Chloral

Other names:	2,2,2-Trichloroacetaldehyde
	2,2,2-Trichloroethanal
	ANHYDROUS CHLORAL
	Acetaldehyde, 2,2,2-trichloro-
	Acetaldehyde, trichloro-
	CCl3CHO
	CHLOAL
	Cloralio
	Grasex
	Rcra waste number U034
	Trichloracetaldehyde
	Trichloroacetaldehyde
	Trichloroethanal
Inchi:	InChI=1S/C2HCl3O/c3-2(4,5)1-6/h1H
InchiKey:	HFFLGKNGCAIQMO-UHFFFAOYSA-N
Formula:	C2HCl3O
SMILES:	O=CC(Cl)(Cl)Cl
Mol. weight [g/mol]:	147.39
CAS:	75-87-6

Physical Properties

Property code	Value	Unit	Source
affp	722.30	kJ/mol	NIST Webbook
basg	690.50	kJ/mol	NIST Webbook
gf	-166.51	kJ/mol	Joback Method
hf	-226.16	kJ/mol	Joback Method
hfl	-218.10	kJ/mol	NIST Webbook
hfus	8.40	kJ/mol	Joback Method
hvap	41.00	kJ/mol	NIST Webbook
ie	10.88	eV	NIST Webbook
ie	10.90	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	1.556		Crippen Method
mcvol	77.330	ml/mol	McGowan Method
pc	4903.92	kPa	Joback Method
rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook

rinpol	715.00		NIST Webbook
rinpol	715.00		NIST Webbook
tb	370.90 ± 0.50	K	NIST Webbook
tb	371.00	K	NIST Webbook
tb	369.55 ± 0.30	K	NIST Webbook
tc	618.25	K	Joback Method
tf	246.48	K	Joback Method
vc	0.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.96	J/mol×K	582.36	Joback Method
cpg	110.05	J/mol×K	402.88	Joback Method
cpg	114.03	J/mol×K	438.78	Joback Method
cpg	117.58	J/mol×K	474.67	Joback Method
cpg	120.73	J/mol×K	510.57	Joback Method
cpg	123.51	J/mol×K	546.46	Joback Method
cpg	128.09	J/mol×K	618.25	Joback Method
cpl	151.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0005710	Pa×s	402.88	Joback Method
dvisc	0.0055677	Pa×s	246.48	Joback Method
dvisc	0.0031770	Pa×s	272.55	Joback Method
dvisc	0.0019994	Pa×s	298.61	Joback Method
dvisc	0.0013554	Pa×s	324.68	Joback Method
dvisc	0.0009735	Pa×s	350.75	Joback Method
dvisc	0.0007320	Pa×s	376.81	Joback Method
hvapt	36.60	kJ/mol	303.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53081e+01
Coeff. B	-3.79402e+03
Coeff. C	-1.60800e+01
Temperature range (K), min.	268.67

Temperature range (K), max.	395.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.45517e+01
Coeff. B	-7.35150e+03
Coeff. C	-1.03261e+01
Coeff. D	7.13919e-06
Temperature range (K), min.	216.00
Temperature range (K), max.	565.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1771
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/mol1771.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75876&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume