

Ethene, chloro-

Other names:	C2H3Cl CHLOROETHENE CHLOROETHYLENE Chlorethene Chlorethylene Chlorure de vinyle Cloruro di vinile Ethylene monochloride Ethylene, chloro- Monochloroethene Monochloroethylene Rcra waste number U043 Trovidur UN 1086 VC VCM Vinyl C monomer Vinyl chloride Vinyl chloride monomer Vinylchlorid Vinyle(chlorure de) Wynylu chlorek
Inchi:	InChI=1S/C2H3Cl/c1-2-3/h2H,1H2
InchiKey:	BZHJMEDXRYGGRV-UHFFFAOYSA-N
Formula:	C2H3Cl
SMILES:	C=CCl
Mol. weight [g/mol]:	62.50
CAS:	75-01-4

Physical Properties

Property code	Value	Unit	Source
af	0.1220		KDB
aigt	745.37	K	KDB
dm	1.45	debye	KDB
fil	4.00	% in Air	KDB
flu	26.00	% in Air	KDB

fpc	194.26	K	KDB
gf	51.54	kJ/mol	KDB
hf	22.00 ± 3.00	kJ/mol	NIST Webbook
hf	35.17	kJ/mol	KDB
hf	38.10 ± 0.84	kJ/mol	NIST Webbook
hf	35.30 ± 1.40	kJ/mol	NIST Webbook
hf	21.00	kJ/mol	NIST Webbook
hf	29.00	kJ/mol	NIST Webbook
hfl	0.90 ± 3.20	kJ/mol	NIST Webbook
hfus	3.85	kJ/mol	Joback Method
hvap	21.00 ± 1.00	kJ/mol	NIST Webbook
ie	9.99	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	10.00 ± 0.01	eV	NIST Webbook
ie	10.00 ± 0.01	eV	NIST Webbook
ie	10.00 ± 0.02	eV	NIST Webbook
ie	9.99 ± 0.02	eV	NIST Webbook
ie	9.98 ± 0.02	eV	NIST Webbook
ie	9.99 ± 0.02	eV	NIST Webbook
ie	10.01	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.00 ± 0.01	eV	NIST Webbook
ie	10.00 ± 0.01	eV	NIST Webbook
log10ws	-1.75		Estimated Solubility Method
log10ws	-1.75		Aqueous Solubility Prediction Method
logp	1.369		Crippen Method
mcvol	46.980	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	5155.00	kPa	KDB
rinpol	378.00		NIST Webbook
rinpol	366.00		NIST Webbook
rinpol	353.00		NIST Webbook
rinpol	362.00		NIST Webbook
rinpol	363.00		NIST Webbook
rinpol	364.00		NIST Webbook
rinpol	366.00		NIST Webbook
rinpol	366.00		NIST Webbook
ripol	603.00		NIST Webbook
ripol	505.00		NIST Webbook

sl	118.00	J/mol×K	NIST Webbook
tb	259.35	K	KDB
tb	259.05 ± 0.40	K	NIST Webbook
tb	259.45 ± 0.20	K	NIST Webbook
tb	259.35	K	NIST Webbook
tb	259.30 ± 0.20	K	NIST Webbook
tc	424.61	K	KDB
tf	113.50 ± 0.20	K	NIST Webbook
tf	94.43 ± 0.10	K	NIST Webbook
tf	119.35	K	NIST Webbook
tf	119.45	K	Aqueous Solubility Prediction Method
tf	119.40	K	KDB
tf	119.36 ± 0.02	K	NIST Webbook
tt	119.31 ± 0.02	K	NIST Webbook
vc	0.177	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	61.82	J/mol×K	366.21	Joback Method
cpg	55.59	J/mol×K	308.25	Joback Method
cpg	52.25	J/mol×K	279.27	Joback Method
cpg	64.71	J/mol×K	395.19	Joback Method
cpg	67.47	J/mol×K	424.17	Joback Method
cpg	70.09	J/mol×K	453.15	Joback Method
cpg	58.78	J/mol×K	337.23	Joback Method
cpl	89.45	J/mol×K	298.15	NIST Webbook
dvisc	0.0009451	Paxs	163.59	Joback Method
dvisc	0.0005978	Paxs	186.73	Joback Method
dvisc	0.0004183	Paxs	209.87	Joback Method
dvisc	0.0003142	Paxs	233.00	Joback Method
dvisc	0.0002485	Paxs	256.13	Joback Method
dvisc	0.0017378	Paxs	140.46	Joback Method
dvisc	0.0002043	Paxs	279.27	Joback Method
hfust	4.92	kJ/mol	119.30	NIST Webbook
hfust	4.92	kJ/mol	119.30	NIST Webbook
hfust	4.92	kJ/mol	119.31	NIST Webbook
hvapt	23.30	kJ/mol	234.50	NIST Webbook
hvapt	22.26	kJ/mol	259.40	KDB
hvapt	22.70	kJ/mol	265.50	NIST Webbook

hvapt	22.90	kJ/mol	243.00	NIST Webbook
pvap	601.50	kPa	313.15	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
pvap	172.00	kPa	273.10	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
rho1	969.00	kg/m ³	259.00	KDB
sfust	41.20	J/mol×K	119.31	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38927e+01
Coeff. B	-2.09601e+03
Coeff. C	-3.33500e+01
Temperature range (K), min.	187.41
Temperature range (K), max.	277.61

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.48913e+01
Coeff. B	-5.42760e+03
Coeff. C	-1.26907e+01
Coeff. D	1.80238e-05
Temperature range (K), min.	119.36
Temperature range (K), max.	432.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Determination of Henry's Law Constants Using Internal Standards	https://www.doi.org/10.1021/je3010535
Low Pressure Solubilities of Vinyl Chloride in Ionic Liquids: The Yaws Handbook of Vapor Pressure:	https://www.doi.org/10.1021/je8005166
Joback Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	https://www.thermo.com/files/research/kdb/mol/mol1731.mol
Aqueous Solubility Prediction Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
	https://www.doi.org/10.1021/je050317k
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75014&Units=SI
	http://link.springer.com/article/10.1007/BF02311772
	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1731

Legend

af:	Acentric Factor
aiqt:	Autoignition Temperature
cp_g:	Ideal gas heat capacity
cp_l:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fl_l:	Lower Flammability Limit
fl_u:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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