Ethane, 1,1-dichloro-

Other names:	1,1-Dichloorethaan
	1,1-Dichloraethan
	1,1-Dichlorethane
	1,1-Dichloroethane
	1,1-Dicloroetano
	Aethylidenchlorid
	Assymmetrical Dichloroethane
	CH3CHCl2
	Chlorure d'ethylidene
	Cloruro di etilidene
	Dichloromethylmethane
	ETHYLIDENE DICHLORIDE
	Ethylidene chloride
	NCI-C04535
	R-150a
	REFRIGERANT-150A
	Rcra waste number U076
	UN 2362
	freon 150a
Inchi:	InChI=1S/C2H4Cl2/c1-2(3)4/h2H,1H3
InchiKey:	SCYULBFZEHDVBN-UHFFFAOYSA-N
Formula:	C2H4Cl2
SMILES:	CC(Cl)Cl
Mol. weight [g/mol]:	98.96
CAS:	75-34-3

Physical Properties

Property code	Value	Unit	Source
af	0.2400		KDB
chl	-1246.80 ± 8.40	kJ/mol	NIST Webbook
dm	2.00	debye	KDB
gf	-73.14	kJ/mol	KDB
hf	-130.00	kJ/mol	KDB
hf	-132.50 ± 3.50	kJ/mol	NIST Webbook
hf	-127.60 ± 1.10	kJ/mol	NIST Webbook
hfl	-163.30 ± 3.50	kJ/mol	NIST Webbook
hfus	5.81	kJ/mol	Joback Method

hvap	30.60 ± 0.10	kJ/mol	NIST Webbook
hvap	30.62 ± 0.14	kJ/mol	NIST Webbook
hvap	30.83 ± 0.08	kJ/mol	NIST Webbook
hvap	30.77	kJ/mol	NIST Webbook
ie	11.06	eV	NIST Webbook
ie	11.04 ± 0.02	eV	NIST Webbook
ie	11.02	eV	NIST Webbook
ie	11.23 ± 0.02	eV	NIST Webbook
log10ws	-1.29		Estimated Solubility Method
log10ws	-1.29		Aqueous Solubility Prediction Method
logp	1.810		Crippen Method
mcvol	63.520	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	5061.00 ± 10.00	kPa	NIST Webbook
pc	5070.00	kPa	KDB
rinpol	592.20		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	570.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	541.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	579.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	563.00		NIST Webbook
rinpol	563.00		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	590.60		NIST Webbook
rinpol	594.20		NIST Webbook
rinpol	598.90		NIST Webbook
rinpol	601.60		NIST Webbook
rinpol	593.30		NIST Webbook
rinpol	585.90		NIST Webbook
rinpol	568.00		NIST Webbook
ripol	901.48		NIST Webbook
ripol	881.00		NIST Webbook
ripol	886.92		NIST Webbook
ripol	901.00		NIST Webbook
ripol	900.52		NIST Webbook

sl	211.75	J/mol×K	NIST Webbook
tb	330.50	K	KDB
tc	523.00	K	KDB
tc	523.40 ± 0.20	K	NIST Webbook
tf	176.19	K	KDB
tf	176.50 ± 0.30	K	NIST Webbook
tf	176.70 ± 1.00	K	NIST Webbook
tf	174.00 ± 1.50	K	NIST Webbook
tf	176.20	K	Aqueous Solubility Prediction Method
tt	176.18 ± 0.02	K	NIST Webbook
vc	0.236	m3/kmol	KDB
zc	0.2751580		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	93.39	J/mol×K	413.00	Joback Method
cpg	81.15	J/mol×K	319.58	Joback Method
cpg	85.42	J/mol×K	350.72	Joback Method
cpg	89.49	J/mol×K	381.86	Joback Method
cpg	100.65	J/mol×K	475.29	Joback Method
cpg	97.11	J/mol×K	444.15	Joback Method
cpg	104.03	J/mol×K	506.43	Joback Method
cpl	120.90	J/mol×K	298.00	NIST Webbook
cpl	127.20	J/mol×K	298.00	NIST Webbook
cpl	126.27	J/mol×K	298.15	NIST Webbook
dvisc	0.0003301	Pa×s	319.58	Joback Method
dvisc	0.0004258	Pa×s	292.51	Joback Method
dvisc	0.0005786	Pa×s	265.43	Joback Method
dvisc	0.0056724	Pa×s	157.14	Joback Method
dvisc	0.0024926	Pa×s	184.21	Joback Method
dvisc	0.0013522	Pa×s	211.29	Joback Method
dvisc	0.0008429	Pa×s	238.36	Joback Method
hfust	7.87	kJ/mol	176.18	NIST Webbook
hfust	7.87	kJ/mol	176.20	NIST Webbook
hfust	7.87	kJ/mol	176.20	NIST Webbook
hvapt	31.00	kJ/mol	293.00	NIST Webbook
hvapt	31.00 ± 29.00	kJ/mol	293.00	NIST Webbook
hvapt	31.90	kJ/mol	262.00	NIST Webbook
hvapt	28.70	kJ/mol	330.70	KDB

hvapt	33.50	kJ/mol	335.50	NIST Webbook
hvapt	34.40	kJ/mol	271.50	NIST Webbook
hvapt	28.20	kJ/mol	449.00	NIST Webbook
hvapt	29.20	kJ/mol	429.00	NIST Webbook
hvapt	28.85	kJ/mol	330.40	NIST Webbook
rhol	1168.00	kg/m3	298.00	KDB
sfust	44.67	J/mol×K	176.18	NIST Webbook
srf	0.02	N/m	293.20	KDB
svapt	105.81	J/mol×K	293.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45193e+01
Coeff. B	-2.92184e+03
Coeff. C	-3.53950e+01
Temperature range (K), min.	240.70
Temperature range (K), max.	523.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.31701e+01
Coeff. B	-5.95760e+03
Coeff. C	-8.86262e+00
Coeff. D	8.18126e-06
Temperature range (K), min.	176.19
Temperature range (K), max.	523.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1572.mol
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
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1572
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75343&Units=SI
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1572
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of 3,7-Dinitro-1,3,5,7-tetraazabicyclo [3.3.1] Nonane in Ethanenitrile, Methanol, 1,1-Dichloroethane, Dimethyl Sulfoxide, Acetone, and Mixed Solvents	https://www.doi.org/10.1021/acs.jced.5b00033

Legend

af:	Acentric Factor
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
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
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
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
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
zc:	Critical Compressibility