Benzene, 1-chloro-2-methyl-

Other names:	1-Chloro-2-methylbenzene
	1-METHYL-2-CHLOROBENZENE
	2-Chloro-1-methylbenzene
	2-Chlorotoluene
	2-Methylchlorobenzene
	Halso 99
	NSC 8766
	O-CHLOROTOLUENE
	O-TOLYL CHLORIDE
	Toluene, o-chloro-
	ortho-Chlorotoluene
Inchi:	InChI=1S/C7H7Cl/c1-6-4-2-3-5-7(6)8/h2-5H,1H3
InchiKey:	IBSQPLPBRSHTTG-UHFFFAOYSA-N
Formula:	C7H7Cl
SMILES:	Cc1ccccc1Cl
Mol. weight [g/mol]:	126.58
CAS:	95-49-8

Physical Properties

Property code	Value	Unit	Source
affp	790.50	kJ/mol	NIST Webbook
basg	761.10	kJ/mol	NIST Webbook
chl	-3750.00 ± 10.00	kJ/mol	NIST Webbook
gf	98.91	kJ/mol	Joback Method
hf	21.51	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	38.50 ± 0.04	kJ/mol	NIST Webbook
hvap	45.30	kJ/mol	NIST Webbook
ie	8.72 ± 0.11	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
ie	8.83 ± 0.02	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	8.62	eV	NIST Webbook
log10ws	-3.52		Estimated Solubility Method
log10ws	-3.52		Aqueous Solubility Prediction Method

logp	2.648		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	940.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	926.10		NIST Webbook
rinpol	151.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	933.60		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	926.10		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	970.00		NIST Webbook
ripol	1277.00		NIST Webbook
ripol	1277.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1288.00		NIST Webbook
tb	431.15 ± 1.50	K	NIST Webbook
tb	157.20 ± 0.50	K	NIST Webbook
tb	432.45 ± 0.50	K	NIST Webbook
tb	432.50 ± 0.50	K	NIST Webbook
tb	432.30 ± 0.20	K	NIST Webbook
tb	432.10 ± 0.20	K	NIST Webbook
tb	432.35 ± 0.30	K	NIST Webbook
tb	432.35 ± 0.50	K	NIST Webbook
tb	432.15 ± 3.00	K	NIST Webbook
tb	532.75 ± 0.20	K	NIST Webbook
tb	432.65 ± 0.30	K	NIST Webbook
tb	431.20	K	NIST Webbook
tb	432.30	K	NIST Webbook
tb	432.30	K	KDB
tb	432.25 ± 0.50	K	NIST Webbook
tc	649.87	K	Joback Method
tf	239.15 ± 2.00	K	NIST Webbook
tf	238.05 ± 0.60	K	NIST Webbook

tf	236.70 ± 0.60	K	NIST Webbook
tf	237.56 ± 0.30	K	NIST Webbook
tf	238.05 ± 0.50	K	NIST Webbook
tf	237.62	K	Aqueous Solubility Prediction Method
tf	236.65 ± 0.60	K	NIST Webbook
tf	236.65 ± 0.30	K	NIST Webbook
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.77	J/mol×K	428.65	Joback Method
cpg	174.12	J/mol×K	465.52	Joback Method
cpg	183.86	J/mol×K	502.39	Joback Method
cpg	193.00	J/mol×K	539.26	Joback Method
cpg	201.57	J/mol×K	576.13	Joback Method
cpg	209.60	J/mol×K	613.00	Joback Method
cpg	217.11	J/mol×K	649.87	Joback Method
dvisc	0.0007850	Pa×s	301.22	Joback Method
dvisc	0.0012200	Pa×s	269.37	Joback Method
dvisc	0.0021341	Pa×s	237.51	Joback Method
dvisc	0.0005496	Pa×s	333.08	Joback Method
dvisc	0.0004094	Pa×s	364.94	Joback Method
dvisc	0.0003198	Pa×s	396.79	Joback Method
dvisc	0.0002591	Pa×s	428.65	Joback Method
hfust	10.30	kJ/mol	237.00	NIST Webbook
hvapt	41.60	kJ/mol	401.00	NIST Webbook
hvapt	42.80	kJ/mol	415.50	NIST Webbook
hvapt	42.50	kJ/mol	387.50	NIST Webbook
hvapt	44.80	kJ/mol	355.00	NIST Webbook
hvapt	45.80	kJ/mol	310.50	NIST Webbook
pvap	0.21	kPa	286.10	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.50	kPa	300.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

pvap	0.43	kPa	297.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.42	kPa	297.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.43	kPa	297.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.35	kPa	294.10	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.29	kPa	291.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.23	kPa	288.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.62	kPa	303.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.16	kPa	283.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.13	kPa	280.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.11	kPa	277.10	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

pvap	0.09	kPa	274.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	93.32	kPa	428.76	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components
pvap	79.99	kPa	422.91	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components
pvap	66.66	kPa	416.25	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components
pvap	53.33	kPa	408.41	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components
pvap	0.73	kPa	306.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	40.00	kPa	398.81	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components
rfi	1.51690		308.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluenes

rfi	1.52190		298.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluenes
rfi	1.51890		303.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluenes
rhol	1082.00	kg/m3	293.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements
rhol	1072.77	kg/m3	303.15	Excess Volumes, Speeds of Sound, Isentropic Compressibilities, and Viscosities of Binary Mixtures of Acetophenone with Chlorotoluenes and Nitrotoluenes at 303.15 K
rhol	1082.22	kg/m3	293.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhol	1077.34	kg/m3	298.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhol	1072.46	kg/m3	303.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures

rhol	1077.30	kg/m3	298.15	Densities, Speeds of Sound, Excess Molar Enthalpies, and Heat Capacities of o-Chlorotoluene and Cyclic Ether Mixtures	
rhol	1072.50	kg/m3	303.15	Densities, Speeds of Sound, Excess Molar Enthalpies, and Heat Capacities of o-Chlorotoluene and Cyclic Ether Mixtures	
rhol	1067.60	kg/m3	308.15	Densities, Speeds of Sound, Excess Molar Enthalpies, and Heat Capacities of o-Chlorotoluene and Cyclic Ether Mixtures	
rhol	1077.30	kg/m3	298.15	Thermodynamic Properties of Ternary Liquid Mixtures Containing o-Chlorotoluene: Excess Molar Volumes and Excess Isentropic Compressibilities	
rhol	1072.50	kg/m3	303.15	Thermodynamic Properties of Ternary Liquid Mixtures Containing o-Chlorotoluene: Excess Molar Volumes and Excess Isentropic Compressibilities	
rhol	1067.60	kg/m3	308.15	Thermodynamic Properties of Ternary Liquid Mixtures Containing o-Chlorotoluene: Excess Molar Volumes and Excess Isentropic Compressibilities	

rhol	1067.60	kg/m3	308.15	Excess molar volumes and excess isentropic compressibilities of binary and ternary mixtures of o-chlorotoluene with cyclic ether and amides or cyclohexane at different temperatures
rhol	1072.50	kg/m3	303.15	Excess molar volumes and excess isentropic compressibilities of binary and ternary mixtures of o-chlorotoluene with cyclic ether and amides or cyclohexane at different temperatures
rhol	1067.60	kg/m3	308.15	Topological and thermodynamic investigations of mixtures containing o-chlorotoluene and lower amides
rhol	1072.50	kg/m3	303.15	Topological and thermodynamic investigations of mixtures containing o-chlorotoluene and lower amides
rhol	1077.30	kg/m3	298.15	Topological and thermodynamic investigations of mixtures containing o-chlorotoluene and lower amides
rhol	1068.21	kg/m3	308.15	FT-IR studies on excess thermodynamic properties of binary liquid mixtures o-chlorotoluene with 1-propanol, 1-butanol, 1-pentanol, 1-hexanol and 1-heptanol at different temperatures

rhol	1072.80	kg/m3	303.15	FT-IR studies on excess thermodynamic properties of binary liquid mixtures o-chlorotoluene with 1-propanol, 1-butanol, 1-pentanol, 1-hexanol and 1-heptanol at different temperatures
rhol	1077.38	kg/m3	298.15	FT-IR studies on excess thermodynamic properties of binary liquid mixtures o-chlorotoluene with 1-propanol, 1-butanol, 1-pentanol, 1-hexanol and 1-heptanol at different temperatures
rhol	1072.82	kg/m3	303.15	Effect of various substituents on benzene ring and their impact on volumetric, acoustic and transport properties of binary liquid mixtures with dimethylacetamide
rhol	1067.60	kg/m3	308.15	Heat capacities of binary and ternary mixtures containing o-chlorotoluene, cyclic ether and aromatic hydrocarbons
rhol	1072.50	kg/m3	303.15	Heat capacities of binary and ternary mixtures containing o-chlorotoluene, cyclic ether and aromatic hydrocarbons
rhol	1077.30	kg/m3	298.15	Heat capacities of binary and ternary mixtures containing o-chlorotoluene, cyclic ether and aromatic hydrocarbons

rhol	1064.01	kg/m3	313.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1068.21	kg/m3	308.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1072.86	kg/m3	303.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1076.47	kg/m3	298.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1068.00	kg/m3	308.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements	
rhol	1073.00	kg/m3	303.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements	
rhol	1077.00	kg/m3	298.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements	

rhol	1077.30	kg/m3	298.15	Excess molar volumes and excess isentropic compressibilities of binary and ternary mixtures of o-chlorotoluene with cyclic ether and amides or cyclohexane at different temperatures

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41771e+01
Coeff. B	-3.53502e+03
Coeff. C	-6.13290e+01
Temperature range (K), min.	315.84
Temperature range (K), max.	460.06

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.83417e+01
Coeff. B	-7.97006e+03
Coeff. C	-9.26611e+00
Coeff. D	5.07756e-06
Temperature range (K), min.	236.65
Temperature range (K), max.	656.00

Datasets

Viscosity, Pa*s

Pressure, kPa - Liquid	Temperature, K - Liquid	Viscosity, Pa*s - Liquid
101.00	303.15	0.0008870

Reference *https://www.doi.org/10.1016/j.jct.2006.04.005*

Sources

Excess heat capacities of mixtures containing 1-methylpyrrolidin-2-one, chlorotoluenes and benzene:	https://www.doi.org/10.1016/j.jct.2014.12.022
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures:	https://www.doi.org/10.1021/je400408w
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Excess molar volumes and excess isentropic compressibilities of binary and ternary mixtures of o-chlorotoluene with cyclic ether and amides at 303.15 K:	https://www.doi.org/10.1016/j.jct.2014.06.030
Determination and correlation of vapor liquid equilibrium for binary systems of chlorotoluene and cyclohexane at different temperatures:	https://www.doi.org/10.1016/j.fluid.2007.01.042
Thermodynamics of binary mixtures containing 2-chlorotoluene and amides:	https://www.doi.org/10.1016/j.fluid.2014.01.019
The effect of substituents in aromatics on their excess properties with benzylalcohol:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1702
Determination of Henry's Law Constants Using Internal Standards and Benchmark Values:	https://www.doi.org/10.1021/je3010535
Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes:	https://www.doi.org/10.1016/j.fluid.2014.07.029
Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluene at 303.15 K:	https://www.doi.org/10.1007/s10765-011-0995-x
Topological and thermodynamic investigations of mixtures containing o-chlorotoluene and lower amides:	https://www.doi.org/10.1016/j.jct.2013.12.006
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Volumetric, ultrasonic and viscometric studies of binary mixtures of dimethyl sulfoxide with chloro and nitro substituted aromatic hydrocarbons at T = 303.15 K: Effect of chlorine atom and nitro group:	https://www.doi.org/10.1016/j.jct.2006.04.005
Excess Volumes, Speeds of Sound, Isentropic Compressibilities, and Excess Isentropic Compressibilities of Binary Mixtures of Chlorotoluenes and 1-Propanol, 1-Butanol, 1-Pentanol, 1-Hexanol, and 1-Heptanol at Different Temperatures and Speed of sound measurements:	https://www.doi.org/10.1021/je050413l
FT-IR studies on excess thermodynamic properties of binary mixtures of chlorotoluenes and 1-propanol at 303.15 K: Influence of chlorine atom position and intermolecular interactions between the components:	https://www.doi.org/10.1016/j.jct.2013.08.013
Miscibility Prediction Method:	https://www.doi.org/10.1016/j.jct.2017.11.003
KDB Vapor Pressure Data:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1702
Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Heat capacities of binary and ternary mixtures containing o-chlorotoluene, cyclic ether and aromatic hydrocarbons:	https://en.wikipedia.org/wiki/Joback_method
Thermodynamic Properties of Ternary Liquid Mixtures Containing o-Chlorotoluene: Excess Molar Volumes, Excess Isentropic Compressibilities, Chlorotoluenes and Cyclic Ethers at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2014.06.024
Densities and ultrasonic studies for binary mixtures of tetrahydrofuran with chlorotoluenes at 298.15 K:	https://www.doi.org/10.1021/je5004719
Effect of various substituents on benzene ring and their impact on volumetric, acoustic and transport properties of binary liquid mixtures with dimethylacetamide:	https://www.doi.org/10.1016/j.fluid.2011.07.018
Volumetric, Speeds of Sound, Excess Molar Enthalpies, and Heat Capacities at 298.15 K for Chlorotoluene and Cyclic Ether Mixtures:	https://www.doi.org/10.1016/j.fluid.2015.03.048
	https://www.doi.org/10.1021/je400722h
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95498&Units=SI

Legend

affp: Proton affinity

basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume