Benzene, 1-chloro-4-methyl-

Other names:	1-Chloro-4-methylbenzene
	1-METHYL-4-CHLOROBENZENE
	4-Chloro-1-methylbenzene
	4-Chlorotoluene
	4-Methylphenyl chloride
	4-Tolyl chloride
	NSC 404114
	P-TOLYL CHLORIDE
	Toluene, p-chloro-
	p-Chlorotoluene
	para-Chlorotoluene
	toluene, 4-chloro-
Inchi:	InChI=1S/C7H7Cl/c1-6-2-4-7(8)5-3-6/h2-5H,1H3
InchiKey:	NPDACUSDTOMAMK-UHFFFAOYSA-N
Formula:	C7H7Cl
SMILES:	Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	126.58
CAS:	106-43-4

Physical Properties

Property code	Value	Unit	Source
affp	762.90	kJ/mol	NIST Webbook
basg	735.20	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	46.00	kJ/mol	NIST Webbook
hvap	38.70 ± 0.02	kJ/mol	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.69 ± 0.02	eV	NIST Webbook
ie	8.70 ± 0.02	eV	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
ie	8.69 ± 0.03	eV	NIST Webbook
log10ws	-3.08		Estimated Solubility Method

log10ws	-3.08		Aqueous Solubility Prediction Method
logp	2.648		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	997.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	944.40		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	938.50		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	944.40		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	961.70		NIST Webbook
rinpol	956.40		NIST Webbook
rinpol	936.30		NIST Webbook
rinpol	151.00		NIST Webbook
rinpol	941.30		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1304.00		NIST Webbook
tb	435.55 ± 0.30	K	NIST Webbook
tb	434.65 ± 1.50	K	NIST Webbook
tb	435.55	K	KDB
tb	435.20	K	NIST Webbook
tb	435.25 ± 0.40	K	NIST Webbook
tb	434.40 ± 0.60	K	NIST Webbook
tb	433.70 ± 3.00	K	NIST Webbook
tb	435.60 ± 0.60	K	NIST Webbook
tb	435.55 ± 0.30	K	NIST Webbook
tb	435.25 ± 0.50	K	NIST Webbook
tb	435.60 ± 0.50	K	NIST Webbook
tb	434.85 ± 0.30	K	NIST Webbook
tb	435.65 ± 0.30	K	NIST Webbook
tb	435.13 ± 0.20	K	NIST Webbook
tc	615.90 ± 0.50	K	NIST Webbook
tf	280.65	K	Aqueous Solubility Prediction Method

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	209.60	J/mol×K	613.00	Joback Method
cpg	201.57	J/mol×K	576.13	Joback Method
cpg	193.00	J/mol×K	539.26	Joback Method
cpg	183.86	J/mol×K	502.39	Joback Method
cpg	174.12	J/mol×K	465.52	Joback Method
cpg	217.11	J/mol×K	649.87	Joback Method
dvisc	0.0012200	Pa×s	269.37	Joback Method
dvisc	0.0007850	Pa×s	301.22	Joback Method
dvisc	0.0002591	Pa×s	428.65	Joback Method
dvisc	0.0003198	Pa×s	396.79	Joback Method
dvisc	0.0005496	Pa×s	333.08	Joback Method
dvisc	0.0004094	Pa×s	364.94	Joback Method
dvisc	0.0021341	Pa×s	237.51	Joback Method
hfust	13.55	kJ/mol	280.70	NIST Webbook
hfust	13.55	kJ/mol	280.70	NIST Webbook
hvapt	41.80	kJ/mol	398.50	NIST Webbook
hvapt	43.50	kJ/mol	385.50	NIST Webbook
hvapt	44.10	kJ/mol	357.00	NIST Webbook
hvapt	41.70	kJ/mol	370.00	NIST Webbook
pvap	0.11	kPa	278.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.12	kPa	280.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.17	kPa	285.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

pvap	0.22	kPa	288.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.22	kPa	288.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.21	kPa	288.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.27	kPa	291.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.33	kPa	294.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.40	kPa	297.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.47	kPa	300.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.09	kPa	276.10	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.57	kPa	303.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.70	kPa	306.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

pvap	40.00	kPa	401.71	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components	
pvap	53.33	kPa	411.34	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components	
pvap	0.83	kPa	309.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes	
pvap	79.99	kPa	425.90	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components	
pvap	93.32	kPa	431.77	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components	
pvap	0.08	kPa	274.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes	
pvap	0.08	kPa	274.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes	
pvap	66.66	kPa	419.20	Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components	

pvap	0.14	kPa	282.10	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
rfi	1.51880		298.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluenes
rfi	1.51380		308.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluenes
rfi	1.51660		303.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluenes
rhol	1064.93	kg/m3	298.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol
rhol	1069.27	kg/m3	293.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhol	1060.54	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	1054.00	kg/m3	308.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements
rhol	1065.00	kg/m3	298.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements
rhol	1069.00	kg/m3	293.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements
rhol	1065.14	kg/m3	298.15	Effect of various substituents on benzene ring and their impact on volumetric, acoustic and transport properties of binary liquid mixtures with dimethylacetamide
rhol	1049.29	kg/m3	313.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol
rhol	1054.27	kg/m3	308.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol

rhol	1059.56	kg/m3	303.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol
rhol	1064.37	kg/m3	298.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhol	1059.46	kg/m3	303.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhol	1060.00	kg/m3	303.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	317.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41461e+01
Coeff. B	-3.55136e+03
Coeff. C	-6.22610e+01
Temperature range (K), min.	318.52
Temperature range (K), max.	464.24

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.00378e+02
Coeff. B	-9.03187e+03
Coeff. C	-1.25791e+01
Coeff. D	7.49089e-06
Temperature range (K), min.	280.65
Temperature range (K), max.	660.00

Datasets

Viscosity, Pa*s

Pressure, kPa - Liquid	Temperature, K - Liquid	Viscosity, Pa*s - Liquid
101.00	303.15	0.0009000

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

Sources

Thermodynamics of binary mixtures:	https://www.doi.org/10.1016/j.fluid.2014.01.019
The effect of substituents in aromatics on their excess properties with benzylalcohol:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Solubility and dissolution mechanism of 4-chlorotoluene in subcritical water investigated in a fused silica capillary reactor by in situ Raman spectroscopy:	https://www.doi.org/10.1016/j.fluid.2016.05.018
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures:	https://www.doi.org/10.1021/je400408w
Measurement and Correlation of Diffusion Coefficients of Aromatic Compounds at Infinite Dilution in Alkane and Cycloalkane Solvents:	https://www.doi.org/10.1021/je6005604
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess heat capacities of mixtures containing 1-methylpyrrolidin-2-one, chlorotoluenes and benzene:	https://www.doi.org/10.1016/j.jct.2014.12.022
Volumetric, ultrasonic and viscometric studies of binary mixtures of dimethyl sulphoxide with chloro and nitro substituted aromatic hydrocarbons at T = 303.15 K:	https://www.doi.org/10.1016/j.jct.2006.04.005
Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluenes:	https://www.doi.org/10.1007/s10765-011-0995-x
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1704.mol
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.2015.03.048
Determination of Henry's Law Constants Using Internal Standards	https://www.doi.org/10.1021/je3010535
NIST Webbook, values:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106434&Units=SI
Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes:	https://www.doi.org/10.1016/j.fluid.2014.07.029

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Densities and ultrasonic studies for binary mixtures of tetrahydrofuran with chlorobenzenes, chlorotoluenes and nitrotoluenes at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2011.07.018
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1704
Excess Volumes, Speeds of Sound, Isentropic Compressibilities, and Viscosities of Binary Mixtures of Acetophenone with Chlorotoluenes and Nitrotoluenes at 303.15 K:	https://www.doi.org/10.1021/je050413l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Determination and correlation of vapor liquid equilibrium for binary systems consisting of close-boiling components:	https://www.doi.org/10.1016/j.fluid.2007.01.042
Diffusion Coefficients of Aromatic Compounds at Infinite Dilution in Binary Mixtures at 298.15 K:	https://www.doi.org/10.1021/je060289l
Influence of chlorine atom on interactions between non-hydrocarbons and 1-alkanol: Density and speed of sound measurements:	https://www.doi.org/10.1016/j.jct.2017.11.003
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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