

Benzene, 1-chloro-3-methyl-

Other names:	1-Chloro-3-methylbenzene
	1-Chloro-5-methylbenzene
	1-METHYL-3-CHLOROBENZENE
	3-Chloro-1-methylbenzene
	3-Chlorotoluene
	M-TOLYL CHLORIDE
	NSC 8767
	Toluene, m-chloro-
	m-Chlorotoluene
	meta-Chlorotoluene
Inchi:	InChI=1S/C7H7Cl/c1-6-3-2-4-7(8)5-6/h2-5H,1H3
InchiKey:	OSOUNOBYRMOXQQ-UHFFFAOYSA-N
Formula:	C7H7Cl
SMILES:	Cc1cccc(Cl)c1
Mol. weight [g/mol]:	126.58
CAS:	108-41-8

Physical Properties

Property code	Value	Unit	Source
affp	783.90	kJ/mol	NIST Webbook
basg	754.50	kJ/mol	NIST Webbook
chl	-3751.00 ± 8.00	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	kJ/mol	Joback Method
ie	8.70 ± 0.10	eV	NIST Webbook
ie	8.83 ± 0.02	eV	NIST Webbook
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	934.90		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	959.00		NIST Webbook

rinpol	932.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	150.00		NIST Webbook
rinpol	160.70		NIST Webbook
rinpol	160.70		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	150.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	927.70		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	933.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1291.00		NIST Webbook
tb	431.20 ± 2.00	K	NIST Webbook
tb	435.20	K	NIST Webbook
tb	434.89 ± 0.20	K	NIST Webbook
tc	649.87	K	Joback Method
tf	224.26 ± 0.60	K	NIST Webbook
tf	246.90	K	NIST Webbook
tf	225.35 ± 2.00	K	NIST Webbook
tf	225.35 ± 0.50	K	NIST Webbook
tf	225.20	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	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
cpg	174.12	J/mol×K	465.52	Joback Method
dvisc	0.0003198	Pa×s	396.79	Joback Method
dvisc	0.0004094	Pa×s	364.94	Joback Method

dvisc	0.0021341	Pa×s	237.51	Joback Method
dvisc	0.0012200	Pa×s	269.37	Joback Method
dvisc	0.0007850	Pa×s	301.22	Joback Method
dvisc	0.0005496	Pa×s	333.08	Joback Method
dvisc	0.0002591	Pa×s	428.65	Joback Method
hvapt	46.20	kJ/mol	310.50	NIST Webbook
hvapt	43.70	kJ/mol	356.50	NIST Webbook
hvapt	41.90	kJ/mol	404.00	NIST Webbook
pvap	0.21	kPa	288.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.26	kPa	291.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.82	kPa	309.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.69	kPa	306.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.58	kPa	303.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.48	kPa	300.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.38	kPa	297.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.31	kPa	294.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

pvap	0.18	kPa	286.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.14	kPa	283.10	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	0.10	kPa	277.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.31	kPa	294.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.08	kPa	274.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
rfi	1.51690		308.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1-Decanol with Isomeric Chlorotoluenes
rfi	1.52070		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
rhoI	1062.33	kg/m3	303.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhoI	1058.00	kg/m3	308.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements
rhoI	1063.00	kg/m3	303.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements
rhoI	1072.00	kg/m3	293.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements
rhoI	1072.15	kg/m3	293.15	Effect of various substituents on benzene ring and their impact on volumetric, acoustic and transport properties of binary liquid mixtures with dimethylacetamide
rhoI	1053.49	kg/m3	313.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol

rhoI	1058.29	kg/m3	308.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol
rhoI	1062.79	kg/m3	303.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol
rhoI	1067.25	kg/m3	298.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol
rhoI	1065.22	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
rhoI	1072.12	kg/m3	293.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhoI	1067.23	kg/m3	298.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhoI	1067.00	kg/m3	298.15	Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41128e+01
Coeff. B	-3.54140e+03
Coeff. C	-6.22050e+01
Temperature range (K), min.	318.36
Temperature range (K), max.	464.58

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	2.97198e+01
Coeff. B	-5.59588e+03
Coeff. C	-2.06159e+00
Coeff. D	1.42367e-06
Temperature range (K), min.	278.15
Temperature range (K), max.	435.15

Datasets

Viscosity, Pa*s

Pressure, kPa - Liquid	Temperature, K - Liquid	Viscosity, Pa*s - Liquid
101.00	303.15	0.0007800
Reference		https://www.doi.org/10.1016/j.jct.2006.04.005

Sources

Influence of chlorine atom on interactions between halo-hydrocarbons and 1-nonanol: Density and speed of sound measurements:

<https://www.doi.org/10.1016/j.jct.2017.11.003>

Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 1,3-dioxolane with Excesses of tetrahydrofuran, 2-methyltetrahydrofuran, 2-methylpyrrolidin-2-one, and benzene:

Effect of various substituents on benzene ring and their impact on aqueous solubility Prediction Method: properties of binary liquid mixtures with dimethylacetamide:

The Yaws Handbook of Vapor Pressure: KDB:

Vaporization enthalpies of a series of the fluoro- and chloro-substituted Methylenes:

Crippen Method:

Densities and ultrasonic studies for binary mixtures of tetrahydrofuran with Excess Volumes, Speeds of Sound, Isoentropic Compressibilities, and Viscosities of Binary Mixtures of studies of binary mixtures of dimethylacetamide with 1,3-dioxolane and 2-methyltetrahydrofuran + 2-methylpyrrolidin-2-one + benzene at 303.15 K. Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol:

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<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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<https://www.doi.org/10.1021/je400408w>

<https://www.doi.org/10.1016/j.fluid.2014.01.019>

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1703>

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
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
rhof:	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

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