

Propane, 1,3-dichloro-

Other names:	1,3-Dichloropropane CH ₂ ClCH ₂ CH ₂ Cl R 270fa TRIMETHYLENE DICHLORIDE
Inchi:	InChI=1S/C3H6Cl2/c4-2-1-3-5/h1-3H2
InchiKey:	YHRUOJUYPBUZOS-UHFFFAOYSA-N
Formula:	C ₃ H ₆ Cl ₂
SMILES:	C1C(C1)Cl
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	41.00	kJ/mol	NIST Webbook
hvap	40.75 ± 0.04	kJ/mol	NIST Webbook
hvap	40.79	kJ/mol	NIST Webbook
hvap	41.00	kJ/mol	NIST Webbook
hvap	40.60 ± 0.10	kJ/mol	NIST Webbook
ie	10.85 ± 0.05	eV	NIST Webbook
ie	10.89 ± 0.04	eV	NIST Webbook
ie	10.93	eV	NIST Webbook
ie	10.93	eV	NIST Webbook
log10ws	-1.62		Estimated Solubility Method
log10ws	-1.62		Aqueous Solubility Prediction Method
logp	1.854		Crippen Method
mvol	77.610	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4010.00	kPa	KDB
rinpol	756.00		NIST Webbook
rinpol	763.00		NIST Webbook

rmpol	774.80		NIST Webbook
rmpol	765.00		NIST Webbook
rmpol	787.00		NIST Webbook
rmpol	747.20		NIST Webbook
rmpol	751.00		NIST Webbook
rmpol	786.00		NIST Webbook
rmpol	760.00		NIST Webbook
rmpol	760.00		NIST Webbook
rmpol	760.00		NIST Webbook
rmpol	765.00		NIST Webbook
rmpol	757.00		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	174.00	K	KDB
tf	173.40	K	Aqueous Solubility Prediction Method
vc	0.301	m ³ /kmol	KDB
zc	0.2412650		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.60	J/mol×K	494.78	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	141.21	J/mol×K	525.16	Joback Method
cpg	110.16	J/mol×K	342.90	Joback Method
cpl	157.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0011766	Paxs	236.57	Joback Method
dvisc	0.0005695	Paxs	289.74	Joback Method
dvisc	0.0037023	Paxs	183.41	Joback Method
dvisc	0.0004342	Paxs	316.32	Joback Method
dvisc	0.0003452	Paxs	342.90	Joback Method
dvisc	0.0007891	Paxs	263.15	Joback Method
dvisc	0.0019411	Paxs	209.99	Joback Method
hvapt	33.89	kJ/mol	393.60	KDB
hvapt	39.00	kJ/mol	371.00	NIST Webbook

hvapt	35.18	kJ/mol	394.00	NIST Webbook
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	1.44600		298.15	Density and refractive index in mixtures of ionic liquids and organic solvents: Correlations and predictions
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 + α,α -alkyl dihalides) I: HE and V E for 25 binary mixtures $\{x\text{Cu-1H}_2\text{u-1CO}_2\text{C}_2\text{H}_5 + (1-x)\alpha,\alpha\text{-ClCH}_2(\text{CH}_2)_v\text{-2CH}_2\text{Cl}\}$, where $u = 1$ to 5, $\alpha = 1$ and $v = x = 2$ to 6
rhol	1191.93	kg/m ³	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	1180.10	kg/m ³	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K

rho	1167.70	kg/m ³	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rho	1154.65	kg/m ³	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
rho	1155.21	kg/m ³	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rho	1167.14	kg/m ³	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
rho	1179.56	kg/m ³	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
rho	1191.92	kg/m ³	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

rhoI	1154.67	kg/m ³	318.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K
rhoI	1167.16	kg/m ³	308.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K
rhoI	1179.20	kg/m ³	298.15	Speed of sound as a function of temperature and pressure for propane derivatives
rhoI	1179.58	kg/m ³	298.15	Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at Temperatures between (288.15 and 318.15) K
rhoI	1180.50	kg/m ³	298.15	Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at T = 298.15 K
speedsI	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	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
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
srf	0.03	N/m	293.15	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	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
srf	0.03	N/m	303.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures (xCu 1H2u
<https://www.doi.org/10.1016/j.jct.2008.10.007>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VI. HE m and VE m for 20 binary mixtures (xCu 1H2u
<https://www.doi.org/10.1021/je020042y>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) V. HE m and VE m for 20 binary mixtures (xCu 1H2u
<https://www.doi.org/10.1021/je200651r>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) IV. HE m and VE m for 20 binary mixtures (xCu 1H2u
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C142289&Units=SI>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) III. HE m and VE m for 20 binary mixtures (xCu 1H2u
<https://www.doi.org/10.1021/je3010535>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) II. HE m and VE m for 20 binary mixtures (xCu 1H2u
<https://www.doi.org/10.1021/je900404r>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I. HE m and VE m for 20 binary mixtures (xCu 1H2u
<https://www.doi.org/10.1021/je901052w>
- Densities and Excess Molar Volumes of the Binary Mixtures of Cyclohexanone with Chloroalkanes at T = (288.15, 298.15, 308.15, and 318.15) K:
<https://www.doi.org/10.1016/j.jct.2005.03.020>
- 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:
<https://www.doi.org/10.1016/j.jct.2005.03.020>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I: HE and VE for 25 binary mixtures (xCu 1H2u-1CO2C2H5 + (1-x)a,x-CICH2(CH2)v-2CH2Cl), where
<https://www.doi.org/10.1016/j.jct.2006.10.008>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) V. Hex and Vex for 20 binary mixtures (xCu 1H2u-1CO2C2H5 + (1-x)a,x-CICH2(CH2)v-2CH2Cl), where
<https://www.doi.org/10.1021/acs.jced.7b00191>
- The Critical Temperatures of a Number of (i) Chloroalkanes (C3-C4) + Esters and (ii) Chloroalkanes + Hydrocarbons (C3-C4) + Esters
http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
- Estimated S₁(T) for Binary Mixtures of Chlorobenzene and Chloroalkanes (C3-C4) + Esters
<https://www.doi.org/10.1016/j.jct.2005.11.003>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) III. HE m and VE m for 20 binary mixtures (xCu 1H2u-1CO2C2H5 + (1-x)a,x-CICH2(CH2)v-2CH2Cl), where
<https://www.doi.org/10.1016/j.jct.2016.12.016>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) II. HE m and VE m for 20 binary mixtures (xCu 1H2u-1CO2C2H5 + (1-x)a,x-CICH2(CH2)v-2CH2Cl), where
<https://www.doi.org/10.1016/j.jct.2018.12.042>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I. HE m and VE m for 20 binary mixtures (xCu 1H2u-1CO2C2H5 + (1-x)a,x-CICH2(CH2)v-2CH2Cl), where
<https://www.doi.org/10.1016/j.jct.2014.04.004>
- Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I. HE m and VE m for 20 binary mixtures (xCu 1H2u-1CO2C2H5 + (1-x)a,x-CICH2(CH2)v-2CH2Cl), where
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- KDB Pure (Korean Thermophysical Properties Databank):
<https://www.thermophysicalproperties.org/>
- 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>

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

Isothermal (vapour + liquid) equilibria and excess Gibbs free energies in <https://www.doi.org/10.1016/j.jct.2007.03.008>

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

Some binary (chloroalkane + chloroalkane) mixtures at temperatures from 298.15 K to 318.15 K: <http://link.springer.com/article/10.1007/BF02311772>

Volumetric Study for the Binary Nitromethane with Chloroalkane <https://www.doi.org/10.1021/je3013342>

Speeds of sound, isotherms in the Range 298.15 to 318.15 K: <https://www.doi.org/10.1016/j.fluid.2014.10.004>

Speeds of sound, isotherms in the Range 298.15 to 318.15 K:

Compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K.

Comparison with theories:

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
rho:	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

Latest version available from:

<https://www.chemeo.com/cid/64-661-7/Propane-1-3-dichloro.pdf>

Generated by Cheméo on 2024-04-19 21:21:45.228380218 +0000 UTC m=+15850954.148957530.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.