

Butane, 2-chloro-

Other names:	1-METHYLPROPYL CHLORIDE 2-CHLOROBUTANE SEC-BUTYL CHLORIDE UN 1127 sec-C4H9Cl
Inchi:	InChI=1S/C4H9Cl/c1-3-4(2)5/h4H,3H2,1-2H3
InchiKey:	BSPCSKHALVHRSR-UHFFFAOYSA-N
Formula:	C4H9Cl
SMILES:	CCC(C)Cl
Mol. weight [g/mol]:	92.57
CAS:	78-86-4

Physical Properties

Property code	Value	Unit	Source
af	0.3000		KDB
chl	-2685.47 ± 0.95	kJ/mol	NIST Webbook
dm	2.10	debye	KDB
gf	-53.51	kJ/mol	KDB
hf	-161.60	kJ/mol	KDB
hf	-166.66 ± 0.99	kJ/mol	NIST Webbook
hfl	-198.43 ± 0.99	kJ/mol	NIST Webbook
hfus	6.79	kJ/mol	Joback Method
hvap	31.53	kJ/mol	NIST Webbook
hvap	31.50 ± 0.10	kJ/mol	NIST Webbook
hvap	31.60 ± 0.10	kJ/mol	NIST Webbook
hvap	31.68	kJ/mol	NIST Webbook
hvap	31.77 ± 0.08	kJ/mol	NIST Webbook
hvap	31.56 ± 0.06	kJ/mol	NIST Webbook
hvap	28.98 ± 0.06	kJ/mol	NIST Webbook
ie	10.72	eV	NIST Webbook
ie	10.59	eV	NIST Webbook
ie	10.53	eV	NIST Webbook
ie	10.50 ± 0.10	eV	NIST Webbook
ie	10.65 ± 0.03	eV	NIST Webbook
ie	10.57 ± 0.06	eV	NIST Webbook
log10ws	-1.96		Aqueous Solubility Prediction Method

log10ws	-1.96		Estimated Solubility Method
logp	2.024		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	3950.00	kPa	KDB
rinpol	598.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	589.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	598.38		NIST Webbook
rinpol	598.87		NIST Webbook
rinpol	598.38		NIST Webbook
tb	340.85 ± 0.60	K	NIST Webbook
tb	341.40 ± 0.30	K	NIST Webbook
tb	341.40	K	KDB
tb	341.26	K	Study of tetrahydropyran-chlorobutane VLE using the a o and o o approaches
tb	341.23	K	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
tb	341.26	K	Vapor-Liquid Equilibrium and Volumetric Measurements for Binary Mixtures of 1,4-Dioxane with Isomeric Chlorobutanes
tb	342.20	K	NIST Webbook
tb	340.90 ± 3.00	K	NIST Webbook
tb	341.40	K	NIST Webbook
tb	341.15 ± 1.50	K	NIST Webbook
tb	341.40 ± 0.20	K	NIST Webbook
tb	341.00 ± 3.00	K	NIST Webbook

tc	520.60	K	NIST Webbook
tc	520.60	K	KDB
tf	137.58	K	Aqueous Solubility Prediction Method
tf	141.80	K	KDB
tf	141.85 ± 0.50	K	NIST Webbook
vc	0.305	m ³ /kmol	KDB
zc	0.2783270		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.95	J/mol×K	504.53	Joback Method
cpg	126.45	J/mol×K	357.35	Joback Method
cpg	141.08	J/mol×K	416.22	Joback Method
cpg	147.98	J/mol×K	445.66	Joback Method
cpg	133.91	J/mol×K	386.78	Joback Method
cpg	118.70	J/mol×K	327.91	Joback Method
cpg	154.60	J/mol×K	475.09	Joback Method
cpl	160.90	J/mol×K	298.15	NIST Webbook
cpl	174.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0003993	Paxs	298.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0003615	Paxs	308.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0004167	Paxs	293.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values

dvisc	0.0004365	Paxs	288.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds
dvisc	0.0004167	Paxs	293.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds
dvisc	0.0003993	Paxs	298.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds
dvisc	0.0003800	Paxs	303.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds
dvisc	0.0004365	Paxs	288.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0003443	Paxs	313.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds
dvisc	0.0003938	Paxs	298.15	Densities and Viscosities of the Binary Mixtures of Tetrahydrofuran with Isomeric Chlorobutanes at 298.15 K and 313.15 K

dvisc	0.0003371	Paxs	313.15	Densities and Viscosities of the Binary Mixtures of Tetrahydrofuran with Isomeric Chlorobutanes at 298.15 K and 313.15 K
dvisc	0.0004631	Paxs	283.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0003800	Paxs	303.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0004631	Paxs	283.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds
dvisc	0.0003615	Paxs	308.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds
dvisc	0.0003443	Paxs	313.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
hvapt	30.90	kJ/mol	328.00	NIST Webbook
hvapt	29.17	kJ/mol	341.40	NIST Webbook
hvapt	33.10	kJ/mol	321.50	NIST Webbook
hvapt	30.70 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	29.10 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	28.20 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	31.80	kJ/mol	292.50	NIST Webbook
hvapt	29.20	kJ/mol	341.20	KDB

hvapt	29.90 ± 0.10	kJ/mol	328.00	NIST Webbook
kvisc	0.0000005	m ² /s	298.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
kvisc	0.0000004	m ² /s	313.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
kvisc	0.0000005	m ² /s	298.15	Thermophysical Properties of Mixtures of Tetrahydropyran with Chlorobutanes
kvisc	0.0000004	m ² /s	313.15	Thermophysical Properties of Mixtures of Tetrahydropyran with Chlorobutanes
kvisc	0.0000005	m ² /s	298.15	Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with 2-Methyltetrahydrofuran
kvisc	0.0000004	m ² /s	313.15	Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with 2-Methyltetrahydrofuran
kvisc	0.0000005	m ² /s	283.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
pvap	59.07	kPa	325.25	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa

pvap	31.55	kPa	308.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers
pvap	13.36	kPa	288.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether
pvap	20.91	kPa	298.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether
pvap	31.55	kPa	308.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether
pvap	13.36	kPa	288.15	Article Previous Article Next Article Articles ASAP Phase Equilibrium of Binary Mixtures of n-Hexane + Branched Chlorobutanes: Experimental Results and Group Contribution Predictions
pvap	20.91	kPa	298.15	Article Previous Article Next Article Articles ASAP Phase Equilibrium of Binary Mixtures of n-Hexane + Branched Chlorobutanes: Experimental Results and Group Contribution Predictions

pvap	31.55	kPa	308.15	Article Previous Article Next Article Articles ASAP Phase Equilibrium of Binary Mixtures of n-Hexane + Branched Chlorobutanes: Experimental Results and Group Contribution Predictions
pvap	93.45	kPa	338.75	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	13.36	kPa	288.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers
pvap	31.55	kPa	308.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether
pvap	74.49	kPa	331.90	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	20.91	kPa	298.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether

pvap	13.36	kPa	288.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether
pvap	102.78	kPa	341.75	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	48.34	kPa	319.80	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	50.22	kPa	320.75	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	96.38	kPa	339.65	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	89.61	kPa	337.34	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	83.29	kPa	335.20	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa

pvap	101.30	kPa	341.23	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	80.00	kPa	334.01	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	78.06	kPa	333.25	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	53.30	kPa	322.42	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	65.21	kPa	328.15	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	61.30	kPa	326.25	Isobaric vapor liquid equilibria for binary systems of butyl chlorides with heptane, toluene and cyclohexane at 101.3, 80.0 and 53.3 kPa
pvap	20.91	kPa	298.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers

rfi	1.39404	298.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rfi	1.38562	313.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rfi	1.38844	308.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rfi	1.39404	298.15	Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes
rfi	1.38573	313.15	Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes
rfi	1.40226	283.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rfi	1.39680	293.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rfi	1.39125	303.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether

rfi	1.39953		288.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rhol	867.37	kg/m3	298.15	Surface Tension of Mixtures of Tetrahydrofuran or Tetrahydropyran with Isomeric Chlorobutanes
rhol	867.37	kg/m3	298.15	Surface study of mixtures containing cyclic ethers and isomeric chlorobutanes
rhol	867.37	kg/m3	298.15	Thermodynamic study of 2-methyl-tetrahydrofuran with isomeric chlorobutanes
rhol	873.00	kg/m3	293.00	KDB
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46808e+01
Coeff. B	-3.17313e+03
Coeff. C	-2.59560e+01
Temperature range (K), min.	246.42
Temperature range (K), max.	364.63

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	5.80053e+01
Coeff. B	-5.45019e+03
Coeff. C	-6.53399e+00
Coeff. D	5.89810e-06
Temperature range (K), min.	141.85

Datasets

Mass density, kg/m³

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m ³ - Liquid
100.00	283.15	884.17
100.00	288.15	878.94
100.00	293.15	872.99
100.00	298.15	867.31
100.00	303.15	861.63
100.00	308.15	856.25
100.00	313.15	850.12
100.00	318.15	844.59
100.00	323.15	838.39
100.00	328.15	832.81
2000.00	283.15	886.22
2000.00	288.15	881.0
2000.00	293.15	875.11
2000.00	298.15	869.59
2000.00	303.15	863.89
2000.00	308.15	858.73
2000.00	313.15	852.55
2000.00	318.15	847.15
2000.00	323.15	841.07
2000.00	328.15	835.59
5000.00	283.15	889.26
5000.00	288.15	884.23
5000.00	293.15	878.43
5000.00	298.15	872.97
5000.00	303.15	867.45
5000.00	308.15	862.31
5000.00	313.15	856.44
5000.00	318.15	850.8
5000.00	323.15	845.19
5000.00	328.15	839.88
7000.00	283.15	891.28
7000.00	288.15	886.25

7000.00	293.15	880.56
7000.00	298.15	875.17
7000.00	303.15	869.74
7000.00	308.15	864.71
7000.00	313.15	858.81
7000.00	318.15	853.7
7000.00	323.15	847.87
7000.00	328.15	842.66
10000.00	283.15	894.16
10000.00	288.15	889.3
10000.00	293.15	883.72
10000.00	298.15	878.41
10000.00	303.15	873.12
10000.00	308.15	868.08
10000.00	313.15	862.43
10000.00	318.15	857.33
10000.00	323.15	851.64
10000.00	328.15	846.54
20000.00	283.15	903.34
20000.00	288.15	898.71
20000.00	293.15	893.43
20000.00	298.15	888.39
20000.00	303.15	883.39
20000.00	308.15	878.72
20000.00	313.15	873.34
20000.00	318.15	868.68
20000.00	323.15	863.29
20000.00	328.15	858.56
30000.00	283.15	911.71
30000.00	288.15	907.27
30000.00	293.15	902.22
30000.00	298.15	897.49
30000.00	303.15	892.74
30000.00	308.15	888.3
30000.00	313.15	883.24
30000.00	318.15	878.85
30000.00	323.15	873.67
30000.00	328.15	869.22
40000.00	283.15	919.47
40000.00	288.15	915.2
40000.00	293.15	910.33
40000.00	298.15	905.79
40000.00	303.15	901.25
40000.00	308.15	897.03

40000.00	313.15	892.21
40000.00	318.15	887.93
40000.00	323.15	883.17
40000.00	328.15	878.94
50000.00	283.15	926.7
50000.00	288.15	922.6
50000.00	293.15	917.87
50000.00	298.15	913.53
50000.00	303.15	909.12
50000.00	308.15	905.05
50000.00	313.15	900.48
50000.00	318.15	896.41
50000.00	323.15	891.75
50000.00	328.15	887.7
60000.00	283.15	933.46
60000.00	288.15	929.48
60000.00	293.15	924.95
60000.00	298.15	920.75
60000.00	303.15	916.44
60000.00	308.15	912.57
60000.00	313.15	908.09
60000.00	318.15	904.23
60000.00	323.15	899.75
60000.00	328.15	895.82
65000.00	283.15	936.67
65000.00	288.15	932.78
65000.00	293.15	928.34
65000.00	298.15	924.15
65000.00	303.15	919.96
65000.00	308.15	916.04
65000.00	313.15	911.73
65000.00	318.15	907.86
65000.00	323.15	903.54
65000.00	328.15	899.7

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Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds: KDB Pure (Korean Thermophysical Properties Databank): Experimental and predicted vapour-liquid equilibrium of the binary mixtures of heptane + chlorobutane isomers: Molar Excess Volume of sec- and tert-Butyl Chloride with Aromatic Hydrocarbons: vapour-liquid equilibria and excess enthalpies for the binary mixtures of binary mixtures of isomeric butanes: Dissociation of Chlorobutanes with 2-methyltetrahydrofuran with isomeric chlorobutanes: Properties of Short-Chain Chloroalkanes: Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with n-hexane: vapour-liquid equilibria for binary systems of butyl chlorides with n-hexane: Handbook of Vapor Pressure: Study of tetrahydropyran-chlorobutane VLE using the α and β approaches: Vapor-Liquid Equilibrium and Volumetric Measurements for Binary Mixtures of Chlorobutane Isomers: Chlorobutanes and isomeric chlorobutanes: ERAS-model and Prigogine-Flory-Patterson theory to describe vapor-liquid equilibria of Tetrahydropyran with n-hexane + n-butanol + isobutanol at T = 298.15 K: Joback Method: Excess properties from p.rho.T data for n-heptane + isomeric chlorobutane systems: Volumetric and acoustic behaviour of systems containing n-hexane, or n-heptane, or n-octane, or n-decane: Articles Previous Article Next Articles Articles ASAP Phase Equilibrium of Binary Mixtures of n-Hexane and the Binary Mixtures of Chlorobutanes with n-Hexane: Vapor-Liquid Equilibrium of Binary Mixtures of Chlorobutanes and n-Hexane: Experimental and Predicted Values: Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and n-hexane: Prediction Method: NIST Webbook: Surface Tension of Mixtures of Tetrahydrofuran or Tetrahydropyran with Isomeric Chlorobutanes:

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Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
kvisc:	Kinematic viscosity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rho:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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