Butane, 1,4-dichloro-

Other names:	1,4-Dichlorobutane
	TETRAMETHYLENE CHLORIDE
Inchi:	InChI=1S/C4H8Cl2/c5-3-1-2-4-6/h1-4H2
InchiKey:	KJDRSWPQXHESDQ-UHFFFAOYSA-N
Formula:	C4H8Cl2
SMILES:	ClCCCCCl
Mol. weight [g/mol]:	127.01
CAS:	110-56-5

Physical Properties

Property code	Value	Unit	Source
chl	-2534.80 ± 1.90	kJ/mol	NIST Webbook
gf	-41.06	kJ/mol	Joback Method
hf	-183.40 ± 1.90	kJ/mol	NIST Webbook
hfl	-229.50	kJ/mol	NIST Webbook
hfl	-229.80 ± 1.90	kJ/mol	NIST Webbook
hfus	14.51	kJ/mol	Joback Method
hvap	33.27	kJ/mol	Joback Method
ie	11.03	eV	NIST Webbook
log10ws	-1.80		Crippen Method
logp	2.244		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	894.10		NIST Webbook
rinpol	898.10		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	867.40		NIST Webbook
tb	428.15	K	KDB
tc	547.67	K	Joback Method
tf	234.50 ± 0.40	K	NIST Webbook
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.05	J/mol×K	426.41	Joback Method
cpg	149.02	J/mol×K	396.09	Joback Method
cpg	169.22	J/mol×K	487.04	Joback Method
cpg	181.25	J/mol×K	547.67	Joback Method
cpg	175.37	J/mol×K	517.35	Joback Method
cpg	162.78	J/mol×K	456.72	Joback Method
cpg	141.67	J/mol×K	365.78	Joback Method
cpl	184.00	J/mol×K	298.15	NIST Webbook
cpl	183.59	J/mol×K	298.15	NIST Webbook
dvisc	0.0041179	Pa×s	194.68	Joback Method
dvisc	0.0004401	Pa×s	337.26	Joback Method
dvisc	0.0005835	Pa×s	308.75	Joback Method
dvisc	0.0008192	Pa×s	280.23	Joback Method
dvisc	0.0012422	Pa×s	251.71	Joback Method
dvisc	0.0020950	Pa×s	223.20	Joback Method
dvisc	0.0003469	Pa×s	365.78	Joback Method
hvapt	43.40	kJ/mol	380.50	NIST Webbook
pvap	2.21	kPa	323.15	Excess molar enthalpies and (vapour + liquid) equilibria for mixtures containing N,N-dialkylamides and a,x-dichloroalkanes
pvap	2.21	kPa	323.15	Excess enthalpies and isothermal (vapour + liquid) equilibria of (1-methyl-2-pyrrolidone + 1-chloroalkane or +,?-dichloroalkane) mixtures
rfi	1.45190		298.15	Isothermal (vapour + liquid) equilibria and excess Gibbs free energies in some binary (cyclopentanone + chloroalkane) mixtures at temperatures from 298.15 K to 318.15 K

rfi	1.45200		298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I: HE and V E for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6
rfi	1.45220		298.15	Isothermal (vapour + liquid) equilibria for (nitromethane or nitroethane + 1,4-dichlorobutane) binary systems at temperatures between (343.15 and 363.15) K
rhol	1112.00	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1133.94	kg/m3	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1123.00	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1132.50	kg/m3	298.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K

rhol	1121.54	kg/m3	308.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K
rhol	1143.43	kg/m3	288.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K
rhol	1110.61	kg/m3	318.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K
rhol	1121.61	kg/m3	308.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K
rhol	1132.57	kg/m3	298.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K

rhol	1110.54	kg/m3	318.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K	
rhol	1143.49	kg/m3	288.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K	
rhol	1135.00	kg/m3	298.15	Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at T = 298.15 K	
speedsl	1251.00	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1215.66	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	

speedsl	1286.64	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
srf	0.03	N/m	303.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	298.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	293.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	313.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	308.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62874e+01
Coeff. B	-4.19096e+03
Coeff. C	-5.08480e+01
Temperature range (K), min.	312.79
Temperature range (K), max.	432.68

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.77758e+01
Coeff. B	-7.95407e+03
Coeff. C	-9.14431e+00
Coeff. D	4.66169e-06
Temperature range (K), min.	235.85
Temperature range (K), max.	641.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
288.15	100.00	1143.7
288.15	500.00	1144.1
288.15	1000.00	1144.5
288.15	1500.00	1144.8
288.15	2000.00	1145.2
288.15	2500.00	1145.5
288.15	3000.00	1145.9
288.15	3600.00	1146.4
288.15	4100.00	1146.7
288.15	4600.00	1147.0
288.15	5100.00	1147.4
288.15	5600.00	1147.7
288.15	6100.00	1148.1
288.15	6600.00	1148.5
288.15	7100.00	1148.9
288.15	7600.00	1149.2
288.15	8100.00	1149.5
288.15	8600.00	1149.9
288.15	9200.00	1150.3
288.15	9600.00	1150.7
288.15	10100.00	1151.0
288.15	10600.00	1151.3
288.15	11100.00	1151.7
288.15	11600.00	1152.0
288.15	12100.00	1152.4

288.15	12600.00	1152.7
288.15	13100.00	1153.1
288.15	13500.00	1153.3
288.15	14200.00	1153.8
288.15	14700.00	1154.1
288.15	15200.00	1154.4
288.15	15700.00	1154.8
288.15	16300.00	1155.2
288.15	16800.00	1155.6
288.15	17300.00	1155.9
288.15	17800.00	1156.2
288.15	18300.00	1156.5
288.15	18800.00	1156.8
288.15	19100.00	1157.1
288.15	19700.00	1157.4
288.15	20200.00	1157.8
298.15	100.00	1133.7
298.15	500.00	1134.0
298.15	1000.00	1134.4
298.15	1500.00	1134.8
298.15	2000.00	1135.2
298.15	2500.00	1135.6
298.15	3100.00	1136.1
298.15	3600.00	1136.4
298.15	4100.00	1136.8
298.15	4600.00	1137.2
298.15	5100.00	1137.6
298.15	5600.00	1137.9
298.15	6100.00	1138.4
298.15	6600.00	1138.7
298.15	7100.00	1139.1
298.15	7600.00	1139.4
298.15	8100.00	1139.8
298.15	8600.00	1140.2
298.15	9200.00	1140.6
298.15	9600.00	1141.0
298.15	10100.00	1141.4
298.15	10700.00	1141.8
298.15	11100.00	1142.1
298.15	11600.00	1142.4
298.15	12100.00	1142.8
298.15	12600.00	1143.2
298.15	13100.00	1143.6
298.15	13600.00	1143.9

298.15	14100.00	1144.2
298.15	14700.00	1144.6
298.15	15200.00	1145.0
298.15	15700.00	1145.4
298.15	16200.00	1145.8
298.15	16700.00	1146.1
298.15	17200.00	1146.5
298.15	17800.00	1146.9
298.15	18300.00	1147.2
298.15	18800.00	1147.6
298.15	19200.00	1147.9
298.15	19700.00	1148.2
298.15	20200.00	1148.7
308.15	100.00	1122.3
308.15	500.00	1122.7
308.15	1000.00	1123.1
308.15	1500.00	1123.5
308.15	2000.00	1123.9
308.15	2500.00	1124.3
308.15	3100.00	1124.8
308.15	3600.00	1125.2
308.15	4100.00	1125.6
308.15	4600.00	1126.0
308.15	5100.00	1126.4
308.15	5600.00	1126.9
308.15	6100.00	1127.2
308.15	6600.00	1127.5
308.15	7100.00	1128.0
308.15	7600.00	1128.4
308.15	8100.00	1128.8
308.15	8600.00	1129.2
308.15	9200.00	1129.6
308.15	9600.00	1130.0
308.15	10100.00	1130.4
308.15	10600.00	1130.9
308.15	11100.00	1131.2
308.15	11600.00	1131.5
308.15	12100.00	1131.9
308.15	12600.00	1132.4
308.15	13100.00	1132.6
308.15	13600.00	1133.1
308.15	14100.00	1133.5
308.15	14700.00	1133.9
308.15	15100.00	1134.2

308.15	15700.00	1134.6
308.15	16200.00	1135.0
308.15	16700.00	1135.3
308.15	17200.00	1135.7
308.15	17800.00	1136.1
308.15	18300.00	1136.5
308.15	18800.00	1136.8
308.15	19200.00	1137.2
308.15	19700.00	1137.6
308.15	20200.00	1138.0
318.15	100.00	1112.0
318.15	500.00	1112.4
318.15	1000.00	1112.8
318.15	1500.00	1113.2
318.15	2000.00	1113.7
318.15	2500.00	1114.1
318.15	3100.00	1114.7
318.15	3500.00	1115.0
318.15	4100.00	1115.5
318.15	4600.00	1115.9
318.15	5100.00	1116.3
318.15	5600.00	1116.8
318.15	6100.00	1117.3
318.15	6600.00	1117.7
318.15	7100.00	1118.1
318.15	7600.00	1118.4
318.15	8100.00	1118.9
318.15	8600.00	1119.3
318.15	9200.00	1119.8
318.15	9600.00	1120.2
318.15	10100.00	1120.6
318.15	10600.00	1121.0
318.15	11100.00	1121.4
318.15	11600.00	1121.8
318.15	12100.00	1122.1
318.15	12600.00	1122.6
318.15	13000.00	1123.0
318.15	13600.00	1123.3
318.15	14200.00	1123.9
318.15	14700.00	1124.4
318.15	15200.00	1124.7
318.15	15700.00	1125.1
318.15	16300.00	1125.4
318.15	16800.00	1126.0

318.15	17300.00	1126.3
318.15	17800.00	1126.5
318.15	18300.00	1127.0
318.15	18800.00	1127.4
318.15	19200.00	1127.7
318.15	19700.00	1128.0
318.15	20200.00	1128.4

Reference *https://www.doi.org/10.1021/je700339f*

Temperature, K	Pressure, kPa	Mass density, kg/m3
298.15	100.00	1133.7

Reference *https://www.doi.org/10.1021/je7003758*

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je901052w
Excess molar enthalpies and (vapour + liquid) equilibria for mixtures containing N,N-dialkylamides and 1-chloroalkanes:	https://www.doi.org/10.1016/j.jct.2007.06.017
Excess enthalpies and isothermal (vapour + liquid) equilibria of (1-methyl-2-pyrrolidone + 1-chloroalkane or + ?-dichloroalkane) mixtures:	https://www.doi.org/10.1016/j.jct.2008.01.024
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110565&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K:	https://www.doi.org/10.1021/je900404r
Densities and Isothermal Compressibilities at Pressures up to 20 MPa of the Systems N,N-Dimethylformamide or N,N-Dimethylacetamide + r,ω-Dichloroalkane:	https://www.doi.org/10.1021/je700339f
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides)III. HE m and V E m for 20 binary mixtures {xCu 1H2u 1CO2C4H9 + (1 - x)a,x-ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = 2 to 6:	https://www.doi.org/10.1016/j.jct.2005.11.003
The additivity of surface and volumetric properties of	https://www.doi.org/10.1016/j.jct.2018.12.042
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures {xCu 1H2u 1CO2C3H7 + (1 x)a,x-ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = x = 2 to 6. An analysis of behavior using the COSMO-RS methodology:	https://www.doi.org/10.1016/j.jct.2008.10.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K:	https://www.doi.org/10.1021/je3013342
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1604.mol
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) V. Hex and Vex for 25 binary mixtures {xCu 1H2u 1CO2CH3 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = 2 to 6:	https://www.doi.org/10.1016/j.jct.2006.10.008
Speeds of sound, isentropic compressibilities and refractive indices	https://www.doi.org/10.1016/j.fluid.2014.10.004
Isothermal (vapour + liquid) equilibria for nitromethane and 1-chloroalkane at temperatures from 298.15 to 318.15 K:	https://www.doi.org/10.1016/j.jct.2012.06.033
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) II. HE and VE for 25 binary mixtures {xCu 1H2u-1CO2C2H5 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6:	https://www.doi.org/10.1016/j.jct.2005.03.020
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1604
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1604
Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2014.04.004

Heat Capacities of alpha,omega-Dichloroalkanes at Temperatures from 284.15 K to 353.15 K and a Study of Additivity Analysis https://www.doi.org/10.1021/je020042y

Densities and Isothermal Compressibilities at Pressures up to 20 MPa of the Systems 1-Methyl-2-pyrrolidone + 1-Chloroalkane or 1,ω-Dichloroalkane: Isothermal (vapour + liquid) equilibria and excess Gibbs free energies in some binary (cyclopentanone + chloroalkane) mixtures at temperatures from 298.15 K to 318.15 K: https://www.doi.org/10.1021/je7003758 https://www.doi.org/10.1016/j.jct.2007.03.008

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
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume