Ethane, 1,1,2-trichloro-

Other names:	1,1,2-Trichlorethane
	1,1,2-Trichloroethane
	1,2,2-Trichloroethane
	CHCl2CH2Cl
	ETHANE TRICHLORIDE
	NCI-C04579
	NSC 405074
	R-140
	Rcra waste number U227
	Rcra waste number U359
	Trichloroethane
	Trojchloroetan(1,1,2)
	VINYL TRICHLORIDE
	freon 140
	vinyltrichloride
	«beta»-T
	«beta»-Trichloroethane
	Â«betaÂ»-T
	Â«betaÂ»-Trichloroethane
Inchi:	InChI=1S/C2H3Cl3/c3-1-2(4)5/h2H,1H2
InchiKey:	UBOXGVDOUJQMTN-UHFFFAOYSA-N
Formula:	C2H3Cl3
SMILES:	ClCC(Cl)Cl
Mol. weight [g/mol]:	133.40
CAS:	79-00-5

Physical Properties

Property code	Value	Unit	Source
chl	-1098.10 ± 4.40	kJ/mol	NIST Webbook
dm	1.25	debye	KDB
gf	-77.54	kJ/mol	KDB
hf	-148.20 ± 4.40	kJ/mol	NIST Webbook
hf	-138.60	kJ/mol	KDB
hf	-148.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-188.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-188.50 ± 4.40	kJ/mol	NIST Webbook
hfus	10.00	kJ/mol	Joback Method

hvap	40.28	kJ/mol	NIST Webbook
hvap	40.20 ± 0.10	kJ/mol	NIST Webbook
hvap	40.30 ± 0.07	kJ/mol	NIST Webbook
hvap	40.10 ± 0.60	kJ/mol	NIST Webbook
hvap	40.30 ± 0.10	kJ/mol	NIST Webbook
hvap	40.28 ± 0.06	kJ/mol	NIST Webbook
ie	11.00	eV	NIST Webbook
ie	11.48	eV	NIST Webbook
log10ws	-1.48		Estimated Solubility Method
log10ws	-1.48		Aqueous Solubility Prediction Method
logp	2.029		Crippen Method
mcvol	75.760	ml/mol	McGowan Method
pc	5140.00	kPa	KDB
rinpol	748.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	747.50		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	741.40		NIST Webbook
rinpol	745.10		NIST Webbook
rinpol	748.10		NIST Webbook
rinpol	743.10		NIST Webbook
rinpol	738.70		NIST Webbook
rinpol	742.80		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1226.00		NIST Webbook

ripol	1236.00		NIST Webbook
ripol	1269.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1282.00		NIST Webbook
tb	386.60	K	KDB
tc	602.00	K	NIST Webbook
tc	606.00	K	KDB
tf	236.55	K	NIST Webbook
tf	236.60 ± 0.02	K	NIST Webbook
tf	236.50 ± 0.20	K	NIST Webbook
tf	237.90 ± 0.20	K	NIST Webbook
tf	235.80	K	KDB
tf	236.58 ± 0.05	K	NIST Webbook
tf	236.95	K	Aqueous Solubility Prediction Method
tt	237.10 ± 0.20	K	NIST Webbook
vc	0.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.75	J/mol×K	521.47	Joback Method
cpg	114.49	J/mol×K	488.58	Joback Method
cpg	120.82	J/mol×K	554.36	Joback Method
cpg	99.38	J/mol×K	357.01	Joback Method
cpg	103.48	J/mol×K	389.90	Joback Method
cpg	107.37	J/mol×K	422.79	Joback Method
cpg	111.03	J/mol×K	455.69	Joback Method
cps	143.10	J/mol×K	251.70	NIST Webbook
dvisc	0.0006996	Pa×s	300.36	Joback Method
dvisc	0.0005175	Pa×s	328.69	Joback Method
dvisc	0.0004016	Pa×s	357.01	Joback Method
dvisc	0.0058194	Pa×s	187.06	Joback Method
dvisc	0.0027805	Pa×s	215.38	Joback Method
dvisc	0.0015774	Pa×s	243.71	Joback Method
dvisc	0.0010070	Pa×s	272.03	Joback Method
hfust	11.38	kJ/mol	237.10	NIST Webbook
hfust	11.38	kJ/mol	237.10	NIST Webbook
hfust	10.90	kJ/mol	237.90	NIST Webbook
hfust	10.88	kJ/mol	237.90	NIST Webbook
hfust	11.38	kJ/mol	237.10	NIST Webbook

hvapt	38.20	kJ/mol	365.00	NIST Webbook
hvapt	38.29 ± 0.63	kJ/mol	330.33	NIST Webbook
hvapt	38.30	kJ/mol	354.50	NIST Webbook
hvapt	33.30	kJ/mol	386.60	KDB
hvapt	34.82	kJ/mol	386.90	NIST Webbook
hvapt	38.60	kJ/mol	350.00	NIST Webbook
rhol	1409.60	kg/m3	313.15	Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane), (Phenylacetonitrile + Trichloroethene), and (Phenylacetonitrile + Tetrachloroethene) at Temperatures of (303.15, 308.15, and 313.15) K
rhol	1416.10	kg/m3	308.15	Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane), (Phenylacetonitrile + Trichloroethene), and (Phenylacetonitrile + Tetrachloroethene) at Temperatures of (303.15, 308.15, and 313.15) K

rhol	1425.00	kg/m3	303.15	Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane), (Phenylacetonitrile + Trichloroethene), and (Phenylacetonitrile + Tetrachloroethene) at Temperatures of (303.15, 308.15, and 313.15) K
rhol	1441.00	kg/m3	293.00	KDB
sfust	48.00	J/mol×K	237.10	NIST Webbook
sfust	45.70	J/mol×K	237.90	NIST Webbook
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44525e+01
Coeff. B	-3.36081e+03
Coeff. C	-4.50510e+01
Temperature range (K), min.	282.31
Temperature range (K), max.	412.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.69520e+01
Coeff. B	-6.70908e+03
Coeff. C	-7.67345e+00
Coeff. D	4.83782e-06
Temperature range (K), min.	236.50
Temperature range (K), max.	602.00

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
308.15	101.00	0.0009030

Reference *https://www.doi.org/10.1016/j.jct.2006.06.009*

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Densities and viscosities of binary liquid mixtures of N-methylacetamide with some chloroethanes and chloroethenes at T = 308.15 K:	https://www.doi.org/10.1016/j.jct.2006.06.009
Determination of Henry's Law Constants Using Internal Standards and Benchmark Values:	https://www.doi.org/10.1021/je3010535
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79005&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1567
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane) at Temperatures of (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je900570e
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1567.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume