Acetaldehyde, chloro-

Other names:	2-CHLORO-1-ETHANAL
	2-Chloroacetaldehyde
	2-Chloroethanal
	Acetaldehyde, 2-chloro-
	CH2ClCHO
	CHLOROETHANAL
	Chloroacetalaldehyde
	Chloroacetaldehyde
	Chloroacetaldehyde monomer
	Monochloroacetaldehyde
	Rcra waste number P023
	UN 2232
Inchi:	InChI=1S/C2H3ClO/c3-1-2-4/h2H,1H2
InchiKey:	QSKPIOLLBIHNAC-UHFFFAOYSA-N
Formula:	C2H3ClO
SMILES:	O=CCCl
Mol. weight [g/mol]:	78.50
CAS:	107-20-0

Physical Properties

Property code	Value	Unit	Source
gf	-145.49	kJ/mol	Joback Method
hf	-185.93	kJ/mol	Joback Method
hfus	7.42	kJ/mol	Joback Method
hvap	31.15	kJ/mol	Joback Method
ie	10.61	eV	NIST Webbook
ie	10.48 ± 0.03	eV	NIST Webbook
ie	10.61	eV	NIST Webbook
log10ws	-0.09		Crippen Method
logp	0.424		Crippen Method
mcvol	52.850	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
tb	358.20	K	NIST Webbook
tc	514.03	K	Joback Method
tf	184.22	K	Joback Method
vc	0.213	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	73.27	J/mol×K	331.25	Joback Method
cpg	89.23	J/mol×K	483.57	Joback Method
cpg	86.31	J/mol×K	453.10	Joback Method
cpg	83.26	J/mol×K	422.64	Joback Method
cpg	80.07	J/mol×K	392.18	Joback Method
cpg	76.75	J/mol×K	361.71	Joback Method
cpg	92.02	J/mol×K	514.03	Joback Method
dvisc	0.0003490	Pa×s	331.25	Joback Method
dvisc	0.0004297	Pa×s	306.75	Joback Method
dvisc	0.0005485	Pa×s	282.24	Joback Method
dvisc	0.0007335	Pa×s	257.74	Joback Method
dvisc	0.0010427	Pa×s	233.23	Joback Method
dvisc	0.0016097	Pa×s	208.72	Joback Method
dvisc	0.0027895	Pa×s	184.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47100e+01
Coeff. B	-3.08284e+03
Coeff. C	-5.27180e+01
Temperature range (K), min.	266.47
Temperature range (K), max.	380.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.71993e+01
Coeff. B	-7.36328e+03
Coeff. C	-1.07117e+01
Coeff. D	7.60151e-06

Temperature range (K), min.	293.00
Temperature range (K), max.	555.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1776
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1776.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107200&Units=SI

Legend

cpg:	Ideal gas 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
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
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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