Acetic acid, dichloro-

Other names:	2,2-Dichloroacetic acid
	2,2-dichloroethanoic acid
	Acetic acid, 2,2-dichloro-
	Bichloracetic acid
	DCA
	DCA (acid)
	DICHLOROACETIC ACID
	DICHLOROETHANOIC ACID
	Dichloracetic acid
	Dichlorethanoic acid
	Kyselina dichloroctova
	NSC 2654
	UN 1764
	Urner's liquid
Inchi:	InChI=1S/C2H2Cl2O2/c3-1(4)2(5)6/h1H,(H,5,6)
InchiKey:	JXTHNDFMNIQAHM-UHFFFAOYSA-N
Formula:	C2H2Cl2O2
SMILES:	O=C(O)C(Cl)Cl
Mol. weight [g/mol]:	128.94
CAS:	79-43-6

Physical Properties

Property code	Value	Unit	Source
chl	-619.70	kJ/mol	NIST Webbook
chl	-624.00 ± 4.00	kJ/mol	NIST Webbook
gf	-326.08	kJ/mol	Joback Method
hf	-386.18	kJ/mol	Joback Method
hfus	11.49	kJ/mol	Joback Method
hvap	51.85	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.875		Crippen Method
mcvol	70.960	ml/mol	McGowan Method
pc	5730.52	kPa	Joback Method
tb	467.20	K	NIST Webbook
tc	659.61	K	Joback Method
tf	284.00 ± 1.50	K	NIST Webbook
tf	283.95 ± 0.10	K	NIST Webbook

tt	286.50 ± 0.20	K	NIST Webbook
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.11	J/mol×K	659.61	Joback Method
cpg	127.64	J/mol×K	627.28	Joback Method
cpg	124.99	J/mol×K	594.95	Joback Method
cpg	122.16	J/mol×K	562.62	Joback Method
cpg	119.15	J/mol×K	530.29	Joback Method
cpg	115.94	J/mol×K	497.96	Joback Method
cpg	112.54	J/mol×K	465.63	Joback Method
cpl	207.00	J/mol×K	307.00	NIST Webbook
cps	182.30	J/mol×K	280.31	NIST Webbook
dvisc	0.0004929	Pa×s	432.67	Joback Method
dvisc	0.0281388	Pa×s	267.89	Joback Method
dvisc	0.0008476	Pa×s	399.72	Joback Method
dvisc	0.0016068	Pa×s	366.76	Joback Method
dvisc	0.0034560	Pa×s	333.80	Joback Method
dvisc	0.0087913	Pa×s	300.85	Joback Method
dvisc	0.0003095	Pa×s	465.63	Joback Method
hfust	7.64	kJ/mol	283.95	NIST Webbook
hfust	12.34	kJ/mol	286.50	NIST Webbook
hfust	12.34	kJ/mol	286.50	NIST Webbook
hfust	12.34	kJ/mol	286.50	NIST Webbook
hvapt	55.70	kJ/mol	392.50	NIST Webbook
pvap	14.00	kPa	408.30	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	13.00	kPa	406.40	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid

pvap	12.00	kPa	404.30	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	15.00	kPa	410.10	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	17.50	kPa	414.10	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	20.00	kPa	417.50	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	25.00	kPa	423.50	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	
pvap	30.00	kPa	428.60	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid	

pvap	40.00	kPa	437.00	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	11.00	kPa	402.40	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	9.00	kPa	397.60	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	8.00	kPa	394.80	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	7.00	kPa	391.80	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	6.00	kPa	388.30	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid

pvap	5.00	kPa	384.30	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
pvap	10.00	kPa	400.20	Isobaric low pressure vapor-liquid equilibrium data for the binary system monochloroacetic acid + dichloroacetic acid
sfust	26.90	J/mol×K	283.95	NIST Webbook
sfust	43.10	J/mol×K	286.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55903e+01
Coeff. B	-4.30223e+03
Coeff. C	-7.50870e+01
Temperature range (K), min.	356.23
Temperature range (K), max.	493.64

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.23660e+02
Coeff. B	-1.17531e+04
Coeff. C	-1.55582e+01
Coeff. D	7.93214e-06
Temperature range (K), min.	286.55
Temperature range (K), max.	586.00

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79436&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1774
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1774

Legend

chl:	Standard liquid 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tt:	Triple Point Temperature
vc:	Critical Volume