Benzene, (trichloromethyl)-

Other names:	(Trichloromethyl)benzene
	.alpha.,.alpha.,.alpha.-trichlorotoluene
	1-(Trichloromethyl)benzene
	BENZOTRICHLORIDE
	Benzenyl chloride
	Benzenyl trichloride
	Benzoic trichloride
	Benzyl trichloride
	Benzylidyne chloride
	Chlorure de benzenyle
	NSC 14663
	PHENYLCHLOROFORM
	Phenyltrichloromethane
	Rcra waste number U023
	TRICHLOROTOLUENE
	Toluene trichloride
	Toluene, «alpha»,«alpha»,«alpha»-trichloro-
	Toluene, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trichloro-
	Trichloormethylbenzeen
	Trichlormethylbenzol
	Trichlorophenylmethane
	Tricloromethilbenzene
	UN 2226
	«alpha»,«alpha»,«alpha»-Trichloromethylbenzene
	«alpha»,«alpha»,«alpha»-Trichlorotoluene
	«omega»,«omega»,«omega»-Trichlorotoluene
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trichloromethylbenzene
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trichlorotoluene
	Â«omegaÂ»,Â«omegaÂ»,Â«omegaÂ»-Trichlorotoluene
Inchi:	InChI=1S/C7H5Cl3/c8-7(9,10)6-4-2-1-3-5-6/h1-5H
InchiKey:	XEMRAKSQROQPBR-UHFFFAOYSA-N
Formula:	C7H5Cl3
SMILES:	ClC(Cl)(Cl)c1ccccc1
Mol. weight [g/mol]:	195.47
CAS:	98-07-7

Physical Properties

Property code	Value	Unit	Source
gf	87.52	kJ/mol	Joback Method
hf	-7.25	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	45.31	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
log10ws	-3.47		Crippen Method
logp	3.513		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	1200.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1187.40		NIST Webbook
tb	493.80	K	NIST Webbook
tc	744.27	K	Joback Method
tf	256.20 ± 0.60	K	NIST Webbook
tf	235.99 ± 0.10	K	NIST Webbook
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.58	J/mol×K	744.27	Joback Method
cpg	212.89	J/mol×K	495.30	Joback Method
cpg	223.35	J/mol×K	536.79	Joback Method
cpg	232.76	J/mol×K	578.29	Joback Method
cpg	241.20	J/mol×K	619.78	Joback Method
cpg	248.77	J/mol×K	661.28	Joback Method
cpg	255.53	J/mol×K	702.77	Joback Method
cpl	210.44	J/mol×K	265.75	Heat capacities of selected chlorohydrocarbons
cpl	209.61	J/mol×K	260.64	Heat capacities of selected chlorohydrocarbons
cpl	209.36	J/mol×K	260.64	Heat capacities of selected chlorohydrocarbons
cpl	209.11	J/mol×K	260.64	Heat capacities of selected chlorohydrocarbons

cpl	210.94	J/mol×K	265.75	Heat capacities of selected chlorohydrocarbons
cpl	223.83	J/mol×K	319.35	Heat capacities of selected chlorohydrocarbons
cpl	210.27	J/mol×K	265.75	Heat capacities of selected chlorohydrocarbons
cpl	211.44	J/mol×K	270.85	Heat capacities of selected chlorohydrocarbons
cpl	211.35	J/mol×K	270.85	Heat capacities of selected chlorohydrocarbons
cpl	211.19	J/mol×K	270.85	Heat capacities of selected chlorohydrocarbons
cpl	212.77	J/mol×K	275.96	Heat capacities of selected chlorohydrocarbons
cpl	212.52	J/mol×K	275.96	Heat capacities of selected chlorohydrocarbons
cpl	212.52	J/mol×K	275.96	Heat capacities of selected chlorohydrocarbons
cpl	214.18	J/mol×K	281.06	Heat capacities of selected chlorohydrocarbons
cpl	213.93	J/mol×K	281.06	Heat capacities of selected chlorohydrocarbons
cpl	213.93	J/mol×K	281.06	Heat capacities of selected chlorohydrocarbons
cpl	215.59	J/mol×K	286.17	Heat capacities of selected chlorohydrocarbons
cpl	226.49	J/mol×K	329.56	Heat capacities of selected chlorohydrocarbons
cpl	215.34	J/mol×K	286.17	Heat capacities of selected chlorohydrocarbons
cpl	217.09	J/mol×K	291.27	Heat capacities of selected chlorohydrocarbons
cpl	217.01	J/mol×K	291.27	Heat capacities of selected chlorohydrocarbons
cpl	216.92	J/mol×K	291.27	Heat capacities of selected chlorohydrocarbons
cpl	217.76	J/mol×K	296.38	Heat capacities of selected chlorohydrocarbons

cpl	217.92	J/mol×K	296.38	Heat capacities of selected chlorohydrocarbons
cpl	218.01	J/mol×K	296.38	Heat capacities of selected chlorohydrocarbons
cpl	219.34	J/mol×K	301.48	Heat capacities of selected chlorohydrocarbons
cpl	219.17	J/mol×K	301.48	Heat capacities of selected chlorohydrocarbons
cpl	219.25	J/mol×K	301.48	Heat capacities of selected chlorohydrocarbons
cpl	220.75	J/mol×K	309.14	Heat capacities of selected chlorohydrocarbons
cpl	230.89	J/mol×K	349.98	Heat capacities of selected chlorohydrocarbons
cpl	215.59	J/mol×K	286.17	Heat capacities of selected chlorohydrocarbons
cpl	228.56	J/mol×K	339.77	Heat capacities of selected chlorohydrocarbons
dvisc	0.0003920	Pa×s	460.62	Joback Method
dvisc	0.0039216	Pa×s	287.25	Joback Method
dvisc	0.0020289	Pa×s	321.93	Joback Method
dvisc	0.0011932	Pa×s	356.60	Joback Method
dvisc	0.0007709	Pa×s	391.27	Joback Method
dvisc	0.0005348	Pa×s	425.95	Joback Method
dvisc	0.0003001	Pa×s	495.30	Joback Method
hfust	10.60	kJ/mol	270.00	NIST Webbook
hfust	13.95	kJ/mol	236.00	NIST Webbook
hvapt	52.00	kJ/mol	402.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.26828e+01
Coeff. B	-3.44439e+03
Coeff. C	-7.64390e+01
Temperature range (K), min.	354.32

Temperature range (K), max.	543.71

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.89647e+00
Coeff. B	-5.52600e+03
Coeff. C	1.59038e+00
Coeff. D	-3.43831e-06
Temperature range (K), min.	268.40
Temperature range (K), max.	737.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98077&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1691
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=1691
Heat capacities of selected chlorohydrocarbons:	https://www.doi.org/10.1016/j.fluid.2012.09.001
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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
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