Chlorine

Other names:	BERTHOLITE
	CHLORE
	Chloor
	Chlor
	Chlorine mol.
	Cl2
	Cloro
	Diatomic chlorine
	Molecular chlorine
	UN 1017
	chlorine, diatomic
Inchi:	InChI=1S/Cl2/c1-2
InchiKey:	KZBUYRJDOAKODT-UHFFFAOYSA-N
Formula:	Cl2
SMILES:	ClCl
Mol. weight [g/mol]:	70.91
CAS:	7782-50-5

Physical Properties

Property code	Value	Unit	Source
af	0.0900		KDB
dm	0.00	debye	KDB
ea	2.52 ± 0.17	eV	NIST Webbook
ea	1.02 ± 0.05	eV	NIST Webbook
ea	2.32 ± 0.10	eV	NIST Webbook
ea	3.20 ± 0.20	eV	NIST Webbook
ea	2.45 ± 0.15	eV	NIST Webbook
ea	2.46 ± 0.14	eV	NIST Webbook
ea	2.50 ± 0.20	eV	NIST Webbook
ea	2.33	eV	NIST Webbook
ea	2.40 ± 0.20	eV	NIST Webbook
ea	2.38 ± 0.10	eV	NIST Webbook
gf	-74.74	kJ/mol	Joback Method
hf	-74.81	kJ/mol	Joback Method
hfus	4.15	kJ/mol	Joback Method
hvap	24.36	kJ/mol	Joback Method
ie	11.49	eV	NIST Webbook

ie	11.59	eV	NIST Webbook
ie	11.49	eV	NIST Webbook
ie	11.48 ± 0.01	eV	NIST Webbook
ie	11.49	eV	NIST Webbook
ie	11.48 ± 0.00	eV	NIST Webbook
ie	11.48 ± 0.01	eV	NIST Webbook
ie	11.50	eV	NIST Webbook
ie	11.51 ± 0.01	eV	NIST Webbook
ie	11.48 ± 0.01	eV	NIST Webbook
log10ws	-1.12		Crippen Method
logp	1.379		Crippen Method
mcvol	35.340	ml/mol	McGowan Method
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=1)		KDB
pc	7991.00	kPa	KDB
pc	7991.40	kPa	NIST Webbook
pc	7977.00 ± 50.00	kPa	NIST Webbook
pt	1.39	kPa	KDB
pt	1.39 ± 0.00	kPa	NIST Webbook
rhoc	576.78	kg/m3	NIST Webbook
sgb	223.08 ± 0.01	J/mol×K	NIST Webbook
tb	239.11	K	KDB
tb	239.50 ± 0.60	K	NIST Webbook
tc	416.90 ± 0.50	K	NIST Webbook
tc	416.96	K	NIST Webbook
tc	416.90	K	KDB
tf	171.60	K	KDB
tt	172.12 ± 0.15	K	NIST Webbook
tt	172.17 ± 0.05	K	NIST Webbook
tt	172.17	K	KDB
vc	0.123	m3/kmol	KDB
zc	0.2835550		KDB
zra	0.28		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	33.70	J/mol×K	454.21	Joback Method
cpg	32.30	J/mol×K	274.26	Joback Method
cpg	32.58	J/mol×K	304.25	Joback Method
cpg	32.84	J/mol×K	334.24	Joback Method

cpg	33.08	J/mol×K	364.23	Joback Method
cpg	33.30	J/mol×K	394.22	Joback Method
cpg	33.51	J/mol×K	424.21	Joback Method
dvisc	0.0002781	Pa×s	274.26	Joback Method
dvisc	0.0020231	Pa×s	149.60	Joback Method
dvisc	0.0011880	Pa×s	170.38	Joback Method
dvisc	0.0007832	Pa×s	191.15	Joback Method
dvisc	0.0005603	Pa×s	211.93	Joback Method
dvisc	0.0004255	Pa×s	232.71	Joback Method
dvisc	0.0003381	Pa×s	253.48	Joback Method
rhol	1563.00	kg/m3	239.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42483e+01
Coeff. B	-2.08776e+03
Coeff. C	-2.23200e+01
Temperature range (K), min.	172.12
Temperature range (K), max.	417.15

Sources

Thermochemistry on crystalline compounds bis-(n-dodecylammonium) tetrachlorometallates (n-C12H25NH3)2MCl4(s) (M = Cu and Cd):	https://www.doi.org/10.1016/j.jct.2013.07.001
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1949
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase equilibria of the systems of CsCl + ErCl3 + H2O and CsCl + ErCl3 + HCl (~10.7% - 14.4%) + H2O at T = 298.15 K and the standard molar enthalpies of formation of solid phase compounds:	https://www.doi.org/10.1016/j.jct.2013.09.016
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7782505&Units=SI
Thermodynamic study on complex of neodymium with glycine:	https://www.doi.org/10.1016/j.jct.2014.11.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Low-Temperature Heat Capacities and Standard Molar Enthalpy of Formation of Ethylenediammonium Tetrachlorocobaltate(II) Chloride (H3NCH2CH2NH3)2[CoCl4]Cl2(s):	https://www.doi.org/10.1021/je901051z
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Isomerism and phase diagram of Pb5(PO4)3F-Pb5(PO4)3Cl system:	https://www.doi.org/10.1016/j.tca.2010.11.020
Thermochemical study of some dichloroacetophenone isomers:	https://www.doi.org/10.1016/j.jct.2010.09.005
Experimental and computational thermochemical studies of benzoxazole and two chlorobenzoxadole derivatives:	https://www.doi.org/10.1016/j.jct.2012.08.028

Standard molar enthalpies of formation of hydroxy-, chlor-, and bromapatite: https://www.doi.org/10.1016/j.jct.2005.01.010
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
sgb:	Molar entropy at standard conditions (1 bar)
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter