	kg/m3	323.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion

rhol	927.70	kg/m3	328.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion
rhol	923.50	kg/m3	333.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion
rhol	952.05	kg/m3	298.15	Cloud Point Phenomena in the (Aniline or N,N-Dimethylaniline + Water) Solutions, and Cosolvent Effects of Liquid Poly(ethylene glycol) Addition: Experimental Measurements and Modeling
rhol	960.60	kg/m3	288.15	Excess molar volumes and viscosity behaviour of binary mixtures of aniline/or N,N-dimethylaniline with imidazolium ionic liquids having triflate or bistriflamide anion
rhol	939.40	kg/m3	313.15	Volumetric and transport properties of binary liquid mixtures of sulfolane with aniline, N,N-dimethylaniline and N,N-diethylaniline at different temperatures and atmospheric pressure

rhol	947.70	kg/m3	303.15	Volumetric and transport properties of binary liquid mixtures of sulfolane with aniline, N,N-dimethylaniline and N,N-diethylaniline at different temperatures and atmospheric pressure	
rhol	935.30	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	939.78	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	943.55	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	948.18	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	956.00	kg/m3	293.00	KDB
rhol	931.45	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
speedsl	1468.00	m/s	303.15	Thermodynamic and acoustic properties of binary mixtures of ethers. IV. Diisopropyl ether or oxolane with N,N-dimethylaniline or N,Ndiethylaniline at 303.15, 313.15 and 323.15 K
speedsl	1393.00	m/s	323.15	Thermodynamic and acoustic properties of binary mixtures of ethers. IV. Diisopropyl ether or oxolane with N,N-dimethylaniline or N,Ndiethylaniline at 303.15, 313.15 and 323.15 K

speedsl	1431.00	m/s	313.15	Thermodynamic and acoustic properties of binary mixtures of ethers. IV. Diisopropyl ether or oxolane with N,N-dimethylaniline or N,Ndiethylaniline at 303.15, 313.15 and 323.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50960e+01
Coeff. B	-4.40969e+03
Coeff. C	-4.51330e+01
Temperature range (K), min.	342.92
Temperature range (K), max.	495.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.20032e+01
Coeff. B	-7.05985e+03
Coeff. C	-3.63909e+00
Coeff. D	4.98882e-07
Temperature range (K), min.	275.60
Temperature range (K), max.	687.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1305.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
THERMODYNAMIC PROPERTIES OF DONOR ACCEPTOR COMPLEXES OF TERTIARY AMINE WITH ARTL KETONES IN DIOXANE MEDIUM:	https://www.doi.org/10.1016/j.tca.2012.02.018
KDB Pure (Koman Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1305
Cloud Point Phenomena in the (Aniline or N,N-Dimethylaniline + Water) Solutions, and Cosolvent Effects of Liquid Poly(ethylene glycol) Addition:	https://www.doi.org/10.1021/je500448j
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1305
Experimental Measurements and Modeling:	https://www.doi.org/10.1016/j.fluid.2013.09.026
Spectroscopic and ultrasonic studies on the molecular interaction of certain aromatic amines with p-chloranil:	https://www.doi.org/10.1021/je200862b
Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K:	https://www.doi.org/10.1016/j.jct.2017.02.007
Excess molar volume and viscosity behaviour of binary mixtures of 1-ethyl-3-methylimidazolium ethylsulfate with aniline/N,N-dimethylaniline at temperatures between 293.15 and 323.15 K:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121697&Units=SI
Vapor-Liquid Equilibrium for the Binary System of N,N-Dimethylaniline with 2-Amino-3-methylpyridine:	https://www.doi.org/10.1021/je101180r
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic and acoustic properties of binary mixtures of ethers. IV. Diisopropyl ether or Oxolane with N,N-dimethylaniline at 303.15 and 313.15 K:	https://www.doi.org/10.1016/j.tca.2011.02.004
Volumetric and transport properties of binary liquid mixtures of sulfolane with N,N-dimethylaniline at 303.15, 313.15 and 323.15 K:	https://www.doi.org/10.1016/j.jct.2015.12.030
Densities and Viscosities for Binary and Ternary Mixtures of 1,4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T = (283.15 to 343.15) K at Different Temperatures and Atmospheric Pressure:	https://www.doi.org/10.1021/je700344f

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
dvisc:	Dynamic viscosity
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
hfust:	Enthalpy of fusion at a given temperature
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume