Ethane, 1,1,1-trichloro-

Other names:

1,1,1-TCE
1,1,1-Trichloraethan
1,1,1-Trichlorethane
1,1,1-Trichloroethane
1,1,1-Tricloroetano
ALPHA-TRICHLOROETHANE
Aerothene TT
CF 2
CH3CCl3
Chloroetene
Chloroethene
Chloroethene NU
Chloroform, methyl-
Chlorotene
Chlorothane NU
Chlorothene
Chlorothene NU
Chlorothene SM
Chlorothene VG
Chlorten
Cleanite
Distillex DS1
Ethana
Ethana NU
F 140a
Freon 140a
Genklene LB
HCC 140a
ICI-CF 2
Inhibisol
METHYLCHLOROFORM
Methyltrichloromethane
NCI-C04626
R-140a
REFRIGERANT-140A
Rcra waste number U226
Solvent 111
Solvethane
Tafclean
Three One A

Three One S
Tri-ethane
Trichloro-1,1,1-ethane
Trichloroethane
Trichloromethylmethane
UN 2831
«alpha»-T
«alpha»-Trichloroethane
Â«alphaÂ»-T
Â«alphaÂ»-Trichloroethane

Inchi: InChI=1S/C2H3Cl3/c1-2(3,4)5/h1H3
InchiKey: UOCLXMDMGBRAIB-UHFFFAOYSA-N
Formula: C2H3Cl3
SMILES: CC(Cl)(Cl)Cl
Mol. weight [g/mol]: 133.40
CAS: 71-55-6

Physical Properties

Property code	Value	Unit	Source
af	0.2170		KDB
chl	-1112.10 ± 1.30	kJ/mol	NIST Webbook
chl	-1108.00 ± 0.79	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
gf	-66.99	kJ/mol	Joback Method
hf	-144.40 ± 1.60	kJ/mol	NIST Webbook
hf	-145.00 ± 2.00	kJ/mol	NIST Webbook
hf	-142.30 ± 1.40	kJ/mol	NIST Webbook
hfl	-174.00	kJ/mol	NIST Webbook
hfl	-177.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-178.60 ± 0.84	kJ/mol	NIST Webbook
hfl	-174.80 ± 1.40	kJ/mol	NIST Webbook
hfus	6.11	kJ/mol	Joback Method
hvap	32.50 ± 0.10	kJ/mol	NIST Webbook
hvap	32.47 ± 0.06	kJ/mol	NIST Webbook
hvap	32.47 ± 0.08	kJ/mol	NIST Webbook
hvap	32.59 ± 0.07	kJ/mol	NIST Webbook
hvap	32.50 ± 0.10	kJ/mol	NIST Webbook
hvap	32.62	kJ/mol	NIST Webbook
ie	11.25	eV	NIST Webbook
ie	11.00	eV	NIST Webbook

log10ws	-2.04		Aqueous Solubility Prediction Method
log10ws	-2.00		Estimated Solubility Method
logp	2.377		Crippen Method
mcvol	75.760	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	4300.00	kPa	KDB
rinpol	636.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	625.98		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	628.60		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	645.10		NIST Webbook
rinpol	623.50		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	642.40		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	637.00		NIST Webbook

rinpol	637.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	621.00		NIST Webbook
ripol	891.00		NIST Webbook
ripol	898.00		NIST Webbook
ripol	898.00		NIST Webbook
ripol	904.35		NIST Webbook
ripol	909.11		NIST Webbook
ripol	897.56		NIST Webbook
ripol	891.00		NIST Webbook
ripol	885.00		NIST Webbook
ripol	908.00		NIST Webbook
ripol	900.00		NIST Webbook
ripol	886.00		NIST Webbook
ripol	898.00		NIST Webbook
ripol	900.00		NIST Webbook
sl	227.48	J/mol×K	NIST Webbook
sl	226.70	J/mol×K	NIST Webbook
tb	347.00	K	Excess volumes and speeds of sound of mixtures of 1,2-dibromoethane with chlorinated ethanes and ethenes at 303.15 K
tb	347.35	K	Excess molar enthalpies of dimethylsulfoxide with chloroethanes and chloroethenes at 298.15K
tb	347.35	K	Vapor-Liquid Equilibria and Excess Molar Enthalpies for N-Methyl-2-pyrrolidone with Chloroethanes and Chloroethenes
tb	347.35	K	Isobaric Vapor Liquid Equilibrium for Dimethylsulfoxide with Chloroethanes and Chloroethenes
tb	347.24	K	KDB
tc	545.00	K	KDB
tc	548.40	K	NIST Webbook
tf	231.90 ± 1.20	K	NIST Webbook
tf	239.20 ± 1.00	K	NIST Webbook
tf	240.90 ± 0.20	K	NIST Webbook
tf	244.95 ± 0.40	K	NIST Webbook
tf	240.50 ± 0.30	K	NIST Webbook

tf	240.80 ± 0.50	K	NIST Webbook
tf	242.01	K	Aqueous Solubility Prediction Method
tf	241.15 ± 1.00	K	NIST Webbook
tf	240.95 ± 0.20	K	NIST Webbook
tf	242.70	K	KDB
tf	242.70 ± 0.02	K	NIST Webbook
tt	243.13	K	KDB
tt	243.13 ± 0.02	K	NIST Webbook
tt	240.10 ± 0.20	K	NIST Webbook
tt	240.20 ± 0.20	K	NIST Webbook
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.94	J/mol×K	457.47	Joback Method
cpg	118.85	J/mol×K	491.88	Joback Method
cpg	122.39	J/mol×K	526.30	Joback Method
cpg	100.77	J/mol×K	354.22	Joback Method
cpg	105.93	J/mol×K	388.64	Joback Method
cpg	110.64	J/mol×K	423.05	Joback Method
cpg	125.60	J/mol×K	560.71	Joback Method
cpl	138.90	J/mol×K	257.29	NIST Webbook
cpl	144.31	J/mol×K	299.59	NIST Webbook
cpl	144.40	J/mol×K	298.15	NIST Webbook
cps	123.00	J/mol×K	225.00	NIST Webbook
dvisc	0.0065153	Pa×s	204.48	Joback Method
dvisc	0.0008725	Pa×s	304.31	Joback Method
dvisc	0.0012605	Pa×s	279.35	Joback Method
dvisc	0.0019574	Pa×s	254.39	Joback Method
dvisc	0.0006385	Pa×s	329.26	Joback Method
dvisc	0.0004883	Pa×s	354.22	Joback Method
dvisc	0.0033450	Pa×s	229.44	Joback Method
hfust	7.47	kJ/mol	224.20	NIST Webbook
hfust	2.35	kJ/mol	243.10	NIST Webbook
hfust	7.49	kJ/mol	224.80	NIST Webbook
hfust	1.88	kJ/mol	240.20	NIST Webbook
hfust	1.88	kJ/mol	240.10	NIST Webbook
hfust	1.88	kJ/mol	240.10	NIST Webbook
hfust	0.21	kJ/mol	205.00	NIST Webbook

hfust	7.45	kJ/mol	223.60	NIST Webbook
hvapt	33.31	kJ/mol	286.53	NIST Webbook
hvapt	29.50	kJ/mol	512.00	NIST Webbook
hvapt	29.40	kJ/mol	443.00	NIST Webbook
hvapt	30.50	kJ/mol	378.50	NIST Webbook
hvapt	32.30	kJ/mol	333.50	NIST Webbook
hvapt	37.60	kJ/mol	247.00	NIST Webbook
hvapt	33.40	kJ/mol	279.00	NIST Webbook
hvapt	33.40 ± 0.10	kJ/mol	284.00	NIST Webbook
hvapt	32.40	kJ/mol	344.00	NIST Webbook
hvapt	29.86	kJ/mol	347.20	NIST Webbook
pvap	37.61	kPa	318.15	(Vapour + liquid) equilibria and excess Gibbs free energies of (cyclohexanone + 1- chlorobutane and + 1,1,1-trichloroethane) binary mixtures at temperatures from (298.15 to 318.15) K
pvap	25.85	kPa	308.15	(Vapour + liquid) equilibria and excess Gibbs free energies of (cyclohexanone + 1- chlorobutane and + 1,1,1-trichloroethane) binary mixtures at temperatures from (298.15 to 318.15) K
pvap	16.64	kPa	298.15	(Vapour + liquid) equilibria and excess Gibbs free energies of (cyclohexanone + 1- chlorobutane and + 1,1,1-trichloroethane) binary mixtures at temperatures from (298.15 to 318.15) K
rfi	1.43590		298.15	Bubble Temperature Measurements on Binary Mixtures Formed by Cyclohexane at 94.7 kPa

rfi	1.43540		298.15	Isothermal (vapour + liquid) equilibria in the binary mixtures (1,2-dichloroethane and 1,1,1-trichloroethane with cyclopentanone) within the temperature range (298.15 to 313.15) K
rfi	1.43790		293.15	Bubble points of the binary mixtures formed by ethylbenzene with some chloroaliphatics and substituted benzenes at p = 94.7 kPa
rfi	1.43590		298.15	Bubble-Temperature Measurements on Some Binary Mixtures Formed by Tetrahydrofuran or Amyl Alcohol with Hydrocarbons, Chlorohydrocarbons, or Butanols at (94.6 or 95.8) kPa
rfi	1.43600		298.15	Bubble Temperature Measurements on the Binary Mixtures of n-Heptane or Nitrobenzene or Chlorobenzene with Some Chloroethanes and Chloroethylenes at (94.6 to 95.8) kPa
rhol	1328.24	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	1329.49	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	1312.65	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	1346.17	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	1294.47	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	1311.45	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

rhol	1328.27	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	1295.66	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	1344.95	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	1294.47	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	1311.45	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	1339.00	kg/m3	298.00	KDB
rhol	1331.30	kg/m3	298.15	Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at T = 298.15 K
sfust	7.84	J/mol×K	240.10	NIST Webbook
sfust	33.31	J/mol×K	223.60	NIST Webbook

sfust	1.02	J/mol×K	205.00	NIST Webbook
sfust	33.30	J/mol×K	224.20	NIST Webbook
sfust	7.80	J/mol×K	240.20	NIST Webbook
sfust	33.30	J/mol×K	224.80	NIST Webbook
sfust	9.67	J/mol×K	243.10	NIST Webbook
speedsl	962.94	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	928.68	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	894.71	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
svapt	116.26	J/mol×K	286.53	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41227e+01
Coeff. B	-2.88621e+03

Coeff. C	-4.35260e+01
Temperature range (K), min.	243.10
Temperature range (K), max.	545.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.02341e+01
Coeff. B	-6.44789e+03
Coeff. C	-9.92362e+00
Coeff. D	8.37906e-06
Temperature range (K), min.	242.75
Temperature range (K), max.	545.00

Sources

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.:	https://www.doi.org/10.1016/j.fluid.2014.10.004
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1566.mol
Bubble-Temperature Measurements on Some Binary Mixtures Formed by Tetrahydrofuran or Amyl Alcohol with Hydrocarbons, Chlorohydrocarbons, or Butanols at (94.0 or 95.8) kPa:	https://www.doi.org/10.1021/je030141r
Isothermal (vapour + liquid) equilibria in the binary mixtures (1,2-dichloroethane and 1,1,1-trichloroethane with cyclopentanone) within the temperature range (298.15 to 313.15) K:	https://www.doi.org/10.1016/j.jct.2005.07.016
Bubble Temperature Measurements on Binary Mixtures Formed by Cyclohexane at 94.7 kPa:	https://www.doi.org/10.1021/je020148t
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/10.1021/je901052w
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71556&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1566
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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess molar enthalpies of dimethylsulfoxide with chloroethanes and chloroethenes at 298.15K:	https://www.doi.org/10.1016/j.tca.2007.08.008
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1566
Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K:	https://www.doi.org/10.1021/je3013342
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Bubble points of the binary mixtures formed by ethylbenzene with some chloroaliphatics and substituted benzenes at p = 94.7 kPa:	https://www.doi.org/10.1016/j.jct.2005.12.009
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Excess volumes and speeds of sound of mixtures of 1,2-dibromoethane with chlorinated ethanes and ethenes at 303.15 K:	https://www.doi.org/10.1016/j.jct.2004.11.013
Isobaric Vapor Liquid Equilibrium for Dimethylsulfoxide with Chloroethanes and Chloroethenes:	https://www.doi.org/10.1021/je700408x
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapor-Liquid Equilibria and Excess Molar Enthalpies for N-Methyl-2-pyrrolidone with Chloroethanes and Chloroethenes:	https://www.doi.org/10.1021/je020065c
Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2014.04.004
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535

Bubble Temperature Measurements on the Binary Mixtures of n-Heptane or Nitrobenzene or Chlorobenzene with some Chloroethanes and 1-chlorobutane at (94.6 to 95.8) kPa

https://www.doi.org/10.1021/je0301085

(Vapour + liquid) equilibria and excess Gibbs free energies of (cyclohexanone + chloroethylenes at (94.6 to 95.8) kPa: 1,1,1-trichloroethane) binary mixtures at temperatures from (298.15 to 318.15) K

https://www.doi.org/10.1016/j.jct.2009.04.006

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dm:	Dipole Moment
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
hfust:	Enthalpy of fusion at a given temperature
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
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume