Octane, 1-chloro-

Other names:	1-Chlorooctane
	1-Octyl chloride
	CAPRYL CHLORIDE
	N-OCTYL CHLORIDE
	Octyl chloride
Inchi:	InChI=1S/C8H17Cl/c1-2-3-4-5-6-7-8-9/h2-8H2,1H3
InchiKey:	CNDHHGUSRIZDSL-UHFFFAOYSA-N
Formula:	C8H17Cl
SMILES:	CCCCCCCCCl
Mol. weight [g/mol]:	148.67
CAS:	111-85-3

Physical Properties

Property code	Value	Unit	Source
chl	-5310.00 ± 1.80	kJ/mol	NIST Webbook
gf	4.55	kJ/mol	Joback Method
hf	-238.90 ± 1.90	kJ/mol	NIST Webbook
hfl	-291.30 ± 1.90	kJ/mol	NIST Webbook
hfus	20.67	kJ/mol	Joback Method
hvap	52.40 ± 0.10	kJ/mol	NIST Webbook
hvap	52.42	kJ/mol	NIST Webbook
hvap	52.42 ± 0.12	kJ/mol	NIST Webbook
hvap	51.40	kJ/mol	NIST Webbook
ie	10.10 ± 0.05	eV	NIST Webbook
ie	9.99	eV	NIST Webbook
log10ws	-3.32		Crippen Method
logp	3.586		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1046.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1059.00		NIST Webbook

rinpol	1059.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1043.80		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1052.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1242.00		NIST Webbook
ripol	1251.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1260.00		NIST Webbook
tb	455.20	K	NIST Webbook
tb	456.95	K	KDB
tb	451.00 ± 1.50	K	NIST Webbook
tb	456.95 ± 0.30	K	NIST Webbook
tc	590.71	K	Joback Method
tf	209.84	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.83	J/mol×K	419.87	Joback Method
cpg	275.59	J/mol×K	448.34	Joback Method
cpg	287.86	J/mol×K	476.82	Joback Method
cpg	299.64	J/mol×K	505.29	Joback Method
cpg	310.96	J/mol×K	533.76	Joback Method
cpg	321.81	J/mol×K	562.24	Joback Method
cpg	332.22	J/mol×K	590.71	Joback Method
cpl	274.70	J/mol×K	298.15	NIST Webbook

cpl	270.79	J/mol×K	286.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	271.83	J/mol×K	289.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	272.66	J/mol×K	291.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	273.66	J/mol×K	294.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	274.53	J/mol×K	296.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	275.61	J/mol×K	299.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	276.52	J/mol×K	301.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	277.29	J/mol×K	304.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	278.37	J/mol×K	306.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	279.28	J/mol×K	309.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	280.50	J/mol×K	311.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	281.58	J/mol×K	314.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	282.47	J/mol×K	316.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	283.79	J/mol×K	319.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	284.92	J/mol×K	321.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	285.45	J/mol×K	324.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	286.81	J/mol×K	326.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	288.43	J/mol×K	329.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	289.95	J/mol×K	331.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	290.13	J/mol×K	334.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	291.34	J/mol×K	336.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	291.91	J/mol×K	339.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	293.56	J/mol×K	341.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	294.16	J/mol×K	344.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	294.82	J/mol×K	346.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	295.79	J/mol×K	349.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	297.21	J/mol×K	351.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	298.14	J/mol×K	353.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	269.76	J/mol×K	284.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
dvisc	0.0052971	Pa×s	209.84	Joback Method
dvisc	0.0022835	Pa×s	244.84	Joback Method
dvisc	0.0012150	Pa×s	279.85	Joback Method
dvisc	0.0007439	Pa×s	314.86	Joback Method
dvisc	0.0005024	Pa×s	349.86	Joback Method
dvisc	0.0003644	Pa×s	384.87	Joback Method
dvisc	0.0002789	Pa×s	419.87	Joback Method
hvapt	50.30	kJ/mol	392.00	NIST Webbook
rfi	1.42820		298.15	Densities, Excess Molar Volumes, Viscosities, and Refractive Indices of Binary Mixtures of n-Butyl Acetate with 1-Chloroalkanes (C4 C8) at 298.15 K
rhol	868.98	kg/m3	298.15	Excess enthalpies and isothermal (vapour + liquid) equilibria of (1-methyl-2-pyrrolidone + 1-chloroalkane or +,?-dichloroalkane) mixtures
rhol	868.98	kg/m3	298.15	(Vapour + liquid) equilibria and excess molar enthalpies for binary mixtures containing N,N-dialkylamides and 1-chloroalkanes
rhol	905.50	kg/m3	253.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K

rhol	897.10	kg/m3	263.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	786.80	kg/m3	393.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	880.60	kg/m3	283.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	872.30	kg/m3	293.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	868.30	kg/m3	298.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	847.40	kg/m3	323.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	830.50	kg/m3	343.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	813.20	kg/m3	363.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	889.00	kg/m3	273.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60368e+01
Coeff. B	-4.38150e+03
Coeff. C	-6.80900e+01
Temperature range (K), min.	346.30
Temperature range (K), max.	476.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.42325e+02
Coeff. B	-1.14740e+04
Coeff. C	-1.87950e+01
Coeff. D	1.20730e-05
Temperature range (K), min.	327.15
Temperature range (K), max.	457.15

Datasets

Mass density, kg/m3

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

288.15	100.00	877.3
288.15	2000.00	878.8
288.15	4000.00	880.2
288.15	6000.00	881.6
288.15	8000.00	883.0
288.15	10000.00	884.4
288.15	11900.00	885.8
288.15	13900.00	887.1
288.15	16000.00	888.4
288.15	18000.00	889.7
288.15	20100.00	891.2
298.15	100.00	868.8
298.15	2000.00	870.2
298.15	4100.00	871.8
298.15	6100.00	873.3
298.15	8100.00	874.8
298.15	10000.00	876.2
298.15	12100.00	877.8
298.15	14200.00	879.3
298.15	16300.00	880.7
298.15	18300.00	882.1
298.15	20200.00	883.4
308.15	100.00	861.4
308.15	2000.00	862.8
308.15	4000.00	864.4
308.15	6000.00	865.9
308.15	7900.00	867.5
308.15	10100.00	869.1
308.15	12000.00	870.5
308.15	14000.00	872.0
308.15	15900.00	873.3
308.15	18000.00	874.8
308.15	20000.00	876.5
318.15	100.00	852.9
318.15	2000.00	854.5
318.15	4000.00	856.2
318.15	6000.00	857.9
318.15	8000.00	859.5
318.15	10000.00	861.2
318.15	12000.00	862.8
318.15	14000.00	864.3
318.15	16000.00	865.8
318.15	18000.00	867.3
318.15	20100.00	868.9

Reference	https://www.doi.org/10.1021/je700096m

Temperature, K	Pressure, kPa	Mass density, kg/m3
298.15	100.00	868.8

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

Sources

(Vapour + liquid) equilibria and excess molar enthalpies for binary mixtures containing N,N-dialkylamides and 1-chloroalkanes:	https://www.doi.org/10.1016/j.jct.2007.01.017
Solubilities of Some Long-Chain n-Alkanes in Dipropyl Ether, Dibutyl Ether, 1-Chlorobutane, and 1-Chlorooctane as Functions of Temperature:	https://www.doi.org/10.1021/je030206q
Densities, Excess Molar Volumes, Viscosities, and Refractive Indices of Binary Mixtures of n-Butyl Acetate with 1-Chloroalkanes (C4 C8) at 298.15 K:	https://www.doi.org/10.1007/s10765-010-0902-x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1644
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1644.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111853&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Excess enthalpies and isothermal (vapour + liquid) equilibria of 1-chloroalkanes + 1-bromoalkanes at 298.15 K:	https://www.doi.org/10.1016/j.jct.2008.01.024
Heat Capacities of 1-Chloroalkanes and 1-Bromoalkanes, within the temperature range 284.15 K to 353.15 K. A Group Additivity and Molecular Connectivity Analysis.:	https://www.doi.org/10.1021/je049652j
Does Alkyl Chain Length Really Matter? Structure Property Relationships in Densities and Isothermal Compressibilities of Ionic Liquids.:	https://www.doi.org/10.1016/j.tca.2013.04.003
Density of Some 1-Chloroalkanes within the Temperature Range from (298.15 to 373.15) K and Compressibilities at Pressures up to 20 MPa of the Systems 1-Methyl-2-pyrrolidone + 1-Chloroalkane or 1,1,1-Trichloroalkane:	https://www.doi.org/10.1021/je7003758
Densities and Isothermal Compressibilities at Pressures up to 20 MPa of the Systems N,N-Dimethylformamide or N,N-Dimethylacetamide + 1-Chloroalkane:	https://www.doi.org/10.1021/je700325c
	https://www.doi.org/10.1021/je700096m

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume