BENZENAMINE, 2-METHYL-

Other names:	(2-methylphenyl)amine
	1-Methyl-2-aminobenzene
	1-amino-2-methylbenzene
	2-amino-1-methylbenzene
	2-aminotoluene
	2-methyl-1-aminobenzene
	2-methylaniline
	2-methylbenzenamine
	2-methylphenylamine
	2-toluidine
	Aniline, 2-methyl-
	C.I. 37077
	NSC 15348
	Rcra waste number U328
	o-Aminotoluene
	o-Methylaniline
	o-Methylbenzenamine
	o-Toluide
	o-Toluidin
	o-Toluidyna
	o-Tolylamine
	o-toluidine
	ortho-aminotoluene
	ortho-methylaniline
	ortho-methylbenzenamine
	ortho-toluidine
	ortho-tolylamine
Inchi:	InChI=1S/C7H9N/c1-6-4-2-3-5-7(6)8/h2-5H,8H2,1H3
InchiKey:	RNVCVTLRINQCPJ-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	Cc1ccccc1N
Mol. weight [g/mol]:	107.16
CAS:	95-53-4

Physical Properties

Property code	Value	Unit	Source

af	0.4328		Cheméo Relay (1.0)
affp	890.90	kJ/mol	NIST Webbook
basg	859.10	kJ/mol	NIST Webbook
chl	-4036.09 ± 0.88	kJ/mol	NIST Webbook
chl	-4034.00	kJ/mol	NIST Webbook
chl	-4064.00	kJ/mol	NIST Webbook
gf	177.29	kJ/mol	Joback Method
hf	54.80	kJ/mol	NIST Webbook
hf	51.40	kJ/mol	NIST Webbook
hf	53.20 ± 0.50	kJ/mol	NIST Webbook
hfl	-4.72 ± 0.96	kJ/mol	NIST Webbook
hfl	-6.49	kJ/mol	NIST Webbook
hfus	12.73	kJ/mol	Joback Method
hvap	57.30 ± 0.20	kJ/mol	NIST Webbook
hvap	57.90	kJ/mol	NIST Webbook
hvap	62.70 ± 0.50	kJ/mol	NIST Webbook
hvap	44.10	kJ/mol	NIST Webbook
hvap	63.10	kJ/mol	NIST Webbook
hvap	56.20	kJ/mol	NIST Webbook
hvap	57.90 ± 0.24	kJ/mol	NIST Webbook
ie	7.84	eV	NIST Webbook
ie	7.69	eV	NIST Webbook
ie	7.47 ± 0.04	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
ie	7.45 ± 0.02	eV	NIST Webbook
ie	7.52	eV	NIST Webbook
ie	7.44 ± 0.02	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
ie	7.70 ± 0.10	eV	NIST Webbook
ie	7.83	eV	NIST Webbook
ie	7.75	eV	NIST Webbook
ie	7.83	eV	NIST Webbook
log10ws	-0.85		Aqueous Solubility Prediction Method
log10ws	-2.21		Estimated Solubility Method
logp	1.577		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	3749.02 ± 253.31	kPa	NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	176.52		NIST Webbook
rinpol	176.52		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1032.70		NIST Webbook
rinpol	1053.90		NIST Webbook

rinpol	176.65		NIST Webbook
rinpol	1032.70		NIST Webbook
rinpol	1040.50		NIST Webbook
rinpol	177.86		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1053.90		NIST Webbook
rinpol	1053.90		NIST Webbook
rinpol	1037.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1789.00		NIST Webbook
tb	473.35 ± 0.30	K	NIST Webbook
tb	469.70 ± 1.00	K	NIST Webbook
tb	473.50 ± 0.30	K	NIST Webbook
tb	473.45 ± 0.07	K	NIST Webbook
tb	470.40 ± 0.50	K	NIST Webbook
tb	472.45 ± 0.60	K	NIST Webbook
tb	473.35 ± 0.50	K	NIST Webbook
tb	473.40	K	NIST Webbook
tb	473.45 ± 0.30	K	NIST Webbook
tb	473.55 ± 0.30	K	NIST Webbook
tb	473.85 ± 0.20	K	NIST Webbook
tb	472.99 ± 0.20	K	NIST Webbook
tb	471.35 ± 0.30	K	NIST Webbook
tb	472.65 ± 0.60	K	NIST Webbook
tb	472.85 ± 0.50	K	NIST Webbook
tb	473.30 ± 0.50	K	NIST Webbook
tc	694.15 ± 2.00	K	NIST Webbook
tf	248.75 ± 0.20	K	NIST Webbook
tf	256.75 ± 0.30	K	NIST Webbook
tf	253.55	K	Aqueous Solubility Prediction Method
tf	250.00 ± 0.20	K	NIST Webbook
tf	248.75 ± 0.30	K	NIST Webbook
tf	256.90 ± 0.30	K	NIST Webbook
tf	245.50 ± 0.40	K	NIST Webbook
tf	249.50 ± 0.02	K	NIST Webbook
tf	249.47 ± 0.05	K	NIST Webbook

tf	256.75 ± 0.50	K	NIST Webbook
tf	257.70 ± 0.60	K	NIST Webbook
tt	258.73 ± 0.01	K	NIST Webbook
tt	258.73 ± 0.01	K	NIST Webbook
vc	0.334	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.04	J/mol×K	463.75	Joback Method
cpg	199.40	J/mol×K	501.76	Joback Method
cpg	210.07	J/mol×K	539.77	Joback Method
cpg	220.08	J/mol×K	577.78	Joback Method
cpg	229.46	J/mol×K	615.79	Joback Method
cpg	238.23	J/mol×K	653.80	Joback Method
cpg	246.42	J/mol×K	691.81	Joback Method
cpl	164.40	J/mol×K	303.15	NIST Webbook
cpl	209.60	J/mol×K	302.50	NIST Webbook
cpl	209.60	J/mol×K	302.50	NIST Webbook
cpl	201.70	J/mol×K	288.00	NIST Webbook
cpl	211.30	J/mol×K	298.00	NIST Webbook
hfust	11.66	kJ/mol	287.60	NIST Webbook
hfust	11.66	kJ/mol	287.60	NIST Webbook
hfust	11.66	kJ/mol	287.60	NIST Webbook
hfust	11.66	kJ/mol	287.60	NIST Webbook
hfust	8.08	kJ/mol	249.60	NIST Webbook
hfust	8.10	kJ/mol	249.55	NIST Webbook
hvapt	45.70	kJ/mol	403.50	NIST Webbook
hvapt	48.60	kJ/mol	403.50	NIST Webbook
hvapt	42.70	kJ/mol	403.50	NIST Webbook
hvapt	48.60	kJ/mol	403.50	NIST Webbook
hvapt	57.80	kJ/mol	403.50	NIST Webbook
hvapt	54.50	kJ/mol	403.50	NIST Webbook
hvapt	51.50	kJ/mol	403.50	NIST Webbook
hvapt	51.50	kJ/mol	403.50	NIST Webbook
hvapt	45.70	kJ/mol	403.50	NIST Webbook
hvapt	42.70	kJ/mol	403.50	NIST Webbook
hvapt	50.00	kJ/mol	432.50	NIST Webbook
hvapt	57.80	kJ/mol	403.50	NIST Webbook
hvapt	54.50	kJ/mol	403.50	NIST Webbook

pvap	0.04	kPa	298.15	Thermodynamic Properties of Binary Mixtures of Tetrahydropyran with Anilines at 308.15 K	
rhol	994.36	kg/m3	298.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquid and Organic Liquids: Excess Molar Volume and Excess Isentropic Compressibility	
rhol	990.23	kg/m3	303.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquid and Organic Liquids: Excess Molar Volume and Excess Isentropic Compressibility	
rhol	994.28	kg/m3	298.15	Molar Excess Volumes and Excess Isentropic Compressibilities of Ternary Mixtures of o-Toluidine	
rhol	994.34	kg/m3	298.15	Thermodynamics of mixtures containing amines VI. Liquid liquid equilibria for mixtures of o-toluidine + selected alkanes	
rhol	994.35	kg/m3	298.15	Thermodynamic studies of molecular interactions in mixtures of o-toulidine with pyridine and picolines: Excess molar volumes, excess molar enthalpies, and excess isentropic compressibilities	

rhol	994.35	kg/m3	298.15	Thermodynamic and topological investigations of ternary mixtures with o-toluidine, tetrahydropyran, and picolines: Excess molar volume and excess isentropic compressibility	
rhol	994.28	kg/m3	298.15	Topological and thermodynamic investigations of binary mixtures: Molar excess volumes, molar excess enthalpies and isentropic compressibility changes of mixing	
rhol	994.20	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	998.43	kg/m3	293.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquid and Organic Liquids: Excess Molar Volume and Excess Isentropic Compressibility	

rhol	994.28	kg/m3	298.15	Molar Excess Volumes and Excess Isentropic Compressibilities of {2-Methylaniline (i) + Benzene (j) + Methylbenzene}, {2-Methylaniline (i) + Benzene (j) + 1,2-Dimethylbenzene (k)}, and {2-Methylaniline (i) + Benzene (j) + 1,4-Dimethylbenzene (k)} at T = 308.15 K
rhol	986.06	kg/m3	308.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquid and Organic Liquids: Excess Molar Volume and Excess Isentropic Compressibility
rhol	986.10	kg/m3	308.15	Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines
rhol	990.20	kg/m3	303.15	Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines
rhol	994.40	kg/m3	298.15	Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines
rhol	998.40	kg/m3	293.15	Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines
sfust	32.00	J/mol×K	249.55	NIST Webbook

speedsl	1558.40	m/s	308.15	Topological investigations of molecular interactions of binary and ternary mixtures containing tetrahydropyran, o-toluidine and N-methyl formamide
speedsl	1558.38	m/s	308.15	Topological investigations of molecular interactions of binary and ternary mixtures containing tetrahydropyran, o-toluidine and N-methyl formamide
speedsl	1577.80	m/s	303.15	Topological investigations of molecular interactions of binary and ternary mixtures containing tetrahydropyran, o-toluidine and N-methyl formamide
speedsl	1602.60	m/s	298.15	Topological investigations of molecular interactions of binary and ternary mixtures containing tetrahydropyran, o-toluidine and N-methyl formamide
speedsl	1501.00	m/s	323.15	Thermodynamic and acoustic properties of binary mixtures of ethers. III. Diisopropyl ether or oxolane with o- or m-toluidines at 303.15, 313.15 and 323.15 K

speedsl	1539.00	m/s	313.15	Thermodynamic and acoustic properties of binary mixtures of ethers. III. Diisopropyl ether or oxolane with o- or m-toluidines at 303.15, 313.15 and 323.15 K
speedsl	1579.00	m/s	303.15	Thermodynamic and acoustic properties of binary mixtures of ethers. III. Diisopropyl ether or oxolane with o- or m-toluidines at 303.15, 313.15 and 323.15 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.43007e+02
Coeff. B	-1.23010e+04
Coeff. C	-1.86082e+01
Coeff. D	9.77089e-06
Temperature range (K), min.	249.47
Temperature range (K), max.	694.15

Sources

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
Molar Excess Volumes and Excess Isentropic Compressibilities of Ternary Mixtures of o-Toluidine:	https://www.doi.org/10.1021/je800100m
Thermodynamic and acoustic properties of binary mixtures of ethers. III. Diisopropyl ether or oxolane with o- or m-toluidines at 303.15, 313.15 and 323.15 K:	https://www.doi.org/10.1016/j.tca.2011.01.019
Topological investigations of molecular interactions of binary and ternary containing tetrahydropyran, o-toluidine and N-methyl formamide:	https://www.doi.org/10.1016/j.tca.2011.06.020
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1297
Excess Molar Enthalpies for Binary and Ternary Mixtures containing Cyclic Ether, 2-Methylaniline and Aromatic Hydrocarbons:	https://www.doi.org/10.1016/j.tca.2011.11.025
Excess molar enthalpies of ternary mixtures containing1-ethyl-3-methylimidazolium tetrafluoroborate and organic solvents:	https://www.doi.org/10.1016/j.tca.2013.07.006

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95534&Units=SI
Thermodynamic Properties of Binary Mixtures of Tetrahydropyran with Anilines at 308.15 K:	https://www.doi.org/10.1021/je1005196
Molecular interactions in binary mixtures containing o-toluidine:	https://www.doi.org/10.1016/j.tca.2007.12.006
Topological and thermodynamic investigations of molecular interactions of aniline and o-toluidine with chloroform:	https://www.doi.org/10.1016/j.tca.2008.02.022
Excess Heat Capacities of Binary and Ternary Mixtures Containing 1-Ethyl-3-methylimidazolium Tetrafluoroborate and Anilines:	https://www.doi.org/10.1021/je401098b
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Chemeo Relay (1.0):	
Excess molar enthalpies of ternary mixtures containing o-toluidine + tetrahydropyran with pyridine or isomeric picolines or benzene or toluene at 308.15K:	https://www.doi.org/10.1016/j.tca.2011.12.023
Chemeo Relay (1.0-beta):	
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1297.mol
Topological and thermodynamic investigations of binary mixtures: Molar excess volumes, molar excess enthalpies and isentropic compressibility changes of mixing:	https://www.doi.org/10.1016/j.tca.2008.06.004
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Thermodynamics of mixtures containing amines VI. Liquid liquid equilibria for mixtures of o-toluidine + selected alkanes:	https://www.doi.org/10.1016/j.fluid.2007.01.022
Molar Excess Volumes and Excess Isentropic Compressibilities of {2-Methylaniline (i) + Benzene (j) + Methylbenzene}, {2-Methylaniline (i) + Benzene (j) + 1,2-Dimethylbenzene (k)}, and {2-Methylaniline (i) + Benzene (j) + 1,4-Dimethylbenzene (k)} at T = 308.15 K:	https://www.doi.org/10.1021/je900237e
Heat capacities of aqueous polar aromatic compounds over a wide range of conditions:	https://www.doi.org/10.1016/j.jct.2004.09.004
Thermodynamic and topological investigations of ternary mixtures with o-toluidine + tetrahydropyran:	https://www.doi.org/10.1016/j.jct.2011.10.002
Thermodynamic Properties of Ternary Mixtures Containing ... Excess Molar Volume and Excess Isentropic Compressibility:	https://www.doi.org/10.1021/je4004965
Thermodynamic studies of molecular interactions in mixtures of o-toluidine with pyridine and picolines: Excess molar volumes, excess molar enthalpies, and excess isentropic compressibilities:	https://www.doi.org/10.1016/j.jct.2010.12.028
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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 changes of mixing:	https://www.doi.org/10.1016/j.tca.2010.07.027
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
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

pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume