Acetic acid, chloro-

Other names:	ALPHA-CHLOROACETIC ACID
	Acetic acid, 2-chloro-
	Acide chloracetique
	Acide monochloracetique
	Acidomonocloroacetico
	CH2ClCOOH
	Chloracetic acid
	Chloroacetic acid
	Chloroethanoic acid
	Kyselina chloroctova
	MCA
	Monochloorazijnzuur
	Monochloracetic acid
	Monochloressigsaeure
	Monochloroacetic acid
	Monochloroethanoic acid
	NCI-C60231
	NSC 142
	UN 1751
	«alpha»-Chloroacetic acid
	Â«alphaÂ»-Chloroacetic acid
Inchi:	InChI=1S/C2H3ClO2/c3-1-2(4)5/h1H2,(H,4,5)
InchiKey:	FOCAUTSVDIKZOP-UHFFFAOYSA-N
Formula:	C2H3ClO2
SMILES:	O=C(O)CCl
Mol. weight [g/mol]:	94.50
CAS:	79-11-8

Physical Properties

Property code	Value	Unit	Source
affp	765.40	kJ/mol	NIST Webbook
basg	734.50	kJ/mol	NIST Webbook
chs	-726.80	kJ/mol	NIST Webbook
chs	-729.00 ± 4.00	kJ/mol	NIST Webbook
gf	-311.71	kJ/mol	Joback Method
hf	-365.16	kJ/mol	Joback Method

hfus	10.82	kJ/mol	Joback Method
hsub	82.20 ± 0.90	kJ/mol	NIST Webbook
hvap	47.86	kJ/mol	Joback Method
ie	10.99	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
log10ws	0.94		Aqueous Solubility Prediction Method
logp	0.310		Crippen Method
mcvol	58.720	ml/mol	McGowan Method
pc	5990.66	kPa	Joback Method
tb	462.50 ± 0.50	K	NIST Webbook
tb	462.20	K	NIST Webbook
tb	461.00 ± 0.07	K	NIST Webbook
tb	462.50 ± 0.30	K	NIST Webbook
tb	462.50 ± 0.35	K	NIST Webbook
tb	462.50	K	KDB
tc	611.88	K	Joback Method
tf	335.53	K	Aqueous Solubility Prediction Method
tf	335.45	K	KDB
vc	0.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	98.95	J/mol×K	459.18	Joback Method
cpg	114.31	J/mol×K	611.88	Joback Method
cpg	111.53	J/mol×K	581.34	Joback Method
cpg	108.62	J/mol×K	550.80	Joback Method
cpg	105.55	J/mol×K	520.26	Joback Method
cpg	102.33	J/mol×K	489.72	Joback Method
cpg	95.41	J/mol×K	428.64	Joback Method
cpl	179.90	J/mol×K	321.05	NIST Webbook
cps	144.00	J/mol×K	303.00	NIST Webbook
dvisc	0.0017657	Pa×s	340.81	Joback Method
dvisc	0.0087857	Pa×s	282.25	Joback Method
dvisc	0.0003619	Pa×s	428.64	Joback Method
dvisc	0.0005681	Pa×s	399.36	Joback Method
dvisc	0.0009576	Pa×s	370.08	Joback Method
dvisc	0.0036526	Pa×s	311.53	Joback Method
dvisc	0.0258931	Pa×s	252.97	Joback Method
hfust	13.93	kJ/mol	329.16	NIST Webbook

hfust	16.30	kJ/mol	334.80	NIST Webbook
hfust	16.30	kJ/mol	334.33	NIST Webbook
hvapt	55.70	kJ/mol	428.00	NIST Webbook
hvapt	56.80	kJ/mol	420.00	NIST Webbook
hvapt	61.10	kJ/mol	399.50	NIST Webbook
pvap	15.00	kPa	406.30	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	14.00	kPa	404.60	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	13.00	kPa	402.70	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	17.50	kPa	410.20	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	20.00	kPa	413.70	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid

pvap	25.00	kPa	419.50	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	30.00	kPa	424.50	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	40.00	kPa	432.60	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	12.00	kPa	400.70	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	10.00	kPa	396.30	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	9.00	kPa	393.80	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	

pvap	8.00	kPa	391.00	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	7.50	kPa	389.50	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	6.00	kPa	384.70	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	5.00	kPa	380.70	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	11.00	kPa	398.70	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
sfust	42.33	J/mol×K	329.16	NIST Webbook	
sfust	48.74	J/mol×K	334.33	NIST Webbook	

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53521e+01
Coeff. B	-3.94767e+03
Coeff. C	-9.44190e+01
Temperature range (K), min.	351.55
Temperature range (K), max.	487.99

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.10585e+01
Coeff. B	-1.04050e+04
Coeff. C	-1.05382e+01
Coeff. D	3.33844e-06
Temperature range (K), min.	333.15
Temperature range (K), max.	686.00

Sources

Isobaric low-pressure vapor liquid equilibrium data of the system monochloroacetic acid + dichloroacetic acid + diethylene glycol dipentyl ether and the constituent binary systems:	https://www.doi.org/10.1016/j.fluid.2012.07.027
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1778
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1778
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79118&Units=SI
Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid:	https://www.doi.org/10.1016/j.fluid.2011.09.020
Isobaric Vapor-Liquid Equilibria for Binary Systems of Acetic Acid + Benzene, Chloroacetic Acid + Benzene, and Dichloroacetic Acid + Benzene at 101.33 kPa:	https://www.doi.org/10.1021/je100144t
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume