Benzene, 1,2,3-trichloro-

Other names:	1,2,3-Trichlorobenzene
	1,2,6-Trichlorobenzene
	UN 2321
	VIC-TRICHLOROBENZENE
Inchi:	InChI=1S/C6H3Cl3/c7-4-2-1-3-5(8)6(4)9/h1-3H
InchiKey:	RELMFMZEBKVZJC-UHFFFAOYSA-N
Formula:	C6H3Cl3
SMILES:	Clc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	181.45
CAS:	87-61-6

Physical Properties

Property code	Value	Unit	Source
chs	-2793.80 ± 1.60	kJ/mol	NIST Webbook
chs	-2789.93	kJ/mol	NIST Webbook
gf	57.00	kJ/mol	Joback Method
hf	8.20 ± 1.80	kJ/mol	NIST Webbook
hf	3.78	kJ/mol	NIST Webbook
hfs	-70.78	kJ/mol	NIST Webbook
hfs	-66.90 ± 1.70	kJ/mol	NIST Webbook
hfus	17.15	kJ/mol	Joback Method
hsub	75.10 ± 0.75	kJ/mol	NIST Webbook
hsub	75.14 ± 0.75	kJ/mol	NIST Webbook
hvap	57.20	kJ/mol	NIST Webbook
ie	9.18 ± 0.03	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
log10ws	-4.22		Aqueous Solubility Prediction Method
log10ws	-3.76		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-4.00		Estimated Solubility Method
logp	3.647		Crippen Method
mcvol	108.360	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	1209.31		NIST Webbook
rinpol	1206.00		NIST Webbook

rinpol	1188.00	NIST Webbook
rinpol	207.00	NIST Webbook
rinpol	1194.94	NIST Webbook
rinpol	1191.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1194.00	NIST Webbook
rinpol	1204.00	NIST Webbook
rinpol	207.00	NIST Webbook
rinpol	1211.00	NIST Webbook
rinpol	1224.60	NIST Webbook
rinpol	1228.50	NIST Webbook
rinpol	1228.50	NIST Webbook
rinpol	1207.90	NIST Webbook
rinpol	1224.28	NIST Webbook
rinpol	1196.19	NIST Webbook
rinpol	1206.69	NIST Webbook
rinpol	1211.00	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1211.00	NIST Webbook
rinpol	1217.00	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1189.00	NIST Webbook
rinpol	1194.94	NIST Webbook
rinpol	1201.02	NIST Webbook
rinpol	1197.00	NIST Webbook
rinpol	1204.00	NIST Webbook
rinpol	1199.00	NIST Webbook
rinpol	1190.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1214.00	NIST Webbook
rinpol	1204.00	NIST Webbook
rinpol	1182.00	NIST Webbook
rinpol	1190.00	NIST Webbook
ripol	1775.00	NIST Webbook
ripol	1743.20	NIST Webbook
ripol	1705.00	NIST Webbook
ripol	1705.00	NIST Webbook
ripol	1735.00	NIST Webbook
ripol	1757.28	NIST Webbook
ripol	1726.64	NIST Webbook
ripol	1744.44	NIST Webbook
ripol	1742.31	NIST Webbook
ripol	1757.28	NIST Webbook

ripol	1768.60		NIST Webbook
tb	491.70	K	NIST Webbook
tc	725.08	K	Joback Method
tf	326.90 ± 0.10	K	NIST Webbook
tf	326.67	K	Aqueous Solubility Prediction Method
tf	323.75 ± 0.20	K	NIST Webbook
tf	325.80 ± 0.20	K	NIST Webbook
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.92	J/mol×K	485.61	Joback Method
cpg	204.95	J/mol×K	725.08	Joback Method
cpg	182.83	J/mol×K	565.43	Joback Method
cpg	189.04	J/mol×K	605.34	Joback Method
cpg	194.78	J/mol×K	645.26	Joback Method
cpg	200.07	J/mol×K	685.17	Joback Method
cpg	176.13	J/mol×K	525.52	Joback Method
cpl	204.00	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	204.38	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	204.75	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	203.62	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	205.52	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	205.91	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	206.30	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	203.25	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	202.88	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	202.52	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	202.16	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	201.80	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	205.14	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	201.44	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
dvisc	0.0003053	Pa×s	485.61	Joback Method
dvisc	0.0003679	Pa×s	454.44	Joback Method
dvisc	0.0004556	Pa×s	423.27	Joback Method
dvisc	0.0016757	Pa×s	298.60	Joback Method
dvisc	0.0011033	Pa×s	329.77	Joback Method
dvisc	0.0007808	Pa×s	360.94	Joback Method
dvisc	0.0005838	Pa×s	392.11	Joback Method
hfust	20.50	kJ/mol	326.90	NIST Webbook
hfust	17.25	kJ/mol	322.90	NIST Webbook
hfust	20.50	kJ/mol	326.90	NIST Webbook
hsubt	65.70	kJ/mol	296.00	NIST Webbook
hsubt	72.70	kJ/mol	285.50	NIST Webbook
hvapt	53.50	kJ/mol	338.00	NIST Webbook
hvapt	54.30	kJ/mol	285.50	NIST Webbook
hvapt	54.50	kJ/mol	325.00	NIST Webbook
hvapt	47.40	kJ/mol	402.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37328e+01
Coeff. B	-3.77196e+03
Coeff. C	-7.78560e+01
Temperature range (K), min.	325.65
Temperature range (K), max.	525.76

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.40186e+02
Coeff. B	-1.21803e+04
Coeff. C	-1.82796e+01
Coeff. D	1.01556e-05

Temperature range (K), min.	349.15
Temperature range (K), max.	493.15

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1671.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1671
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87616&Units=SI
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes:	https://www.doi.org/10.1021/je600573w
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume