Ethene, 1,1-dichloro-

Other names:	1,1-DCE
	1,1-DICHLOROETHENE
	1,1-Dichloroethylene
	1,1-dichloroethylene (vinylidene chloride)
	1,1-dichloroethylene (vinylidine chloride)
	CH2=CCl2
	Chlorure de vinylidene
	Ethylene, 1,1-dichloro-
	NCI-C54262
	Rcra waste number U078
	VDC
	VINYLIDENE CHLORIDE
	Vinylidene dichloride
	Vinylidine chloride
Inchi:	InChI=1S/C2H2Cl2/c1-2(3)4/h1H2
InchiKey:	LGXVIGDEPROXKC-UHFFFAOYSA-N
Formula:	C2H2Cl2
SMILES:	C=C(Cl)Cl
Mol. weight [g/mol]:	96.94
CAS:	75-35-4

Physical Properties

Property code	Value	Unit	Source
af	0.1790		KDB
chl	-1096.00 ± 1.40	kJ/mol	NIST Webbook
chl	-1095.90	kJ/mol	NIST Webbook
ea	0.10	eV	NIST Webbook
gf	21.39	kJ/mol	Joback Method
hf	2.00 ± 2.00	kJ/mol	NIST Webbook
hf	2.20 ± 1.40	kJ/mol	NIST Webbook
hfl	-24.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-25.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-24.30 ± 1.40	kJ/mol	NIST Webbook
hfus	6.74	kJ/mol	Joback Method
hvap	26.48 ± 0.08	kJ/mol	NIST Webbook
hvap	26.48 ± 0.08	kJ/mol	NIST Webbook
hvap	26.74 ± 0.09	kJ/mol	NIST Webbook

hvap	26.74	kJ/mol	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.74	eV	NIST Webbook
ie	9.83	eV	NIST Webbook
ie	9.81 ± 0.04	eV	NIST Webbook
ie	9.79	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.99 ± 0.02	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
log10ws	-1.64		Aqueous Solubility Prediction Method
log10ws	-1.64		Estimated Solubility Method
logp	1.935		Crippen Method
mcvol	59.220	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	4680.00	kPa	KDB
rinpol	513.00		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	489.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	521.10		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	511.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	520.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	521.10		NIST Webbook
rinpol	519.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	511.00		NIST Webbook
ripol	750.44		NIST Webbook
ripol	715.00		NIST Webbook
ripol	744.00		NIST Webbook
ripol	744.91		NIST Webbook

ripol	736.00		NIST Webbook
ripol	715.00		NIST Webbook
ripol	736.00		NIST Webbook
ripol	736.00		NIST Webbook
ripol	734.18		NIST Webbook
ripol	744.00		NIST Webbook
ripol	744.00		NIST Webbook
sl	201.54	J/mol×K	NIST Webbook
tb	304.20	K	NIST Webbook
tb	304.70	K	KDB
tb	304.70	K	NIST Webbook
tb	304.55 ± 0.20	K	NIST Webbook
tc	489.00	K	KDB
tf	150.65	K	Aqueous Solubility Prediction Method
tf	156.00	K	KDB
tt	150.59 ± 0.02	K	NIST Webbook
vc	0.219	m3/kmol	KDB
zc	0.2520840		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	81.88	J/mol×K	443.47	Joback Method
cpg	84.42	J/mol×K	475.19	Joback Method
cpg	69.91	J/mol×K	316.58	Joback Method
cpg	73.19	J/mol×K	348.30	Joback Method
cpg	76.27	J/mol×K	380.02	Joback Method
cpg	79.17	J/mol×K	411.75	Joback Method
cpg	86.80	J/mol×K	506.91	Joback Method
cpl	111.29	J/mol×K	298.15	NIST Webbook
hfust	6.51	kJ/mol	150.90	NIST Webbook
hfust	6.51	kJ/mol	150.90	NIST Webbook
hfust	6.51	kJ/mol	150.59	NIST Webbook
hvapt	28.40	kJ/mol	275.00	NIST Webbook
hvapt	26.48	kJ/mol	298.15	NIST Webbook
hvapt	30.18	kJ/mol	304.70	KDB
hvapt	26.14	kJ/mol	304.70	NIST Webbook
sfust	43.26	J/mol×K	150.59	NIST Webbook
svapt	88.80	J/mol×K	298.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50904e+01
Coeff. B	-2.91479e+03
Coeff. C	-2.58590e+01
Temperature range (K), min.	222.77
Temperature range (K), max.	324.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.64762e+01
Coeff. B	-6.23863e+03
Coeff. C	-1.27358e+01
Coeff. D	1.56756e-05
Temperature range (K), min.	150.65
Temperature range (K), max.	482.00

Sources

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

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C75354&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1722

Determination of Henry's Law Constants Using Internal Standards with Benchmark Values: https://www.doi.org/10.1021/je3010535

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB: https://www.cheric.org/files/research/kdb/mol/mol1722.mol

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
ea:	Electron affinity
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
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
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