Propane, 1-chloro-2-methyl-

Other names: 1-Chloro-2-methylpropane
Isobutyl chloride
iso-C4H9Cl
Inchi: InChI=1S/C4H9Cl/c1-4(2)3-5/h4H,3H2,1-2H3
InchiKey: QTBFPMKWQKYFLR-UHFFFAOYSA-N
Formula: C4H9Cl
SMILES: CC(C)CCl
Mol. weight [g/mol]: 92.57
CAS: 513-36-0

Physical Properties

Property code	Value	Unit	Source
chl	-2692.80 ± 8.40	kJ/mol	NIST Webbook
gf	-31.57	kJ/mol	Joback Method
hf	-146.91	kJ/mol	Joback Method
hfus	6.79	kJ/mol	Joback Method
hvap	31.81	kJ/mol	NIST Webbook
hvap	31.67 ± 0.06	kJ/mol	NIST Webbook
hvap	31.70 ± 0.10	kJ/mol	NIST Webbook
ie	10.66 ± 0.03	eV	NIST Webbook
ie	10.50 ± 0.10	eV	NIST Webbook
ie	10.80	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
ie	10.73 ± 0.07	eV	NIST Webbook
log10ws	-2.00		Estimated Solubility Method
log10ws	-2.00		Aqueous Solubility Prediction Method
logp	1.881		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	605.00		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	619.00		NIST Webbook

rinpol	603.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	596.00		NIST Webbook
tb	342.05	K	Vapor-Liquid Equilibrium and Volumetric Measurements for Binary Mixtures of 1,4-Dioxane with Isomeric Chlorobutanes
tb	342.05	K	Study of tetrahydropyran-chlorobutane VLE using the a o and o o approaches
tc	504.53	K	Joback Method
tf	149.76	K	Joback Method
vc	0.302	m3/kmol	Joback Method

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	133.91	J/mol×K	386.78	Joback Method
cpg	141.08	J/mol×K	416.22	Joback Method
cpg	147.98	J/mol×K	445.66	Joback Method
cpg	154.60	J/mol×K	475.09	Joback Method
cpg	118.70	J/mol×K	327.91	Joback Method
cpl	158.60	J/mol×K	298.00	NIST Webbook
dvisc	0.0003921	Pa×s	308.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values

dvisc	0.0004833	Pa×s	288.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0004540	Pa×s	293.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0004296	Pa×s	298.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0004112	Pa×s	303.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0005155	Pa×s	283.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0003726	Pa×s	313.15	Viscosities of Binary Mixtures Containing Isomeric Chlorobutanes and Diisopropylether: Experimental and Predicted Values
dvisc	0.0005155	Pa×s	283.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds

dvisc	0.0004833	Pa×s	288.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds	
dvisc	0.0004540	Pa×s	293.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds	
dvisc	0.0004296	Pa×s	298.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds	
dvisc	0.0004112	Pa×s	303.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds	
dvisc	0.0003921	Pa×s	308.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds	
dvisc	0.0003726	Pa×s	313.15	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds	
dvisc	0.0004295	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	0.0003664	Pa×s	313.15	Densities and Viscosities of the Binary Mixtures of Tetrahydrofuran with Isomeric Chlorobutanes at 298.15 K and 313.15 K
hvapt	29.22	kJ/mol	341.60	NIST Webbook
hvapt	36.10	kJ/mol	280.50	NIST Webbook
kvisc	0.0000004	m2/s	313.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
kvisc	0.0000004	m2/s	313.15	Thermophysical Properties of Mixtures of Tetrahydropyran with Chlorobutanes
kvisc	0.0000005	m2/s	298.15	Thermophysical Properties of Mixtures of Tetrahydropyran with Chlorobutanes
kvisc	0.0000004	m2/s	313.15	Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with 2-Methyltetrahydrofuran
kvisc	0.0000006	m2/s	283.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
kvisc	0.0000005	m2/s	298.15	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures
kvisc	0.0000005	m2/s	298.15	Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with 2-Methyltetrahydrofuran

pvap	13.00	kPa	288.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether	
pvap	20.35	kPa	298.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether	
pvap	30.45	kPa	308.15	Isothermal vapour-liquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether	
pvap	13.00	kPa	288.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers	
pvap	20.35	kPa	298.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers	
pvap	30.45	kPa	308.15	Experimental and predicted vapour-liquid equilibrium of the binary mixtures n-heptane + chlorobutane isomers	
pvap	13.00	kPa	288.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether	

pvap	20.35	kPa	298.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether	
pvap	30.45	kPa	308.15	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether	
pvap	13.00	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	20.35	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	30.45	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	1.39528	298.15	Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes	
rfi	1.38686	313.15	Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes	
rfi	1.40354	283.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.40080	288.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.38683	313.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.39529	298.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.39245	303.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	
rfi	1.38963	308.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether	

rfi	1.39802		293.15	Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether
rhol	870.89	kg/m3	298.15	Thermodynamic study of 2-methyl-tetrahydrofuran with isomeric chlorobutanes
rhol	871.13	kg/m3	298.15	Surface Tension of Mixtures of Tetrahydrofuran or Tetrahydropyran with Isomeric Chlorobutanes
rhol	871.13	kg/m3	298.15	Surface study of mixtures containing cyclic ethers and isomeric chlorobutanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41015e+01
Coeff. B	-2.81263e+03
Coeff. C	-4.53090e+01
Temperature range (K), min.	248.92
Temperature range (K), max.	365.29

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid

100.00	283.15	888.74
100.00	288.15	883.47
100.00	293.15	877.41
100.00	298.15	871.72
100.00	303.15	865.91
100.00	308.15	860.63
100.00	313.15	854.27
100.00	318.15	848.89
100.00	323.15	842.52
100.00	328.15	837.0
2000.00	283.15	890.75
2000.00	288.15	885.59
2000.00	293.15	879.49
2000.00	298.15	873.82
2000.00	303.15	868.26
2000.00	308.15	863.03
2000.00	313.15	856.75
2000.00	318.15	851.46
2000.00	323.15	845.19
2000.00	328.15	839.85
5000.00	283.15	893.77
5000.00	288.15	888.71
5000.00	293.15	882.8
5000.00	298.15	877.2
5000.00	303.15	871.68
5000.00	308.15	866.72
5000.00	313.15	860.48
5000.00	318.15	855.36
5000.00	323.15	849.19
5000.00	328.15	844.08
7000.00	283.15	895.72
7000.00	288.15	890.75
7000.00	293.15	884.93
7000.00	298.15	879.37
7000.00	303.15	873.97
7000.00	308.15	869.17
7000.00	313.15	862.93
7000.00	318.15	857.9
7000.00	323.15	851.95
7000.00	328.15	846.74
10000.00	283.15	898.62
10000.00	288.15	893.72
10000.00	293.15	888.0
10000.00	298.15	882.59

10000.00	303.15	877.32
10000.00	308.15	872.31
10000.00	313.15	866.38
10000.00	318.15	861.51
10000.00	323.15	855.62
10000.00	328.15	850.7
20000.00	283.15	907.63
20000.00	288.15	903.03
20000.00	293.15	897.62
20000.00	298.15	892.47
20000.00	303.15	887.46
20000.00	308.15	882.89
20000.00	313.15	877.3
20000.00	318.15	872.7
20000.00	323.15	867.15
20000.00	328.15	862.58
30000.00	283.15	915.91
30000.00	288.15	911.59
30000.00	293.15	906.26
30000.00	298.15	901.48
30000.00	303.15	896.65
30000.00	308.15	892.36
30000.00	313.15	887.04
30000.00	318.15	882.71
30000.00	323.15	877.47
30000.00	328.15	873.25
40000.00	283.15	923.6
40000.00	288.15	919.26
40000.00	293.15	914.31
40000.00	298.15	909.72
40000.00	303.15	905.09
40000.00	308.15	901.1
40000.00	313.15	895.94
40000.00	318.15	891.92
40000.00	323.15	886.79
40000.00	328.15	882.68
50000.00	283.15	930.74
50000.00	288.15	926.55
50000.00	293.15	921.75
50000.00	298.15	917.36
50000.00	303.15	912.92
50000.00	308.15	909.05
50000.00	313.15	904.09
50000.00	318.15	900.17

50000.00	323.15	895.27
50000.00	328.15	889.88
60000.00	283.15	937.43
60000.00	288.15	933.39
60000.00	293.15	928.75
60000.00	298.15	924.47
60000.00	303.15	920.14
60000.00	308.15	916.5
60000.00	313.15	911.72
60000.00	318.15	907.95
60000.00	323.15	903.21
60000.00	328.15	899.53
65000.00	283.15	940.6
65000.00	288.15	936.76
65000.00	293.15	932.1
65000.00	298.15	927.91
65000.00	303.15	923.66
65000.00	308.15	920.02
65000.00	313.15	915.32
65000.00	318.15	911.65
65000.00	323.15	906.99
65000.00	328.15	903.34

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

Sources

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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
Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether:	https://www.doi.org/10.1021/je100765j

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
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume