Propane, 1,3-dichloro-

Other names:	1,3-Dichloropropane
	CH2ClCH2CH2Cl
	R 270fa
	TRIMETHYLENE DICHLORIDE
Inchi:	InChI=1S/C3H6Cl2/c4-2-1-3-5/h1-3H2
InchiKey:	YHRUOJUYPBUZOS-UHFFFAOYSA-N
Formula:	C3H6Cl2
SMILES:	ClCCCCl
Mol. weight [g/mol]:	112.99
CAS:	142-28-9

Physical Properties

Property code	Value	Unit	Source
af	0.2880		KDB
chl	-1885.30 ± 8.40	kJ/mol	NIST Webbook
gf	-49.48	kJ/mol	Joback Method
hf	-136.73	kJ/mol	Joback Method
hfus	11.92	kJ/mol	Joback Method
hvap	40.60 ± 0.10	kJ/mol	NIST Webbook
hvap	41.00	kJ/mol	NIST Webbook
hvap	40.79	kJ/mol	NIST Webbook
hvap	40.75 ± 0.04	kJ/mol	NIST Webbook
hvap	41.00	kJ/mol	NIST Webbook
ie	10.93	eV	NIST Webbook
ie	10.93	eV	NIST Webbook
ie	10.89 ± 0.04	eV	NIST Webbook
ie	10.85 ± 0.05	eV	NIST Webbook
log10ws	-1.62		Aqueous Solubility Prediction Method
log10ws	-1.62		Estimated Solubility Method
logp	1.854		Crippen Method
mcvol	77.610	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4010.00	kPa	KDB
rinpol	760.00		NIST Webbook
rinpol	756.00		NIST Webbook

rinpol	765.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	747.20		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	774.80		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	787.00		NIST Webbook
ripol	1188.00		NIST Webbook
tb	393.60	K	KDB
tc	602.70	K	KDB
tf	239.00 ± 0.02	K	NIST Webbook
tf	173.40	K	Aqueous Solubility Prediction Method
tf	174.00	K	KDB
vc	0.301	m3/kmol	KDB
zc	0.2412650		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.21	J/mol×K	525.16	Joback Method
cpg	115.92	J/mol×K	373.28	Joback Method
cpg	121.44	J/mol×K	403.65	Joback Method
cpg	126.72	J/mol×K	434.03	Joback Method
cpg	131.77	J/mol×K	464.41	Joback Method
cpg	136.60	J/mol×K	494.78	Joback Method
cpg	110.16	J/mol×K	342.90	Joback Method
cpl	157.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0004342	Pa×s	316.32	Joback Method
dvisc	0.0005695	Pa×s	289.74	Joback Method
dvisc	0.0007891	Pa×s	263.15	Joback Method
dvisc	0.0011766	Pa×s	236.57	Joback Method
dvisc	0.0019411	Pa×s	209.99	Joback Method
dvisc	0.0003452	Pa×s	342.90	Joback Method
dvisc	0.0037023	Pa×s	183.41	Joback Method
hvapt	39.00	kJ/mol	371.00	NIST Webbook
hvapt	35.18	kJ/mol	394.00	NIST Webbook

hvapt	33.89	kJ/mol	393.60	KDB
rfi	1.44620		298.15	Isothermal Vapor Liquid Equilibria for Nitromethane and Nitroethane + 1,3-Dichloropropane Binary Systems at Temperatures between (343.15 and 363.15) K
rfi	1.44590		298.15	Isothermal (vapour + liquid) equilibria and excess Gibbs free energies in some binary (cyclopentanone + chloroalkane) mixtures at temperatures from 298.15 K to 318.15 K
rfi	1.44550		298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I: HE and V E for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6
rfi	1.44600		298.15	Density and refractive index in mixtures of ionic liquids and organic solvents: Correlations and predictions
rhol	1154.67	kg/m3	318.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K
rhol	1191.92	kg/m3	288.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K

rhol	1180.50	kg/m3	298.15	Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at T = 298.15 K	
rhol	1167.14	kg/m3	308.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K	
rhol	1154.65	kg/m3	318.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K	
rhol	1179.58	kg/m3	298.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K	
rhol	1191.93	kg/m3	288.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K	
rhol	1179.20	kg/m3	298.15	Speed of sound as a function of temperature and pressure for propane derivatives	

rhol	1155.21	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1167.70	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1180.10	kg/m3	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1179.56	kg/m3	298.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclopentanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K
rhol	1167.16	kg/m3	308.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K

speedsl	1236.45	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1163.22	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1199.72	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
srf	0.03	N/m	303.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	298.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	293.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	313.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

srf	0.03	N/m	308.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44611e+01
Coeff. B	-3.43171e+03
Coeff. C	-4.53460e+01
Temperature range (K), min.	287.47
Temperature range (K), max.	420.41

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.24683e+01
Coeff. B	-7.89152e+03
Coeff. C	-1.15542e+01
Coeff. D	8.02366e-06
Temperature range (K), min.	173.65
Temperature range (K), max.	603.00

Sources

The Critical Temperatures of a Number of (i) (Chloroalkane (C3 C4) + Hydrocarbon (C6-C7)) Binary Mixtures	https://www.doi.org/10.1021/acs.jced.7b00191
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides). VII. HE m and VE m	https://www.doi.org/10.1016/j.jct.2008.10.007
for 20 binary mixtures	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides). VI. HE and VE for 25	https://www.doi.org/10.1016/j.jct.2005.03.020
for 20 binary mixtures	https://www.doi.org/10.1021/je901052w
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides). III. HE m and V E m	https://www.doi.org/10.1016/j.jct.2005.11.003
for 20 binary mixtures	https://www.doi.org/10.1016/j.fluid.2014.10.004
Comprehensive isentropic compressibilities and refractive indices	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination of Henry's Law	https://www.doi.org/10.1021/je3010535
Constants Using Internal Standards with Benchmark Values:	

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1589
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142289&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Density and refractive index in mixtures of ionic liquids and organic solvents: Correlations and predictions:	https://www.doi.org/10.1016/j.jct.2008.01.023
The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes:	https://www.doi.org/10.1016/j.jct.2018.12.042
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1589
Isothermal (vapour + liquid) equilibria and excess Gibbs free energies in some binary (cyclopentanone + chloroalkane) mixtures at temperatures from 298.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2007.03.008
Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at 298.15 K:	https://www.doi.org/10.1016/j.jct.2014.04.004
Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K:	https://www.doi.org/10.1021/je900404r
Isothermal Vapor Liquid Equilibria for Nitromethane and Nitroethane + 1,3-Dichloropropane Binary Systems at Temperatures between (343.15 and 363.15) K:	https://www.doi.org/10.1021/je200651r
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) V. Hex and Vex for 28 binary mixtures {xCu-1H2u-1COOCH3 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6:	https://www.doi.org/10.1016/j.jct.2006.10.008
Speed of sound as a function of temperature and pressure for propane derivatives:	https://www.doi.org/10.1016/j.jct.2016.12.016
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1589.mol
Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (288.15 to 318.15) K:	https://www.doi.org/10.1021/je3013342
Heat Capacities of alpha,omega-Dichloroalkanes at Temperatures from 284.15 K to 353.15 K and a Group Additivity Analysis:	https://www.doi.org/10.1021/je020042y

Legend

af:	Acentric Factor
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
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
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility