Benzene, 1,2,3,4-tetrachloro-

Other names: 1,2,3,4-Tetrachlorobenzene
Inchi: InChI=1S/C6H2Cl4/c7-3-1-2-4(8)6(10)5(3)9/h1-2H
InchiKey: GBDZXPJXOMHESU-UHFFFAOYSA-N
Formula: C6H2Cl4
SMILES: Clc1ccc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 215.89
CAS: 634-66-2

Physical Properties

Property code	Value	Unit	Source
chs	-2642.22 ± 0.74	kJ/mol	NIST Webbook
gf	35.44	kJ/mol	Joback Method
hf	-25.40	kJ/mol	NIST Webbook
hfus	20.96	kJ/mol	Joback Method
hsub	78.80 ± 0.20	kJ/mol	NIST Webbook
hsub	60.84	kJ/mol	NIST Webbook
hvap	60.10	kJ/mol	NIST Webbook
ie	9.11	eV	NIST Webbook
ie	9.23 ± 0.03	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-4.57		Estimated Solubility Method
log10ws	-4.63		Aqueous Solubility Prediction Method
logp	4.300		Crippen Method
mcvol	120.600	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1342.00		NIST Webbook
rinpol	1362.21		NIST Webbook
rinpol	1369.92		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1352.40		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1366.00		NIST Webbook

rinpol	1375.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	237.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	219.20		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1359.50		NIST Webbook
rinpol	1343.88		NIST Webbook
rinpol	1377.18		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1385.30		NIST Webbook
rinpol	1385.40		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1402.30		NIST Webbook
rinpol	1388.00		NIST Webbook
ripol	1944.44		NIST Webbook
ripol	1914.10		NIST Webbook
ripol	1920.95		NIST Webbook
ripol	1914.10		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1968.20		NIST Webbook
ripol	1908.00		NIST Webbook
ripol	1941.00		NIST Webbook
ripol	1951.96		NIST Webbook
ripol	1931.77		NIST Webbook
tb	527.20	K	NIST Webbook
tc	774.01	K	Joback Method
tf	320.40	K	Aqueous Solubility Prediction Method
tf	320.00 ± 0.20	K	NIST Webbook
tt	319.68 ± 0.03	K	NIST Webbook
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.78	J/mol×K	569.02	Joback Method
cpg	217.36	J/mol×K	774.01	Joback Method

cpg	213.23	J/mol×K	733.01	Joback Method
cpg	208.73	J/mol×K	692.01	Joback Method
cpg	203.83	J/mol×K	651.01	Joback Method
cpg	198.52	J/mol×K	610.02	Joback Method
cpg	186.59	J/mol×K	528.02	Joback Method
cpl	227.13	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	227.46	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	227.80	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	228.13	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	228.47	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	228.81	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	225.17	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	225.49	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	225.82	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	226.14	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	226.47	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	226.80	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	229.50	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	229.16	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
dvisc	0.0009401	Pa×s	372.20	Joback Method
dvisc	0.0006972	Pa×s	403.37	Joback Method
dvisc	0.0005397	Pa×s	434.53	Joback Method
dvisc	0.0004323	Pa×s	465.69	Joback Method
dvisc	0.0003561	Pa×s	496.86	Joback Method
dvisc	0.0003001	Pa×s	528.02	Joback Method
dvisc	0.0013389	Pa×s	341.04	Joback Method
hfust	17.00	kJ/mol	319.70	NIST Webbook
hfust	17.00	kJ/mol	320.00	NIST Webbook
hfust	17.00	kJ/mol	320.00	NIST Webbook
hfust	16.96	kJ/mol	319.68	NIST Webbook
hvapt	56.70	kJ/mol	434.00	NIST Webbook
sfust	53.10	J/mol×K	319.68	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	527.20	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39017e+01
Coeff. B	-4.07979e+03
Coeff. C	-8.77250e+01
Temperature range (K), min.	387.40
Temperature range (K), max.	562.66

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C634662&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes: https://www.doi.org/10.1021/je600573w

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume