Benzene, 1-chloro-2-(trichloromethyl)-

Other names:	1-Chloro-2-(trichloromethyl)benzene
	2-Chlorobenzotrichloride
	Toluene, o,«alpha»,«alpha»,«alpha»-tetrachloro-
	Toluene, o,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-tetrachloro-
	o-Chlorobenzotrichloride
	o-Chlorobenzylidyne chloride
	o-Chlorophenyltrichloromethane
	«alpha»,«alpha»,«alpha»,2-Tetrachlorotoluene
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,2-Tetrachlorotoluene
Inchi:	InChI=1S/C7H4Cl4/c8-6-4-2-1-3-5(6)7(9,10)11/h1-4H
InchiKey:	MFHPYLFZSCSNST-UHFFFAOYSA-N
Formula:	C7H4Cl4
SMILES:	Clc1ccccc1C(Cl)(Cl)Cl
Mol. weight [g/mol]:	229.92
CAS:	2136-89-2

Physical Properties

Property code	Value	Unit	Source
gf	65.96	kJ/mol	Joback Method
hf	-34.46	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.167		Crippen Method
mcvol	134.690	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1413.70		NIST Webbook
tb	535.20	K	NIST Webbook
tb	537.50	K	NIST Webbook
tc	792.94	K	Joback Method
tf	302.50 ± 0.02	K	NIST Webbook
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.69	J/mol×K	792.94	Joback Method
cpg	269.61	J/mol×K	750.40	Joback Method
cpg	263.93	J/mol×K	707.86	Joback Method
cpg	257.55	J/mol×K	665.32	Joback Method
cpg	250.40	J/mol×K	622.79	Joback Method
cpg	242.39	J/mol×K	580.25	Joback Method
cpg	233.44	J/mol×K	537.71	Joback Method
dvisc	0.0024728	Pa×s	329.69	Joback Method
dvisc	0.0002731	Pa×s	537.71	Joback Method
dvisc	0.0003475	Pa×s	503.04	Joback Method
dvisc	0.0004580	Pa×s	468.37	Joback Method
dvisc	0.0006310	Pa×s	433.70	Joback Method
dvisc	0.0009192	Pa×s	399.03	Joback Method
dvisc	0.0014383	Pa×s	364.36	Joback Method
hvapt	55.00	kJ/mol	505.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40774e+01
Coeff. B	-4.20588e+03
Coeff. C	-9.05610e+01
Temperature range (K), min.	395.56
Temperature range (K), max.	570.36

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2136892&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume