n-Propyl chloride

Other names:	1-Chloropropane
	Chloropropane
	PROPYL CHLORIDE
	Propane, 1-chloro-
	UN 1278
	n-C3H7Cl
Inchi:	InChI=1S/C3H7Cl/c1-2-3-4/h2-3H2,1H3
InchiKey:	SNMVRZFUUCLYTO-UHFFFAOYSA-N
Formula:	C3H7Cl
SMILES:	CCCCl
Mol. weight [g/mol]:	78.54
CAS:	540-54-5

Physical Properties

Property code	Value	Unit	Source
af	0.2350		KDB
chg	-2072.10 ± 0.79	kJ/mol	NIST Webbook
chl	-2025.00 ± 8.00	kJ/mol	NIST Webbook
dm	2.00	debye	KDB
gf	-50.70	kJ/mol	KDB
hf	-132.50 ± 0.92	kJ/mol	NIST Webbook
hf	-132.50	kJ/mol	NIST Webbook
hf	-130.20	kJ/mol	KDB
hf	-131.20 ± 0.84	kJ/mol	NIST Webbook
hfus	7.72	kJ/mol	Joback Method
hvap	28.50 ± 0.21	kJ/mol	NIST Webbook
hvap	28.50 ± 0.20	kJ/mol	NIST Webbook
hvap	28.56	kJ/mol	NIST Webbook
hvap	29.00	kJ/mol	NIST Webbook
ie	10.82	eV	NIST Webbook
ie	10.79	eV	NIST Webbook
ie	10.80 ± 0.10	eV	NIST Webbook
ie	10.78 ± 0.04	eV	NIST Webbook
ie	10.88	eV	NIST Webbook
ie	10.88	eV	NIST Webbook
ie	10.70 ± 0.05	eV	NIST Webbook
ie	10.82 ± 0.03	eV	NIST Webbook

log10ws	-1.47		Aqueous Solubility Prediction Method
log10ws	-1.47		Estimated Solubility Method
logp	1.635		Crippen Method
mcvol	65.370	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4577.86 ± 50.66	kPa	NIST Webbook
pc	4580.00	kPa	KDB
rinpol	533.00		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	570.00		NIST Webbook
rinpol	570.00		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	542.10		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	533.10		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	526.90		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	535.00		NIST Webbook
rinpol	535.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	528.79		NIST Webbook
rinpol	529.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	538.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	511.00		NIST Webbook
rinpol	528.77		NIST Webbook
rinpol	531.00		NIST Webbook
ripol	739.00		NIST Webbook
ripol	739.00		NIST Webbook
ripol	740.00		NIST Webbook

tb	319.60	K	KDB
tb	319.60	K	Study of isobaric vapour liquid equilibrium of some cyclic ethers with 1-chloropropane: Experimental results and SAFT-VR modelling
tc	503.00	K	KDB
tc	503.20 ± 0.30	K	NIST Webbook
tf	150.20 ± 0.70	K	NIST Webbook
tf	150.30	K	KDB
tf	150.55	K	Aqueous Solubility Prediction Method
vc	0.254	m3/kmol	KDB
zc	0.2781600		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.40	J/mol×K	305.47	Joback Method
cpg	121.35	J/mol×K	477.06	Joback Method
cpg	116.51	J/mol×K	448.46	Joback Method
cpg	111.48	J/mol×K	419.86	Joback Method
cpg	100.84	J/mol×K	362.67	Joback Method
cpg	106.26	J/mol×K	391.26	Joback Method
cpg	95.22	J/mol×K	334.07	Joback Method
cpl	131.88	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	132.94	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	133.40	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	132.37	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	133.92	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	134.38	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	130.50	J/mol×K	297.00	NIST Webbook	
cpl	128.63	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	
cpl	128.99	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	129.53	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	130.10	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	130.47	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	130.95	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	131.33	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	131.40	J/mol×K	298.00	NIST Webbook	
cpl	132.20	J/mol×K	298.00	NIST Webbook	
dvisc	0.0008886	Pa×s	204.15	Joback Method	
dvisc	0.0005878	Pa×s	229.48	Joback Method	
dvisc	0.0004222	Pa×s	254.81	Joback Method	
dvisc	0.0003219	Pa×s	280.14	Joback Method	

dvisc	0.0002567	Pa×s	305.47	Joback Method
dvisc	0.0030571	Pa×s	153.49	Joback Method
dvisc	0.0015101	Pa×s	178.82	Joback Method
hvapt	28.90 ± 0.84	kJ/mol	318.70	NIST Webbook
hvapt	27.18	kJ/mol	319.60	NIST Webbook
hvapt	31.00	kJ/mol	284.00	NIST Webbook
hvapt	33.10	kJ/mol	262.00	NIST Webbook
hvapt	27.24	kJ/mol	319.70	KDB
pvap	45.85	kPa	298.15	Thermophysical Study of the n-Hexane or n-Heptane with 1-Chloropropane Systems
rfi	1.38560		298.15	Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes
rfi	1.38800		293.15	Speed of Sound and Density of 1-Chloropropane in the Range of Temperatures 180-373 K and Pressures up to 196.1 MPa
rfi	1.37673		313.15	Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes
rhol	883.81	kg/m3	298.15	High-pressure phase equilibrium in the {carbon dioxide (1) + 1-chloropropane (2)} binary system
rhol	891.00	kg/m3	293.00	KDB
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.43244e+01
Coeff. B	-2.77486e+03
Coeff. C	-3.41110e+01
Temperature range (K), min.	231.80
Temperature range (K), max.	503.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.12803e+01
Coeff. B	-5.68990e+03
Coeff. C	-8.61530e+00
Coeff. D	8.07867e-06
Temperature range (K), min.	150.35
Temperature range (K), max.	503.15

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	283.15	902.63
100.00	288.15	896.23
100.00	293.15	890.21
100.00	298.15	883.84
100.00	303.15	877.47
100.00	308.15	870.93
100.00	313.15	864.52
100.00	318.15	857.87
2000.00	283.15	904.69
2000.00	288.15	898.45
2000.00	293.15	892.48
2000.00	298.15	886.15
2000.00	303.15	879.88
2000.00	308.15	873.45
2000.00	313.15	867.21
2000.00	318.15	860.65
5000.00	283.15	907.93

5000.00	288.15	901.79
5000.00	293.15	895.94
5000.00	298.15	889.74
5000.00	303.15	883.66
5000.00	308.15	877.45
5000.00	313.15	871.28
5000.00	318.15	864.78
7000.00	283.15	909.98
7000.00	288.15	903.93
7000.00	293.15	898.21
7000.00	298.15	892.15
7000.00	303.15	886.15
7000.00	308.15	879.96
7000.00	313.15	873.89
7000.00	318.15	867.55
10000.00	283.15	913.08
10000.00	288.15	907.07
10000.00	293.15	901.51
10000.00	298.15	895.54
10000.00	303.15	889.67
10000.00	308.15	883.53
10000.00	313.15	877.67
10000.00	318.15	871.55
20000.00	283.15	922.59
20000.00	288.15	916.99
20000.00	293.15	911.64
20000.00	298.15	906.01
20000.00	303.15	900.59
20000.00	308.15	894.81
20000.00	313.15	889.31
20000.00	318.15	883.58
30000.00	283.15	931.43
30000.00	288.15	925.99
30000.00	293.15	920.91
30000.00	298.15	915.65
30000.00	303.15	910.36
30000.00	308.15	904.99
30000.00	313.15	899.78
30000.00	318.15	894.34
40000.00	283.15	939.52
40000.00	288.15	934.32
40000.00	293.15	929.44
40000.00	298.15	924.4
40000.00	303.15	919.39

40000.00	308.15	914.15
40000.00	313.15	909.27
40000.00	318.15	904.1
50000.00	283.15	947.07
50000.00	288.15	942.03
50000.00	293.15	937.36
50000.00	298.15	932.48
50000.00	303.15	927.7
50000.00	308.15	922.69
50000.00	313.15	918.01
50000.00	318.15	913.08
60000.00	283.15	954.12
60000.00	288.15	949.19
60000.00	293.15	944.77
60000.00	298.15	940.12
60000.00	303.15	935.41
60000.00	308.15	930.56
60000.00	313.15	926.13
60000.00	318.15	921.31
65000.00	283.15	957.51
65000.00	288.15	952.7
65000.00	293.15	948.3
65000.00	298.15	943.68
65000.00	303.15	939.08
65000.00	308.15	934.35
65000.00	313.15	929.93
65000.00	318.15	925.2

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

Sources

High-pressure phase equilibrium in the {carbon dioxide (1) + 1-chloropropane (2)} binary system: https://www.doi.org/10.1016/j.jct.2015.07.039

Speed of Sound and Density of 1-Chloropropane in the Range of Temperatures 180-373 K and Pressures up to 196.1 MPa: https://www.doi.org/10.1021/acs.jced.7b00443

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Phase equilibrium and thermophysical properties of mixtures containing a cyclic ether and 1-chloropropane: https://www.doi.org/10.1016/j.fluid.2010.04.017

Activity Coefficients at Infinite Dilution for Hydrocarbons in Fatty Alcohols Determined by Gas-Liquid Chromatography: https://www.doi.org/10.1021/je1005517

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Volumetric and refractive properties of binary mixtures containing 1,4-dioxane and chloroalkanes: https://www.doi.org/10.1016/j.jct.2006.05.003

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:	https://www.doi.org/10.1021/je049652j
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Volumetric Properties of Short-Chain Chloroalkanes:	https://www.doi.org/10.1021/je3003805
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1594.mol
Study of isobaric vapour liquid equilibrium of some cyclic ethers with 1-chloropropane: Experimental results and SAFT-VR modelling:	https://www.doi.org/10.1016/j.fluid.2009.01.010
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C540545&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1594
Thermophysical Study of the n-Hexane or n-Heptane with 1- Chloropropane Systems:	https://www.doi.org/10.1016/j.tca.2011.07.023

Legend

af:	Acentric Factor
chg:	Standard gas enthalpy of combustion
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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	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