Propane, 2-chloro-2-methyl-

Other names:	1,1-dimethylethyl chloride
	1-chloro-1,1-dimethylethane
	2-CHLORO-2-METHYLPROPANE
	2-CHLOROISOBUTANE
	2-Methyl-2-chloropropane
	2-Methyl-2-propyl chloride
	Chlorotrimethylmethane
	NSC 6527
	TRIMETHYLCHLOROMETHANE
	Tertiary-butyl chloride
	tert-Butyl Chloride
	tert-C4H9Cl
Inchi:	InChI=1S/C4H9Cl/c1-4(2,3)5/h1-3H3
InchiKey:	NBRKLOOSMBRFMH-UHFFFAOYSA-N
Formula:	C4H9Cl
SMILES:	CC(C)(C)Cl
Mol. weight [g/mol]:	92.57
CAS:	507-20-0

Physical Properties

Property code	Value	Unit	Source
af	0.1900		KDB
chl	-2675.20 ± 8.40	kJ/mol	NIST Webbook
dm	2.10	debye	KDB
gf	-64.14	kJ/mol	KDB
hf	-179.90	kJ/mol	NIST Webbook
hf	-183.40	kJ/mol	KDB
hfl	-211.20 ± 2.30	kJ/mol	NIST Webbook
hfus	2.90	kJ/mol	Joback Method
hvap	29.00 ± 0.10	kJ/mol	NIST Webbook
hvap	28.60	kJ/mol	NIST Webbook
hvap	29.19	kJ/mol	NIST Webbook
ie	10.69	eV	NIST Webbook
ie	10.61 ± 0.03	eV	NIST Webbook
ie	10.30 ± 0.10	eV	NIST Webbook
ie	10.58	eV	NIST Webbook
ie	10.76	eV	NIST Webbook

log10ws	-1.76		Crippen Method
logp	2.024		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	3950.00	kPa	KDB
rinpol	540.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	525.00		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	530.04		NIST Webbook
rinpol	530.04		NIST Webbook
rinpol	530.66		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	530.00		NIST Webbook
tb	324.15 ± 0.30	K	NIST Webbook
tb	324.80 ± 0.50	K	NIST Webbook
tb	324.80 ± 0.50	K	NIST Webbook
tb	323.90 ± 0.40	K	NIST Webbook
tb	323.85 ± 0.30	K	NIST Webbook
tb	323.70 ± 0.30	K	NIST Webbook
tb	324.00 ± 0.30	K	NIST Webbook
tb	323.40 ± 0.50	K	NIST Webbook
tb	323.85 ± 0.30	K	NIST Webbook
tb	324.00 ± 0.40	K	NIST Webbook
tb	324.00	K	NIST Webbook
tb	325.20	K	NIST Webbook
tb	323.88	K	Vapor-Liquid Equilibrium and Volumetric Measurements for Binary Mixtures of 1,4-Dioxane with Isomeric Chlorobutanes
tb	323.88	K	Study of tetrahydropyran-chlorobutane VLE using the a o and o o approaches
tb	324.00	K	KDB

tb	324.00 ± 2.00	K	NIST Webbook
tb	324.15 ± 1.50	K	NIST Webbook
tc	507.00	K	KDB
tf	250.30 ± 1.00	K	NIST Webbook
tf	246.10 ± 0.40	K	NIST Webbook
tf	248.20 ± 0.20	K	NIST Webbook
tf	247.80	K	KDB
tf	246.05 ± 0.40	K	NIST Webbook
tf	246.10 ± 0.60	K	NIST Webbook
tf	246.15 ± 1.00	K	NIST Webbook
tf	244.65 ± 0.20	K	NIST Webbook
tf	247.80 ± 0.30	K	NIST Webbook
tt	247.53 ± 0.02	K	NIST Webbook
tt	184.80	K	Solid binary mixtures of neopentanol with tert-Butyl chloride and carbon tetrachloride studied by thermal, X-ray and dielectric techniques
vc	0.295	m3/kmol	KDB
zc	0.2764230		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.81	J/mol×K	325.12	Joback Method
cpg	127.87	J/mol×K	355.88	Joback Method
cpg	136.43	J/mol×K	386.64	Joback Method
cpg	144.52	J/mol×K	417.41	Joback Method
cpg	152.16	J/mol×K	448.17	Joback Method
cpg	159.37	J/mol×K	478.93	Joback Method
cpg	166.16	J/mol×K	509.69	Joback Method
cpl	152.70	J/mol×K	259.60	NIST Webbook
cpl	162.00	J/mol×K	298.15	NIST Webbook
cpl	172.80	J/mol×K	272.73	NIST Webbook
dvisc	0.0005135	Pa×s	293.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values

dvisc	0.0004438	Pa×s	303.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0004196	Pa×s	308.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0003904	Pa×s	313.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0004751	Pa×s	298.15	Densities and Viscosities of the Binary Mixtures of Tetrahydrofuran with Isomeric Chlorobutanes at 298.15 K and 313.15 K
dvisc	0.0003907	Pa×s	313.15	Densities and Viscosities of the Binary Mixtures of Tetrahydrofuran with Isomeric Chlorobutanes at 298.15 K and 313.15 K
dvisc	0.0005980	Pa×s	283.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0005538	Pa×s	288.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values

dvisc	0.0004768	Pa×s	298.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
hfust	1.97	kJ/mol	248.10	NIST Webbook
hfust	1.89	kJ/mol	247.80	NIST Webbook
hfust	1.99	kJ/mol	248.40	NIST Webbook
hfust	1.87	kJ/mol	182.90	NIST Webbook
hfust	1.97	kJ/mol	248.10	NIST Webbook
hfust	5.88	kJ/mol	219.30	NIST Webbook
hvapt	27.55	kJ/mol	324.00	NIST Webbook
hvapt	32.30	kJ/mol	305.50	NIST Webbook
hvapt	27.80	kJ/mol	309.00	NIST Webbook
hvapt	27.00	kJ/mol	309.00	NIST Webbook
hvapt	29.10	kJ/mol	289.00	NIST Webbook
kvisc	0.0000007	m2/s	283.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
kvisc	0.0000005	m2/s	313.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
kvisc	0.0000006	m2/s	298.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
kvisc	0.0000006	m2/s	298.15	Thermophysical Properties of Mixtures of Tetrahydropyran with Chlorobutanes
kvisc	0.0000005	m2/s	313.15	Thermophysical Properties of Mixtures of Tetrahydropyran with Chlorobutanes

kvisc	0.0000006	m2/s	298.15	Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with 2-Methyltetrahydrofuran
pvap	40.13	kPa	298.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers
pvap	26.42	kPa	288.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers
pvap	40.13	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	40.13	kPa	298.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether
pvap	26.42	kPa	288.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether

pvap	26.42	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	59.52	kPa	308.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether	
pvap	40.13	kPa	298.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether	
pvap	26.42	kPa	288.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether	
pvap	59.52	kPa	308.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers	
pvap	59.52	kPa	308.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether	

pvap	59.52	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	
rfi	1.37312		313.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.37314		313.15	Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes	
rfi	1.39115		283.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.38821		288.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.38522		293.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.38225		298.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	

rfi	1.37921		303.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rfi	1.38224		298.15	Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes
rfi	1.37619		308.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rhol	835.67	kg/m3	298.15	Thermodynamic study of 2-methyl-tetrahydrofuran with isomeric chlorobutanes
rhol	842.00	kg/m3	293.00	KDB
rhol	836.45	kg/m3	298.15	Surface Tension of Mixtures of Tetrahydrofuran or Tetrahydropyran with Isomeric Chlorobutanes
rhol	836.45	kg/m3	298.15	Surface study of mixtures containing cyclic ethers and isomeric chlorobutanes
sfust	26.82	J/mol×K	219.30	NIST Webbook
sfust	10.25	J/mol×K	182.90	NIST Webbook
sfust	7.95	J/mol×K	248.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39693e+01
Coeff. B	-2.69943e+03

Coeff. C	-3.54210e+01
Temperature range (K), min.	232.72
Temperature range (K), max.	347.21

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.61650e+01
Coeff. B	-5.86752e+03
Coeff. C	-9.39992e+00
Coeff. D	8.62699e-06
Temperature range (K), min.	235.00
Temperature range (K), max.	507.00

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	283.15	855.04
100.00	288.15	849.49
100.00	293.15	842.98
100.00	298.15	836.8
100.00	303.15	830.82
100.00	308.15	824.5
100.00	313.15	818.16
100.00	318.15	812.44
100.00	323.15	805.63
2000.00	283.15	857.34
2000.00	288.15	851.9
2000.00	293.15	845.52
2000.00	298.15	839.47
2000.00	303.15	833.52
2000.00	308.15	827.85
2000.00	313.15	821.21
2000.00	318.15	815.53
2000.00	323.15	808.87
5000.00	283.15	860.89

5000.00	288.15	855.68
5000.00	293.15	849.29
5000.00	298.15	843.49
5000.00	303.15	837.7
5000.00	308.15	832.26
5000.00	313.15	825.78
5000.00	318.15	820.32
5000.00	323.15	813.81
7000.00	283.15	863.25
7000.00	288.15	858.07
7000.00	293.15	851.78
7000.00	298.15	846.04
7000.00	303.15	840.35
7000.00	308.15	835.02
7000.00	313.15	828.59
7000.00	318.15	823.22
7000.00	323.15	816.94
10000.00	283.15	866.58
10000.00	288.15	861.54
10000.00	293.15	855.47
10000.00	298.15	849.77
10000.00	303.15	844.23
10000.00	308.15	839.07
10000.00	313.15	832.78
10000.00	318.15	827.64
10000.00	323.15	821.51
20000.00	283.15	877.11
20000.00	288.15	872.26
20000.00	293.15	866.52
20000.00	298.15	861.25
20000.00	303.15	855.99
20000.00	308.15	851.28
20000.00	313.15	845.4
20000.00	318.15	840.68
20000.00	323.15	834.91
30000.00	283.15	886.39
30000.00	288.15	881.97
30000.00	293.15	876.42
30000.00	298.15	871.55
30000.00	303.15	866.5
30000.00	308.15	862.19
30000.00	313.15	856.61
30000.00	318.15	852.24
30000.00	323.15	846.65

40000.00	283.15	895.03
40000.00	288.15	890.79
40000.00	293.15	885.44
40000.00	298.15	880.72
40000.00	303.15	875.98
40000.00	308.15	871.88
40000.00	313.15	866.61
40000.00	318.15	862.53
40000.00	323.15	857.22
50000.00	283.15	903.08
50000.00	288.15	898.94
50000.00	293.15	893.59
50000.00	298.15	889.39
50000.00	303.15	884.66
50000.00	308.15	880.77
50000.00	313.15	875.72
50000.00	318.15	871.96
50000.00	323.15	866.77
60000.00	283.15	910.34
60000.00	288.15	906.48
60000.00	293.15	901.48
60000.00	298.15	897.22
60000.00	303.15	892.77
60000.00	308.15	889.06
60000.00	313.15	884.23
60000.00	318.15	880.5
60000.00	323.15	875.56
65000.00	283.15	913.66
65000.00	288.15	910.15
65000.00	293.15	905.24
65000.00	298.15	900.97
65000.00	303.15	896.61
65000.00	308.15	892.9
65000.00	313.15	888.28
65000.00	318.15	884.5
65000.00	323.15	879.7

Reference *https://www.doi.org/10.1021/je3003805*

Sources

Thermodynamic study of 2-methyl-tetrahydrofuran with isomeric chlorobutanes: https://www.doi.org/10.1016/j.tca.2004.11.034

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1610
Surface Tension of Mixtures of Tetrahydrofuran or Tetrahydropyran with Isomeric Chlorobutanes:	https://www.doi.org/10.1007/s10765-007-0169-z
Solid-liquid mixtures of neopentanol with tert-Butyl chloride and carbon tetrachloride studied by thermal, X-ray and dielectric techniques:	https://www.doi.org/10.1016/j.tca.2016.03.003
Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether:	https://www.doi.org/10.1021/je100765j
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Excess properties from p.rho.T data for n-heptane + isomeric chlorobutane mixtures:	https://www.doi.org/10.1016/j.tca.2015.06.017
Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes:	https://www.doi.org/10.1016/j.jct.2006.05.003
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with 2-Methylfuran:	https://www.doi.org/10.1021/je030167i
Volumetric Properties of Short-Chain 2-Alkanols + Tetrahydrofuran:	https://www.doi.org/10.1021/je3003805
Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether:	https://www.doi.org/10.1016/j.jct.2012.02.039
Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers:	https://www.doi.org/10.1016/j.fluid.2015.09.031
Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures:	https://www.doi.org/10.1021/je200213h
Molar Excess Volume of sec- and tert-Butyl Chloride with Aromatic Hydrocarbons at T = 298.15 K:	https://www.doi.org/10.1021/je7002918
Thermophysical Properties of Mixtures of Tetrahydropyran with Chlorobutanes:	https://www.doi.org/10.1007/s10765-006-0100-z
Article Previous Article Next Article Articles ASAP Phase Equilibrium of Binary Mixtures of n-Hexane + Branched Chlorobutanes: Experimental Results and Group Contribution Predictions:	https://www.doi.org/10.1021/je500116z
Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes + Diethyl Ether: Experimental and Predicted Values:	https://www.doi.org/10.1007/s10765-010-0737-5
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Surface study of mixtures containing cyclic ethers and isomeric chlorobutanes:	https://www.doi.org/10.1016/j.jct.2006.10.003
Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether:	https://www.doi.org/10.1016/j.fluid.2011.06.001
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapor-Liquid Equilibrium and Volumetric Measurements for Binary Mixtures of 1,4-Dioxane with Isomeric Chlorobutanes:	https://www.doi.org/10.1021/je020185k
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1610
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C507200&Units=SI
Volumetric and acoustic behaviour of systems containing n-hexane, or n-heptane and isomeric chlorobutanes:	https://www.doi.org/10.1016/j.jct.2010.06.008
Study of tetrahydropyran+chlorobutane VLE using the a o and o o approaches:	https://www.doi.org/10.1016/j.fluid.2005.02.014
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1610.mol
Densities and Viscosities of the Binary Mixtures of Tetrahydrofuran with Isomeric Chlorobutanes at 298.15 K and 313.15 K:	https://www.doi.org/10.1021/je0600653
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
kvisc:	Kinematic viscosity
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility