Benzene, 1,3-dichloro-

Other names:	1,3-DICHLOROBENZENE
	Benzene, m-dichloro-
	Metadichlorobenzene
	Rcra waste number U071
	m-Dichlorobenzene
	m-Dichlorobenzol
	m-Phenylene dichloride
Inchi:	InChI=1S/C6H4Cl2/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	ZPQOPVIELGIULI-UHFFFAOYSA-N
Formula:	C6H4Cl2
SMILES:	Clc1cccc(Cl)c1
Mol. weight [g/mol]:	147.00
CAS:	541-73-1

Physical Properties

Property code	Value	Unit	Source
chl	-2955.76 ± 0.96	kJ/mol	NIST Webbook
chl	-2952.00 ± 8.00	kJ/mol	NIST Webbook
chl	-2960.30	kJ/mol	NIST Webbook
gf	78.56	kJ/mol	Joback Method
hf	28.10	kJ/mol	NIST Webbook
hfl	-20.50 ± 0.96	kJ/mol	NIST Webbook
hfpi	903.30	kJ/mol	NIST Webbook
hfpiz	915.90	kJ/mol	NIST Webbook
hfus	13.34	kJ/mol	Joback Method
hvap	53.90	kJ/mol	NIST Webbook
hvap	47.00	kJ/mol	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	9.10 ± 0.02	eV	NIST Webbook
ie	9.14 ± 0.03	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.12 ± 0.02	eV	NIST Webbook
ie	9.11 ± 0.01	eV	NIST Webbook
ie	9.10 ± 0.02	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	9.12 ± 0.01	eV	NIST Webbook

log10ws	-3.04		Estimated Solubility Method
log10ws	-3.05		Aqueous Solubility Prediction Method
logp	2.993		Crippen Method
mcvol	96.120	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	4151.61	kPa	Joback Method
rinpol	1002.37		NIST Webbook
rinpol	1036.20		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1024.65		NIST Webbook
rinpol	1004.07		NIST Webbook
rinpol	1013.30		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1014.97		NIST Webbook
rinpol	1015.34		NIST Webbook
rinpol	1017.77		NIST Webbook
rinpol	1018.92		NIST Webbook
rinpol	975.40		NIST Webbook
rinpol	1020.90		NIST Webbook
rinpol	986.21		NIST Webbook
rinpol	985.10		NIST Webbook
rinpol	1022.50		NIST Webbook
rinpol	997.98		NIST Webbook
rinpol	999.87		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1007.00		NIST Webbook

rinpol	1005.00	NIST Webbook
rinpol	1002.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1014.00	NIST Webbook
rinpol	1022.00	NIST Webbook
rinpol	1022.50	NIST Webbook
rinpol	988.00	NIST Webbook
rinpol	1005.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	986.00	NIST Webbook
rinpol	982.00	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	981.00	NIST Webbook
rinpol	981.00	NIST Webbook
rinpol	981.00	NIST Webbook
rinpol	982.00	NIST Webbook
rinpol	162.00	NIST Webbook
rinpol	160.40	NIST Webbook
rinpol	1025.00	NIST Webbook
rinpol	1004.00	NIST Webbook
rinpol	1017.40	NIST Webbook
rinpol	1022.50	NIST Webbook
rinpol	1004.07	NIST Webbook
rinpol	964.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1007.00	NIST Webbook
rinpol	1013.80	NIST Webbook
rinpol	1022.00	NIST Webbook
rinpol	975.40	NIST Webbook
rinpol	997.98	NIST Webbook
rinpol	985.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1005.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	1027.35	NIST Webbook
rinpol	1027.05	NIST Webbook
rinpol	1020.06	NIST Webbook
rinpol	1017.40	NIST Webbook
rinpol	162.00	NIST Webbook
rinpol	964.00	NIST Webbook
ripol	1418.00	NIST Webbook
ripol	1477.00	NIST Webbook
ripol	1453.00	NIST Webbook

ripol	1455.40		NIST Webbook
ripol	1474.10		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1445.33		NIST Webbook
ripol	1438.32		NIST Webbook
ripol	1417.70		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1451.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1418.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1455.40		NIST Webbook
ripol	1445.33		NIST Webbook
tb	446.15	K	Excess molar volumes of ternary mixtures of 1,3-dichlorobenzene and methyl ethyl ketone with 1-alkanols at 303.15K
tb	446.20	K	NIST Webbook
tb	446.15	K	KDB
tb	446.15 ± 0.07	K	NIST Webbook
tc	674.86	K	Joback Method
tf	248.25	K	Aqueous Solubility Prediction Method
tf	248.39	K	KDB
tf	248.39 ± 0.05	K	NIST Webbook
tf	248.75 ± 0.50	K	NIST Webbook
tf	246.90 ± 0.20	K	NIST Webbook
tf	249.00 ± 2.00	K	NIST Webbook
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.77	J/mol×K	674.86	Joback Method
cpg	149.05	J/mol×K	443.20	Joback Method
cpg	157.36	J/mol×K	481.81	Joback Method
cpg	165.09	J/mol×K	520.42	Joback Method

cpg	172.26	J/mol×K	559.03	Joback Method
cpg	178.92	J/mol×K	597.64	Joback Method
cpg	185.08	J/mol×K	636.25	Joback Method
cpl	183.20	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	167.15	J/mol×K	283.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	167.54	J/mol×K	285.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	167.93	J/mol×K	287.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	168.32	J/mol×K	289.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	168.72	J/mol×K	291.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	169.13	J/mol×K	293.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	169.55	J/mol×K	295.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	169.97	J/mol×K	297.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	170.90	J/mol×K	298.15	NIST Webbook
cpl	170.82	J/mol×K	301.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	171.25	J/mol×K	303.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	171.69	J/mol×K	305.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	172.14	J/mol×K	307.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	172.58	J/mol×K	309.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	173.04	J/mol×K	311.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	173.49	J/mol×K	313.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	173.95	J/mol×K	315.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	174.41	J/mol×K	317.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	174.88	J/mol×K	319.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	175.35	J/mol×K	321.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	175.83	J/mol×K	323.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.30	J/mol×K	325.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.78	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.26	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.75	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	178.24	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.73	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.22	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.71	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	180.20	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	180.70	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.20	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.70	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	182.20	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	182.70	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	170.39	J/mol×K	299.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
dvisc	0.0003668	Pa×s	412.03	Joback Method
dvisc	0.0021588	Pa×s	256.16	Joback Method
dvisc	0.0012985	Pa×s	287.33	Joback Method
dvisc	0.0008628	Pa×s	318.51	Joback Method
dvisc	0.0006166	Pa×s	349.68	Joback Method
dvisc	0.0002989	Pa×s	443.20	Joback Method
dvisc	0.0004656	Pa×s	380.85	Joback Method
hfust	12.60	kJ/mol	248.30	NIST Webbook
hfust	12.64	kJ/mol	248.40	NIST Webbook
hfust	12.64	kJ/mol	248.40	NIST Webbook
hfust	12.59	kJ/mol	248.75	NIST Webbook
hvapt	44.70	kJ/mol	430.50	NIST Webbook
hvapt	50.40	kJ/mol	248.00	NIST Webbook
hvapt	50.00	kJ/mol	262.00	NIST Webbook
hvapt	44.10	kJ/mol	402.50	NIST Webbook
rfi	1.54400		298.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Octanol with Chlorobenzenes
rfi	1.54100		303.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Octanol with Chlorobenzenes

rfi	1.53800		308.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Octanol with Chlorobenzenes
rfi	1.54320		298.15	Liquid-Liquid Equilibria for Mixtures of (Furfural + a Chlorinated Aromatic Compound + an Alkane) at T = 298.15 K
rhol	1282.87	kg/m3	298.15	Experimental and predicted data of excess molar enthalpies and excess molar volumes for the ternary system (1,3-dichlorobenzene + benzene + 1-chlorohexane) at T = 298.15 K
rhol	1277.16	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
sfust	50.60	J/mol×K	248.75	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45419e+01
Coeff. B	-3.97801e+03
Coeff. C	-4.53350e+01
Temperature range (K), min.	324.41
Temperature range (K), max.	476.30

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.72737e+01
Coeff. B	-7.22933e+03
Coeff. C	-6.05176e+00
Coeff. D	2.34995e-06
Temperature range (K), min.	248.39
Temperature range (K), max.	683.95

Datasets

Viscosity, Pa*s

Pressure, kPa - Liquid	Temperature, K - Liquid	Viscosity, Pa*s - Liquid
101.00	303.15	0.0010250
Reference		*https://www.doi.org/10.1016/j.jct.2006.04.005*

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1678.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1678
Liquid-Liquid Equilibria for Mixtures of (Furfural + a Chlorinated Aromatic Compound + an Alkane) at T = 298.15 K:	https://www.doi.org/10.1021/je020107x
Measurement and Prediction of Excess Molar Enthalpies and Excess Molar Volumes of the Ternary System 1,3-dichlorobenzene + Benzene + Hexane at 298.15 K.:	https://www.doi.org/10.1021/je034237x
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of Ethanol with Chlorobenzenes:	https://www.doi.org/10.1007/s10765-011-1087-7
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
The Critical Temperatures of a Number of (i) (Chloroalkane (C3 C4) + Hydrocarbon (C6 C7)) Binary Mixtures and (ii) (Aromatic Halocarbon (Chlorobenzene, Fluorobenzene, 1,2-Dichlorobenzene, or 1,3-Dichlorobenzene) + Alkane (C8)) Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00191

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Effect of various substituents on benzene ring and their impact on volumetric, acoustic and transport properties of binary liquid mixtures with dimethylformamide: 1-alkanols at 303.15K:	https://www.doi.org/10.1016/j.fluid.2015.03.048
Excess molar volumes of ternary mixtures of 1,3-dichlorobenzene and methanol, 1-propanol, and 1-hexanol at 303.15K:	https://www.doi.org/10.1016/j.fluid.2006.04.010
Heat Capacities and Densities of Some Fluoro-, Chloro-, Bromo-, and Bromochloro-Substituted Benzenes:	https://www.doi.org/10.1021/je600573w
Experimental and predicted data of excess molar enthalpies and excess molar volumes for the ternary system (1,3-dichlorobenzene + benzene + 1-chlorohexane) at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2013.12.024

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfpiz:	Enthalpy of formation of positive ion at 0K
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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