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A COMPILATION OF SOME PHYSICO-CHEMICAL PROPERTIES FOR CHLOROBENZENES

R-M. Dannenfelser, M. Paric, M. White, and S.H. Yalkowsky

College of Pharmacy, University of Arizona, Tucson, Arizona 85721

ABSTRACT

A compilation of some physico-chemical properties for chlorobenzenes are given. The literature values for the solution properties have been evaluated and whenever possible average values are given.

INTRODUCTION

Chlorobenzenes represent an important class of environmental pollutants. Although their physico-chemical properties have been studied extensively, there is no single source in which the data can be found.

This work provides a compilation of those physico-chemical properties of the chlorobenzenes that are determinant of their biological and toxicological properties. These properties can be divided into three classifications:

1) Molecular properties, i.e., properties of the isolated molecules, these include surface area, volume, and dipole moment;
2) Pure component properties, i.e., properties of the pure compounds; these include melting point, enthalpy and entropy of melting, vapor pressure, molar volume and solubility parameter; and
3) Aqueous solution properties, i.e., properties of the compounds in an aqueous solution which is in equilibrium with another phase, these include water solubility, octanol-water partition coefficient, organic-matter partition coefficient, and Henry's law constant.

The values for each property are taken from literature and are converted to common units for ease of comparison. Average values for the 20°C to 30°C temperature range are given for each property where there are two or more values present.

MOLECULAR PROPERTIES FOR THE CHLOROBENZENES

Some molecular properties can be measured experimentally, however many others are not measured but rather are calculated from known atomic and bond parameters. The values of molecular properties are generally independent of the environment of the molecules.

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Table I shows the molecular surface area and molecular volume. As can be seen in the table there are differences among the values for surface area and volume, this can be attributed to different measurement and/or calculation methods of these properties. For example, the surface area using the zero solvent radius is smaller (and closer to the true surface area) than the solvent radius (or solvent accessible) method. Volume, too, can be defined differently, for example the volume can include or exclude void volume. Including the void volume would give a larger volume than excluding the void volume. Thus it is not possible to calculate an average value for these properties. For similarly defined volume and surface area the values are in agreement. As expected volume and surface area increase as the number of chlorines increase.

As seen in Table II there is only a small amount of dipole moment data available for the chlorobenzenes. The dipole moments whether in the gas phase or in benzene are fairly close to one another. Where more than one dipole moment is cited the data are in agreement.

TABLE I:
MOLECULAR SURFACE AREA AND VOLUME OF CHLOROBENZENES

CHLOROBENZENE	SURFACE AREA (A^2)	VOLUME (A^3/molecule)	REF
Mono-		169.4	2
Mono-		169.4	15
Mono-		169.4	17
Mono-	280.3	399.2	18 *
Mono-		194.1	26
Mono-	127.9		35
Mono-		194.3	55
Mono-		168.9	82
Mono-	127.1		83
Mono-	127.5	177.6	AVERAGE
1,2-Di-		187.6	15
1,2-Di-		187.6	17
1,2-Di-		228.8	26
1,2-Di-	143.3		35
1,2-Di-		229.1	55
1,2-Di-		190.0	82
1,2-Di-	142.7		83
1,2-Di-	143.0	204.6	AVERAGE
1,3-Di-		189.3	15
1,3-Di-		189.3	17
1,3-Di-		228.8	26
1,3-Di-	145.4		35
1,3-Di-		229.1	55
1,3-Di-	144.7		83
1,3-Di-	145.1	209.1	AVERAGE
1,4-Di-		195.9	2
1,4-Di-		195.9	15
1,4-Di-		195.9	17
1,4-Di-	303.5	441.9	18 *
1,4-Di-		228.8	26
1,4-Di-	144.9		35
1,4-Di-		229.1	55
1,4-Di-	144.7		83
1,4-Di-	144.8	209.1	AVERAGE

TABLE I: continued
MOLECULAR SURFACE AREA AND VOLUME OF CHLOROBENZENES

CHLOROBENZENE	SURFACE AREA (A^2)	VOLUME (A^3/molecule)	REF
1,2,3-Tri-		207.5	17
1,2,3-Tri-		263.5	26
1,2,3-Tri-	158.7		35
1,2,3-Tri-		264.0	55
1,2,3-Tri-	158.3		83
1,2,3-Tri-	158.5	245.0	AVERAGE
1,2,4-Tri-		207.5	15
1,2,4-Tri-		207.5	17
1,2,4-Tri-	314.7	463.0	18 *
1,2,4-Tri-		263.5	26
1,2,4-Tri-	160.3		35
1,2,4-Tri-		264.0	55
1,2,4-Tri-	160.2		83
1,2,4-Tri-	160.2	235.6	AVERAGE
1,3,5-Tri-		207.5	17
1,3,5-Tri-		263.5	26
1,3,5-Tri-	162.9		35
1,3,5-Tri-		264.0	55
1,3,5-Tri-	162.2		83
1,3,5-Tri-	162.5	245.0	AVERAGE
1,2,3,4-Tetra-		235.8	17
1,2,3,4-Tetra-	173.5		27
1,2,3,4-Tetra-		298.9	55
1,2,3,4-Tetra-	173.8		83
1,2,3,4-Tetra-	173.6	267.4	AVERAGE
1,2,3,5-Tetra-		235.8	17
1,2,3,5-Tetra-	337.6	507.4	18 *
1,2,3,5-Tetra-		298.2	26
1,2,3,5-Tetra-	176.1		35
1,2,3,5-Tetra-		298.9	55
1,2,3,5-Tetra-	175.8		83
1,2,3,5-Tetra-	175.9	277.6	AVERAGE
1,2,4,5-Tetra-		235.8	17
1,2,4,5-Tetra-		298.2	26
1,2,4,5-Tetra-	175.7		35
1,2,4,5-Tetra-		298.9	55
1,2,4,5-Tetra-	175.8		83
1,2,4,5-Tetra-	175.7	277.6	AVERAGE
Penta-		275.6	17
Penta-	355.3	546.3	18 *
Penta-		332.9	26
Penta-	188.9		35
Penta-		333.7	55
Penta-	189.4		83
Penta-	189.1	314.1	AVERAGE
Hexa-		308.8	17
Hexa-	372.6	584.9	18 *
Hexa-		367.6	26
Hexa-	202.2		35
Hexa-		366.9	55
Hexa-	203.0		83
Hexa-	202.6	347.8	AVERAGE

* solvent accessible and not used for the average values

TABLE II:
DIPOLE MOMENTS FOR CHLOROBENZENES

CHLOROBENZENE	DIPOLE MOMENT IN THE GAS PHASE (debyes)	DIPOLE MOMENT IN BENZENE (debyes)	REF
Mono-	1.70E18	1.58E18	72
Mono-	1.69E18		80
Mono-	1.69E18		AVERAGE
1,2-Di-	2.53E18	2.27E18	72
1,2-Di-	2.50E18		80
1,2-Di-	2.51E18		AVERAGE
1,3-Di-	1.67E18	1.48E18	72
1,3-Di-	1.72E18		80
1,3-Di-	1.69E18		AVERAGE
1,4-Di-	0.00E18	0.00E18	72
1,4-Di-	0.00E18		80
1,4-Di-	0.00E18		AVERAGE
1,2,3-Tri-		2.31E18	72
1,2,4-Tri-		1.25E18	72
1,3,5-Tri-		0.00E18	72
1,2,3,4-Tetra-		1.90E18	72
1,2,3,5-Tetra-		0.65E18	72
1,2,4,5-Tetra-		0.00E18	72
Penta-		0.88E18	72
Hexa-		0.00E18	72

PURE COMPONENT PROPERTIES FOR THE CHLOROBENZENES

Pure component properties usually characterize changes in the physical state of a substance. All of these properties are obtained experimentally. Entropy is calculated by dividing the measured enthalpy by the measured melting or boiling point. There is very little data available for both enthalpy and entropy.

The melting properties are shown in Table III. Melting points for the chlorobenzenes are readily found in the literature. While few values are found for the enthalpy and entropy of melting. The reported melting points are in agreement and tend to increase as more chlorines are added. [It appears that the paper by Miller et al. has a typographical error in the reported melting points of chlorobenzene (22.74K) and 1,2-dichlorobenzene (156K). For this work the melting point for chlorobenzene was taken as 227.4K and for 1,2-dichlorobenzene 256K.]

Table IV shows the boiling properties for the chlorobenzenes. The observed boiling points are in good agreement with one another. Boiling point increases as the number of chlorines increase. No data were found for the entropy of boiling and only 1,2-dichlorobenzene has a value for enthalpy of boiling.

Vapor pressure for the chlorobenzenes are presented in Table V. The vapor pressure decreases as the number of chlorines increase. Data for chlorobenzene and 1,2-dichlorobenzene are readily available. The vapor pressure data are evaluated according to the evaluation scheme described below. Average vapor pressures (between 20°C and 30°C) are given for the chlorobenzenes.

Molar volumes and solubility parameters for the chlorobenzenes are presented in Table VI. These properties are generally calculated. Few solubility parameters are available for the chlorobenzenes, the only values that were found are for chlorobenzene and 1,2-dichlorobenzene. The molar volumes presented in this table are calculated by dividing the molecular weight by its density.

TABLE III:
MELTING POINT, ENTHALPY AND ENTROPY OF MELTING FOR CHLOROBENZENES

CHLOROBENZENE	MELTING POINT (°C)	ENTHALPY OF MELTING (J/m)	ENTROPY OF MELTING (J/deg·mol)	REF
Mono-	-45.2			19
Mono-	-45.7			26
Mono-	-45.6			35
Mono-	-45.6			47
Mono-	-45.8			55*
Mono-	-45.0			76
Mono-	-45.5			AVERAGE
1,2-Di-	-17.6			19
1,2-Di-	-52.9			26***
1,2-Di-	-17.0			35
1,2-Di-	-17.0			47
1,2-Di-		12,936		52
1,2-Di-	-17.0			55**
1,2-Di-	-17.0	12,935	50.50	66
1,2-Di-	-16.7			76
1,2-Di-	-17.1	12,935		AVERAGE
1,3-Di-	-24.8			26
1,3-Di-	-24.4			35
1,3-Di-	-24.7			47
1,3-Di-	-24.9			55
1,3-Di-	-24.0	12,642	50.75	66
1,3-Di-	-24.8			76
1,3-Di-	-24.6			AVERAGE
1,4-Di-	53.0			26
1,4-Di-	53.1			35
1,4-Di-	53.1			47
1,4-Di-	53.5	19,000	58.16	54
1,4-Di-	52.9			55
1,4-Di-	53.0	18,377	56.32	66
1,4-Di-	53.0			76
1,4-Di-		18,159		79
1,4-Di-	53.1	18,512	57.24	AVERAGE

TABLE III: continued
MELTING POINT, ENTHALPY AND ENTROPY OF MELTING FOR CHLOROBENZENES

CHLOROBENZENE	MELTING POINT (°C)	ENTHALPY OF MELTING (J/m)	ENTROPY OF MELTING (J/deg·mol)	REF
1,2,3-Tri-	52.7			26
1,2,3-Tri-	52.6			35
1,2,3-Tri-	53.0			47
1,2,3-Tri-	52.6	18,500	56.90	54
1,2,3-Tri-	52.6			55
1,2,3-Tri-	52.0			76
1,2,3-Tri-	52.6			AVERAGE
1,2,4-Tri-	16.9			26
1,2,4-Tri-	17.0			35
1,2,4-Tri-	17.0			47
1,2,4-Tri-	17.0			55
1,2,4-Tri-	18.0			70
1,2,4-Tri-	17.0			76
1,2,4-Tri-	17.2			AVERAGE
1,3,5-Tri-	63.9			26
1,3,5-Tri-	63.4			35
1,3,5-Tri-	63.0			47
1,3,5-Tri-	63.1	18,800	56.07	54
1,3,5-Tri-	64.0			55
1,3,5-Tri-	63.0			76
1,3,5-Tri-	63.4			AVERAGE
1,2,3,4-Tetra-	47.5			35
1,2,3,4-Tetra-	47.5			47
1,2,3,4-Tetra-	47.0	17,000	53.14	54
1,2,3,4-Tetra-	47.0			55
1,2,3,4-Tetra-	47.3			AVERAGE
1,2,3,5-Tetra-	50.8			26
1,2,3,5-Tetra-	54.5			35
1,2,3,5-Tetra-	54.5			47
1,2,3,5-Tetra-	50.7	19,000	58.58	54
1,2,3,5-Tetra-	50.7			55
1,2,3,5-Tetra-	52.2			AVERAGE
1,2,4,5-Tetra-	139.1			26
1,2,4,5-Tetra-	140.0			35
1,2,4,5-Tetra-	140.0			47
1,2,4,5-Tetra-	139.0	24,100	58.58	54
1,2,4,5-Tetra-	139.0			55
1,2,4,5-Tetra-	139.4			AVERAGE
Penta-	84.6			26
Penta-	86.0			35
Penta-	86.0			47
Penta-	84.5	20,600	57.94	54
Penta-	84.5			55
Penta-	85.0	16,100		64
Penta-	85.1	18,350		AVERAGE
Hexa-	228.4			26
Hexa-	230.0			35
Hexa-	230.0			47
Hexa-	227.9	22,400	44.77	54
Hexa-	228.3			55
Hexa-	228.0	18,700		64
Hexa-	228.0			70
Hexa-	227.0			76
Hexa-	228.5	20,550		AVERAGE

* MP reported as 22.74K, typographical error used 227.4K
** MP reported as 156K, typographical error used 256K
*** MP reported as 220.2K

TABLE IV:
BOILING POINT, ENTHALPY AND ENTROPY OF BOILING FOR CHLOROBENZENES

CHLOROBENZENE	BOILING POINT (°C)	ENTHALPY OF BOILING (J/m)	ENTROPY OF BOILING	REF
Mono-	130.00			19
Mono-	132.00			47
Mono-	132.00			54
Mono-	131.70			69
Mono-	132.00			76
Mono-	131.54			AVERAGE
1,2-Di-	177.00			19
1,2-Di-	180.50			47
1,2-Di-	179.60	39,978		52
1,2-Di-	180.50			54
1,2-Di-	180.50			69
1,2-Di-	179.00			76
1,2-Di-	179.52			AVERAGE
1,3-Di-	173.00			47
1,3-Di-	173.00			54
1,3-Di-	173.00			69
1,3-Di-	172.00			76
1,3-Di-	172.75			AVERAGE
1,4-Di-	174.00			47
1,4-Di-	174.00			54
1,4-Di-	173.40			76
1,4-Di-	173.80			AVERAGE
1,2,3-Tri-	218.00			47
1,2,3-Tri-	218.00			54
1,2,3-Tri-	219.00			76
1,2,3-Tri-	218.33			AVERAGE
1,2,4-Tri-	213.50			47
1,2,4-Tri-	214.00			70
1,2,4-Tri-	213.00			76
1,2,4-Tri-	213.50			AVERAGE
1,3,5-Tri-	208.00			47
1,3,5-Tri-	208.00			54
1,3,5-Tri-	208.50			76
1,3,5-Tri-	208.17			AVERAGE
1,2,3,4-Tetra-	254.00			47
1,2,3,4-Tetra-	254.00			54
1,2,3,4-Tetra-	254.00			AVERAGE
1,2,3,5-Tetra-	246.00			47
1,2,3,5-Tetra-	246.00			54
1,2,3,5-Tetra-	246.00			AVERAGE
1,2,4,5-Tetra-	243.00			47
1,2,4,5-Tetra-	243.00			54
1,2,4,5-Tetra-	243.00			AVERAGE
Penta-	277.00			47
Penta-	277.00			54
Penta-	277.00			AVERAGE
Hexa-	322.00			47
Hexa-	322.00			54
Hexa-	318.00			70
Hexa-	322.00			76
Hexa-	321.00			AVERAGE

TABLE V:
VAPOR PRESSURES FOR CHLOROBENZENES

CHLOROBENZENE	VAPOR PRESSURE (atm)	TEMP (°C)	EVAL	REF
Mono-	1.16E-2	20	2	76
Mono-	1.60E-2	25	3	46
Mono-	1.58E-2	25	2	47
Mono-	1.55E-2	25	2	76
Mono-	1.98E-2	30	1	19
Mono-	1.66E-2	30	8	34
Mono-	1.97E-2	30	3	76
Mono-	1.57E-2	35	2	47
Mono-	1.89E-2	40	8	34
Mono-	2.18E-2	50	8	34
Mono-	2.93E-2	60	8	34
Mono-	2.93E-2	70	8	34
Mono-	3.79E-2	80	8	34
Mono-	3.84E-2	90	8	34
Mono-	1.00E-2	131.7	2	56
Mono-	1.56E-2	ns	2	3
Mono-	1.54E-2	ns	2	20
Mono-	1.62E-2	20-30		AVERAGE
1,2-Di-	1.32E-3	20	1	76
1,2-Di-	1.93E-3	25	2	47
1,2-Di-	1.69E-3	25	2	56
1,2-Di-	1.97E-3	25	1	76
1,2-Di-	3.95E-3	30	1	19
1,2-Di-	2.50E-3	30	2	76
1,2-Di-	1.97E-3	52	0	47
1,2-Di-	1.00E-0	180.5	2	56
1,2-Di-	1.32E-3	ns	0	20
1,2-Di-	2.10E-3	20-30		AVERAGE
1,3-Di-	3.03E-3	25	2	47
1,3-Di-	1.00E-0	173	2	56
1,3-Di-	3.00E-3	ns	2	20
1,3-Di-	3.02E-3	20-30		AVERAGE
1,4-Di-	7.90E-4	20	1	76
1,4-Di-	9.00E-4	25	2	46
1,4-Di-	8.90E-4	25	2	47
1,4-Di-	1.32E-3	25	1	48
1,4-Di-	5.26E-4	25	2	56
1,4-Di-	2.37E-3	30	2	76
1,4-Di-	1.00E-0	174	2	56
1,4-Di-	1.55E-3	ns	2	20
1,4-Di-	1.19E-3	20-30		AVERAGE
1,2,3-Tri-	5.23E-4	25	2	47
1,2,3-Tri-	1.32E-3	40	2	56
1,2,3-Tri-	2.76E-4	ns	1	20
1,2,3-Tri-	4.00E-4	20-30		AVERAGE
1,2,4-Tri-	3.75E-4	20	2	70
1,2,4-Tri-	5.98E-4	25	2	47
1,2,4-Tri-	3.82E-4	ns	1	20
1,2,4-Tri-	4.52E-4	20-30		AVERAGE
1,3,5-Tri-	7.60E-4	25	2	47
1,3,5-Tri-	7.63E-4	ns	1	20
1,3,5-Tri-	7.62E-4	20-30		AVERAGE
1,2,3,4-Tetra-	8.65E-5	25	2	47
1,2,3,4-Tetra-	5.26E-5	ns	0	20
1,2,3,4-Tetra-	6.96E-5	20-30		AVERAGE

TABLE V: continued
VAPOR PRESSURES FOR CHLOROBENZENES

CHLOROBENZENE	VAPOR PRESSURE (atm)	TEMP (°C)	EVAL	REF
1,2,3,5-Tetra-	1.84E-4	25	2	47
1,2,3,5-Tetra-	9.21E-5	ns	0	20
1,2,3,5-Tetra-	1.38E-4	20-30		AVERAGE
1,2,4,5-Tetra-	9.97E-5	25	2	47
1,2,4,5-Tetra-	7.11E-6	ns	2	20
1,2,4,5-Tetra-	5.34E-5	20-30		AVERAGE
Penta-	8.77E-5	25	2	47
Penta-	7.89E-6	ns	0	20
Penta-	4.78E-5	20-30		AVERAGE
Hexa-	1.28E-8	20	3	70
Hexa-	3.39E-6	25	2	47
Hexa-	1.43E-8	ns	2	20
Hexa-	1.14E-6	20-30		AVERAGE

TABLE VI:
MOLAR VOLUME AND SOLUBILITY PARAMETERS FOR CHLOROBENZENES

CHLOROBENZENE	MW	DENSITY	TEMP (°C)	MOLAR VOLUME	SOLUBILITY PARAMETER	REF
Mono-					9.60	82
Mono-	112.56	1.1058	20	101.8		31, 80
1,2-Di-					9.80	82
1,2-Di-	147.01	1.3048	20	112.7		31, 80
1,3-Di-	147.01	1.2884	20	114.1		31, 80
1,4-Di-	147.01	1.2457	20	118.0		31, 80
1,2,3-Tri-	181.45	1.4533	40	124.9		31, 80
1,2,4-Tri-	181.45	1.4542	20	124.8		31, 80
1,3,5-Tri-	181.45	1.3865	64	130.9		31, 80
1,2,3,4-Tetra-	215.90					31, 80
1,2,3,5-Tetra-	215.90					31, 80
1,2,4,5-Tetra-	215.90	1.858	22	116.2		31, 80
Penta-	250.34	1.8342	16.5	136.5		31, 80
Hexa-	284.79	1.5691	23.6	181.5		31, 80

SOLUTION PROPERTIES FOR THE CHLOROBENZENES

Several important properties of the chlorobenzenes involve an aqueous solution in equilibrium with some other phase. The value characterizing the equilibrium between the aqueous solution and the pure chlorobenzene is the aqueous solubility. The equilibrium between the aqueous solution and an octanol solution is the octanol-water partition coefficient. The equilibrium involving organic carbon is the organic matter-water partition coefficient. The equilibrium between the aqueous solution and the vapor phase is the Henry's law constant.

These solution properties are generally derived experimentally and presented in logarithmic form. The logarithmic values for the above solution properties are given in Tables VII, VIII, IX, and X. Each of the reported values are objectively evaluated according to the scheme given in Table XI. The objective evaluation scheme has already been approved by the Environmental Protection Agency. Using the scheme each data point is given a total evaluation between 0 and 10 as described below.

Table VII shows the aqueous solubility of the chlorobenzenes. As the number of chlorines increase the less soluble the chlorobenzene becomes. The solubility data were taken from the AQUASOL dATAbASE of Aqueous Solubility (84). As can be seen in the table there is an abundance of solubility data for the chlorobenzenes. In general the values are in good agreement with each other. An average value for the log solubility between 20°C and 30°C is given for each of the chlorobenzenes.

The octanol-water partition coefficients in Table VIII are reported between the temperatures of 20°C and 25°C. Log K_{ow} values increase as the number of chlorines increase. All of the values correlate well with one another. Each of the chlorobenzenes are given an average log K_{ow} value.

As seen in Table IX, not as much data have been published for the organic matter-water partition coefficients as for the octanol-water partition coefficients. Log K_{oc} also tends to increase as the chlorines increase. Wherever two or more values between 20°C and 30°C are cited an average of the log organic matter-water partition coefficient (log K_{oc}) is given.

Literature values for the Henry's law constant are given in Table X. Average values are not given for the Henry's law constant because the data varies greatly from one reference to the next.

TABLE VII:
WATER SOLUBILITY FOR CHLOROBENZENES

CHLOROBENZENE	SOLUBILITY LOG(M/L)	TEMP (°C)	EVAL	REF
Mono-	-2.37	20.00	3	35
Mono-	-2.32	21.00	8	12
Mono-	-2.35	25.00	7	1
Mono-	-2.38	25.00	6	2
Mono-	-2.35	25.00	8	5
Mono-	-2.51	25.00	5	42
Mono-	-2.42	25.00	9	67
Mono-	-2.35	25.00	7	77
Mono-	-2.01	25.50	7	65
Mono-	-3.05	26.70	8	43
Mono-	-2.40	30.00	7	22
Mono-	-2.36	30.00	2	23
Mono-	-2.36	30.00	10	27
Mono-	-2.40	30.00	3	29
Mono-	-2.40	30.00	8	30
Mono-	-2.36	30.00	5	34
Mono-	-2.38	30.00	8	49
Mono-	-2.38	30.00	8	50
Mono-	-2.20	40.00	5	34
Mono-	-2.45	45.00	7	59
Mono-	-2.07	50.00	5	34
Mono-	-2.01	60.00	5	34
Mono-	-1.85	70.00	5	34
Mono-	-1.79	80.00	5	34
Mono-	-1.65	90.00	5	34
Mono-	-2.38	ns	2	20
Mono-	-2.58	ns	4	54
Mono-	-2.41	20-30		AVERAGE
1,2-Di-	-3.04	3.50	3	13
1,2-Di-	-2.99	20.00	3	13
1,2-Di-	-3.02	20.00	3	35
1,2-Di-	-3.04	20.00	6	36
1,2-Di-	-2.98	25.00	8	4
1,2-Di-	-3.03	25.00	8	5
1,2-Di-	-2.98	25.00	7	14
1,2-Di-	-3.01	25.00	6	36
1,2-Di-	-2.94	25.00	5	42
1,2-Di-	-2.93	30.00	6	36
1,2-Di-	-2.99	30.00	8	49
1,2-Di-	-3.01	30.00	8	50
1,2-Di-	-2.90	35.00	6	36
1,2-Di-	-2.88	40.00	6	36
1,2-Di-	-2.86	45.00	6	36
1,2-Di-	-2.82	55.00	6	36
1,2-Di-	-2.80	60.00	6	36
1,2-Di-	-2.98	ns	2	3
1,2-Di-	-3.17	ns	2	20
1,2-Di-	-3.20	ns	4	54
1,2-Di-	-2.98	ns	4	75
1,2-Di-	-3.02	20-30		AVERAGE
1,3-Di-	-3.10	20.00	3	35
1,3-Di-	-3.12	20.00	6	36
1,3-Di-	-3.04	25.00	8	4
1,3-Di-	-3.01	25.00	8	5
1,3-Di-	-3.04	25.00	7	14
1,3-Di-	-3.08	25.00	6	36
1,3-Di-	-3.02	30.00	6	36
1,3-Di-	-3.07	30.00	8	49
1,3-Di-	-3.07	30.00	8	50
1,3-Di-	-2.99	35.00	6	36
1,3-Di-	-2.94	40.00	6	36
1,3-Di-	-2.92	45.00	6	36
1,3-Di-	-2.88	55.00	6	36
1,3-Di-	-2.86	60.00	6	36
1,3-Di-	-3.04	ns	2	3
1,3-Di-	-3.08	ns	2	20
1,3-Di-	-3.07	ns	4	54
1,3-Di-	-3.05	ns	4	75
1,3-Di-	-3.06	20-30		AVERAGE

TABLE VII: continued
WATER SOLUBILITY FOR CHLOROBENZENES

CHLOROBENZENE	SOLUBILITY LOG(M/L)	TEMP (°C)	EVAL	REF
1,4-Di-	-3.52	20.00	3	35
1,4-Di-	-3.33	20.00	6	36 **
1,4-Di-	-3.28	22.20	10	79 **
1,4-Di-	-3.25	24.60	10	79 **
1,4-Di-	-3.29	25.00	5	1
1,4-Di-	-3.23	25.00	6	2
1,4-Di-	-3.30	25.00	8	4
1,4-Di-	-3.35	25.00	8	5
1,4-Di-	<-2.47	25.00	4	7
1,4-Di-	-3.27	25.00	6	22
1,4-Di-	-3.27	25.00	2	29
1,4-Di-	-3.27	25.00	6	36 **
1,4-Di-	-3.25	25.00	3	46
1,4-Di-	-3.25	25.00	3	47
1,4-Di-	-3.26	25.00	2	48
1,4-Di-	-4.16	25.00	5	60
1,4-Di-	-3.23	25.50	10	79 **
1,4-Di-	-3.28	30.00	7	27
1,4-Di-	-3.20	30.00	6	36 **
1,4-Di-	-3.20	30.00	8	49
1,4-Di-	-3.19	30.00	8	50
1,4-Di-	-3.20	30.00	10	79 **
1,4-Di-	-3.16	34.50	10	79 **
1,4-Di-	-3.23	35.00	6	36 **
1,4-Di-	-3.08	38.40	10	79
1,4-Di-	-3.16	40.00	6	36 **
1,4-Di-	-3.08	45.00	6	36 **
1,4-Di-	-2.97	47.50	10	79
1,4-Di-	-2.93	50.10	10	79 **
1,4-Di-	-2.97	55.00	6	36
1,4-Di-	-2.85	59.20	10	79
1,4-Di-	-2.96	60.00	6	36
1,4-Di-	-2.83	60.70	10	79 **
1,4-Di-	-2.81	65.10	10	79 **
1,4-Di-	-2.79	65.20	10	79 **
1,4-Di-	-2.72	73.40	10	79
1,4-Di-	-3.27	ns	2	20
1,4-Di-	-3.27	ns	1	32
1,4-Di-	-3.68	ns	4	54
1,4-Di-	-3.30	ns	4	75
1,4-Di-	-3.30	rt	4	68
1,4-Di-	-3.32	20-30		AVERAGE
1,2,3-Tri-	-4.11	20.00	3	35
1,2,3-Tri-	-4.00	25.00	8	5
1,2,3-Tri-	-4.00	25.00	8	16
1,2,3-Tri-	-4.04	25.00	3	47
1,2,3-Tri-	-3.76	25.00	8	83
1,2,3-Tri-	-4.18	ns	2	20
1,2,3-Tri-	-4.17	ns	4	54
1,2,3-Tri-	-4.04	20-30		AVERAGE
1,2,4-Tri-	-3.78	19.00	1	51
1,2,4-Tri-	-3.71	20.00	3	35
1,2,4-Tri-	-3.76	25.00	8	5
1,2,4-Tri-	-3.57	25.00	7	14
1,2,4-Tri-	-3.72	25.00	8	83
1,2,4-Tri-	-3.45	30.00	8	49
1,2,4-Tri-	-3.45	30.00	8	50
1,2,4-Tri-	-3.78	ns	2	20
1,2,4-Tri-	-3.78	ns	1	32
1,2,4-Tri-	-3.60	ns	4	54
1,2,4-Tri-	-3.65	20-30		AVERAGE
1,3,5-Tri-	-4.62	20.00	3	35
1,3,5-Tri-	-4.48	25.00	8	5
1,3,5-Tri-	-4.44	25.00	8	83
1,3,5-Tri-	-4.50	ns	2	20
1,3,5-Tri-	-4.64	ns	4	54
1,3,5-Tri-	-4.54	20-30		AVERAGE

TABLE VII: continued
WATER SOLUBILITY FOR CHLOROBENZENES

CHLOROBENZENE	SOLUBILITY LOG(M/L)	TEMP (°C)	EVAL	REF
1,2,3,4-Tetra-	-4.80	20.00	3	35
1,2,3,4-Tetra-	-4.56	25.00	8	5
1,2,3,4-Tetra-	-4.70	25.00	8	83
1,2,3,4-Tetra-	-4.79	ns	2	20
1,2,3,4-Tetra-	-4.82	ns	6	33
1,2,3,4-Tetra-	-4.25	ns	4	54
1,2,3,4-Tetra-	-4.65	20-30		AVERAGE
1,2,3,5-Tetra-	-5.00	20.00	3	35
1,2,3,5-Tetra-	-4.73	25.00	8	4
1,2,3,5-Tetra-	-4.63	25.00	8	5
1,2,3,5-Tetra-	-4.79	25.00	6	83
1,2,3,5-Tetra-	-4.95	ns	2	20
1,2,3,5-Tetra-	-4.89	ns	6	33
1,2,3,5-Tetra-	-4.87	ns	4	54
1,2,3,5-Tetra-	-4.72	ns	4	75
1,2,3,5-Tetra-	-4.82	20-30		AVERAGE
1,2,4,5-Tetra-	-5.84	20.00	3	35
1,2,4,5-Tetra-	-5.56	23.00	0	25
1,2,4,5-Tetra-	-5.67	25.00	8	5
1,2,4,5-Tetra-	-5.56	25.00	8	83
1,2,4,5-Tetra-	-5.74	ns	3	6
1,2,4,5-Tetra-	-4.56	ns	2	20
1,2,4,5-Tetra-	-4.56	ns	0	32
1,2,4,5-Tetra-	-5.59	ns	5	33
1,2,4,5-Tetra-	-4.96	ns	4	54
1,2,4,5-Tetra-	-5.34	20-30		AVERAGE
Penta-	-6.00	20.00	3	35
Penta-	-5.27	25.00	8	4
Penta-	-5.65	25.00	8	83
Penta-	-6.27	ns	2	20
Penta-	-6.27	ns	2	32
Penta-	-5.48	ns	4	54
Penta-	-5.27	ns	4	75
Penta-	-5.74	20-30		AVERAGE
Hexa-	-7.76	20.00	4	14
Hexa-	-7.72	20.00	7	28*
Hexa-	-7.59	20.00	7	28*
Hexa-	-7.69	20.00	3	35
Hexa-	-7.76	25.00	5	81
Hexa-	-7.68	26.70	8	43
Hexa-	<-5.46	30.00	6	50
Hexa-	-7.68	ns	2	20
Hexa-	-6.91	ns	1	32
Hexa-	-7.15	ns	1	39
Hexa-	-7.98	ns	2	53
Hexa-	-6.78	ns	4	54
Hexa-	-7.52	20-30		AVERAGE

* different methods
** average

TABLE VIII:
OCTANOL-WATER PARTITION COEFFICIENTS FOR CHLOROBENZENES

CHLOROBENZENE	LOG(K_{OW})	TEMP (°C)	EVAL	REF
Mono-	2.84	20	8	22
Mono-	2.90	25	7	10
Mono-	2.98	25	4	54
Mono-	2.98	25	6	77
Mono-	2.84	rt	5	40
Mono-	2.84	ns	2	20
Mono-	2.18	ns	5	43
Mono-	3.79	ns	3	73
Mono-	3.79	ns	2	74
Mono-	3.02	20-30		AVERAGE
1,2-Di-	3.43	25	7	10
1,2-Di-	3.40	20	10	75
1,2-Di-	3.55	22	7	37
1,2-Di-	3.40	23	10	4
1,2-Di-	3.38	25	4	54
1,2-Di-	3.38	25	6	77
1,2-Di-	3.40	25	10	78
1,2-Di-	3.38	rt	5	40
1,2-Di-	3.60	ns	2	20
1,2-Di-	3.44	20-30		AVERAGE
1,3-Di-	3.44	20	10	75
1,3-Di-	3.60	22	7	37
1,3-Di-	3.44	23	10	4
1,3-Di-	3.53	25	7	10
1,3-Di-	3.48	25	4	54
1,3-Di-	3.48	25	6	77
1,3-Di-	3.53	25	10	78
1,3-Di-	3.38	rt	5	40
1,3-Di-	3.60	ns	2	20
1,3-Di-	3.44	ns	2	74
1,3-Di-	3.49	20-30		AVERAGE
1,4-Di-	3.38	20	8	22
1,4-Di-	3.53	20	2	38 **
1,4-Di-	3.37	20	10	75
1,4-Di-	3.62	22	7	37
1,4-Di-	3.37	23	10	4
1,4-Di-	3.44	25	7	10
1,4-Di-	3.38	25	4	54
1,4-Di-	3.37	25	6	77
1,4-Di-	3.52	25	10	78
1,4-Di-	3.39	rt	5	40
1,4-Di-	3.60	ns	2	20
1,4-Di-	3.38	ns	2	58
1,4-Di-	3.38	ns	3	73
1,4-Di-	3.37	ns	2	74
1,4-Di-	3.44	20-30		AVERAGE
1,2,3-Tri-	4.20	20	2	38 **
1,2,3-Tri-	4.11	22	7	37
1,2,3-Tri-	4.14	25	7	10
1,2,3-Tri-	4.04	25	4	54
1,2,3-Tri-	4.05	25	10	78
1,2,3-Tri-	4.14	rt	3	17
1,2,3-Tri-	4.11	ns	2	20
1,2,3-Tri-	4.11	20-30		AVERAGE
1,2,4-Tri-	3.93	22	7	37
1,2,4-Tri-	4.05	25	7	10
1,2,4-Tri-	4.02	25	5	24
1,2,4-Tri-	3.98	25	4	54
1,2,4-Tri-	3.97	25	10	78
1,2,4-Tri-	4.02	rt	3	17
1,2,4-Tri-	4.02	ns	4	14
1,2,4-Tri-	4.30	ns	0	20
1,2,4-Tri-	4.03	ns	2	31 *
1,2,4-Tri-	4.18	ns	1	32
1,2,4-Tri-	2.33	ns	2	70
1,2,4-Tri-	4.23	ns	3	73
1,2,4-Tri-	4.52	ns	2	74
1,2,4-Tri-	3.97	20-30		AVERAGE

TABLE VIII: continued
OCTANOL-WATER PARTITION COEFFICIENTS FOR CHLOROBENZENES

CHLOROBENZENE	LOG(K_{OW})	TEMP (°C)	EVAL	REF
1,3,5-Tri-	4.20	20	2	38 **
1,3,5-Tri-	4.15	22	7	37
1,3,5-Tri-	4.19	25	7	10
1,3,5-Tri-	4.02	25	4	54
1,3,5-Tri-	4.19	25	10	78
1,3,5-Tri-	4.31	rt	3	17
1,3,5-Tri-	4.15	ns	2	20
1,3,5-Tri-	4.17	20-30		AVERAGE
1,2,3,4-Tetra-	4.68	20	10	8
1,2,3,4-Tetra-	4.46	22	7	37
1,2,3,4-Tetra-	4.64	25	7	10
1,2,3,4-Tetra-	4.55	25	4	54
1,2,3,4-Tetra-	4.37	25	10	78
1,2,3,4-Tetra-	4.60	rt	3	17
1,2,3,4-Tetra-	4.75	ns	7	9
1,2,3,4-Tetra-	4.46	ns	2	20
1,2,3,4-Tetra-	4.46	ns	2	74
1,2,3,4-Tetra-	4.55	20-30		AVERAGE
1,2,3,5-Tetra-	4.94	20	2	38 **
1,2,3,5-Tetra-	4.46	20	10	75
1,2,3,5-Tetra-	4.50	22	7	37
1,2,3,5-Tetra-	4.46	23	10	4
1,2,3,5-Tetra-	4.66	25	7	10
1,2,3,5-Tetra-	4.65	25	4	54
1,2,3,5-Tetra-	4.59	rt	3	17
1,2,3,5-Tetra-	4.46	ns	2	20
1,2,3,5-Tetra-	4.59	20-30		AVERAGE
1,2,4,5-Tetra-	4.52	22	7	37
1,2,4,5-Tetra-	4.60	25	7	10
1,2,4,5-Tetra-	4.51	25	4	54
1,2,4,5-Tetra-	4.56	25	10	78
1,2,4,5-Tetra-	4.70	rt	3	17
1,2,4,5-Tetra-	4.67	ns	2	20
1,2,4,5-Tetra-	4.67	ns	1	32
1,2,4,5-Tetra-	4.60	20-30		AVERAGE
Penta-	5.69	20	2	38 **
Penta-	4.94	20	10	75
Penta-	4.88	22	7	37
Penta-	4.94	23	10	4
Penta-	5.18	25	7	10
Penta-	4.88	25	5	24
Penta-	5.03	25	4	54
Penta-	5.17	25	10	78
Penta-	5.20	rt	3	17
Penta-	5.19	ns	2	20
Penta-	5.19	ns	2	32
Penta-	5.12	20-30		AVERAGE
Hexa-	5.44	20	10	8
Hexa-	6.44	20	2	38 **
Hexa-	5.00	22	7	37
Hexa-	5.73	25	7	10
Hexa-	5.38	25	5	24 *
Hexa-	5.47	25	4	54
Hexa-	5.31	25	10	78
Hexa-	5.50	rt	3	17
Hexa-	5.50	ns	4	14
Hexa-	5.23	ns	2	20
Hexa-	5.23	ns	2	32
Hexa-	4.13	ns	5	43
Hexa-	5.40	ns	1	70 *
Hexa-	5.23	ns	3	73
Hexa-	6.18	ns	2	74
Hexa-	5.41	20-30		AVERAGE

* average
** calculated

TABLE IX:
ORGANIC MATTER-WATER PARTION COEFFICIENTS FOR CHLOROBENZENES

CHLOROBENZENE	LOG(K_{OC})*	TEMP (°C)	EVAL	REF
Mono-	2.68	20	7	15
Mono-	2.52	ns	2	20
Mono-	2.60	20-30		AVERAGE
1,2-Di-	3.27	20	7	15
1,2-Di-	2.25	ns	2	13
1,2-Di-	3.23	ns	2	20
1,2-Di-	2.92	20-30		AVERAGE
1,3-Di-	3.23	20	7	15
1,3-Di-	3.23	ns	2	20
1,3-Di-	3.23	20-30		AVERAGE
1,4-Di-	3.20	20	7	15
1,4-Di-	3.23	ns	2	20
1,4-Di-	3.22	20-30		AVERAGE
1,2,3-Tri-	3.87	ns	2	20
1,2,4-Tri-	3.70	20	7	15
1,2,4-Tri-	3.96	ns	2	20
1,2,4-Tri-	3.83	20-30		AVERAGE
1,3,5-Tri-	3.79	ns	2	20
1,3,5-Tri-	2.67	ns	4	71 **
1,3,5-Tri-	3.23	20-30		AVERAGE
1,2,3,4-Tetra-	3.25	20	10	8
1,2,3,4-Tetra-	4.26	ns	2	20
1,2,3,4-Tetra-	3.76	20-30		AVERAGE
1,2,3,5-Tetra-	4.25	ns	2	20
1,2,4,5-Tetra-	3.20	ns	2	20
Penta-	4.11	ns	2	20
Hexa-	4.25	20	10	8
Hexa-	3.59	ns	2	20
Hexa-	3.92	20-30		AVERAGE

* ml/g
** average

TABLE X:
HENRY'S LAW CONSTANTS FOR CHLOROBENZENES

CHLOROBENZENE	HENRY'S LAW CONSTANT (Log(atm L/mole))	TEMP (°C)	EVAL	REF
Mono-	0.576	25	4	44 *
Mono-	0.568	25	2	46
Mono-	0.491	25	3	47
Mono-	0.515	ns	2	20
1,2-Di-	0.079	20	5	63
1,2-Di-	0.279	25	3	47
1,2-Di-	0.286	ns	2	20
1,3-Di-	0.255	20	5	63
1,3-Di-	0.555	ns	2	20
1,4-Di-	0.176	20	5	63
1,4-Di-	0.204	25	2	46
1,4-Di-	0.375	25	3	47
1,4-Di-	0.461	ns	2	20

TABLE X:
HENRY'S LAW CONSTANTS FOR CHLOROBENZENES

CHLOROBENZENE	HENRY'S LAW CONSTANT (Log(atm L/mole)	TEMP (°C)	EVAL	REF
1,2,3-Tri-	-0.051	20	5	63
1,2,3-Tri-	0.097	25	3	47
1,2,3-Tri-	0.626	ns	2	20
1,2,4-Tri-	0.079	20	5	63
1,2,4-Tri-	0.364	ns	2	20
1,3,5-Tri-	0.279	20	5	63
1,3,5-Tri-	1.378	ns	2	20
1,2,3,4-Tetra-	-0.161	20	5	63
1,2,3,5-Tetra-	0.196	25	3	47
1,2,4,5-Tetra-	0.000	20	5	63
Penta-	-0.149	20	5	63
Hexa-	-0.319	20	5	63
Hexa-	-0.167	ns	2	20

* calculated

TABLE XI:
EVALUATION SCHEME

Objective data evaluation will be based on the following point system:

PARAMETER	NUMBER OF POINTS		
	0	1	2
Temperature	Not given, ambient, or room temp.	Given with no range	Given with range
Purity of Solute	Not stated or as received	Stated with no range or as received with range	Stated with range or altered or calculated
Equilibration Time/agitation	Not stated	Stated briefly	Described in detail
Analysis	Not stated	Stated briefly or stated in other paper	Described in detail
Accuracy and/or Precision	1 significant figure or range > 20%	2 significant figure or range 5-20%	3 significant figure or range 1-5%

EVALUATION

Solution property values and vapor pressures are evaluated as objectively as possible according to the evaluation scheme in Table XI. This scheme has already been approved by the Environmental Protection Agency. The evaluation consists of five areas: temperature, purity of the solute, sample equilibration, analysis, and the accuracy or precision of the data point. Each area is given a rating of 0 (worst), 1, or 2 (best). For example, the temperature score is 0 if temperature is not given; 1 if it is given; and 2 if it is given with a range. The scores for the five criteria are added for the total evaluation which lies between 0 and 10. This evaluation tells how good the reporting of the value is and not how good the number is.

SUMMARY

The molecular, pure component and aqueous solution properties are summarized in Tables XII, XIII, and XIV. Parenthesis indicate when only one value is listed in the previous tables and the brackets indicate values where a large scatter in the data exists.

Table XII shows the molecular properties. As would be expected both the surface area and the volume increase as more chlorines are added to the benzene ring.

The pure component properties are listed in Table XIII. As the number of chlorines increase the boiling points generally increase. Vapor pressure, on the other hand, decreases as more chlorines are added to the benzene ring. This can be attributed to the fact that vapor pressure is low for high melting compounds. Melting point is symmetry dependent and therefore has some fluctuations, but the general trend is an increase in melting point as the number of chlorines increase. Both enthalpy and entropy of melting are also dependent on symmetry and tend to fluctuate with chlorine number.

Table XIV shows the average values for the solution properties for the chlorobenzenes. The aqueous solubility values decrease with the addition of chlorines while octanol-water partition coefficient values increase. Log_{oc} for the chlorobenzenes have a general upward trend as the number of chlorine atoms increase. Scatter is seen among the Henry's law constants (denoted by the values enclosed in brackets). This can be attributed to the difficulty of vapor phase measurements.

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TABLE XII:
SUMMARY OF THE MOLECULAR PROPERTIES FOR THE CHLOROBENZENES

CHLOROBENZENE	SURFACE AREA (A^2)	VOLUME (A^3/molecule)	DIPOLE MOMENT IN GAS PHASE ($x10^{-18}$ debyes)	DIPOLE MOMENT IN BENZENE ($x10^{-18}$ debyes)
Mono-	127.5	177.6	1.69	(1.58)
1,2-Di-	143.0	204.6	2.52	(2.27)
1,3-Di-	145.1	209.1	1.70	(1.48)
1,4-Di-	144.8	209.1	0.00	(0.00)
1,2,3-Tri-	158.5	245.0		(2.31)
1,2,4-Tri-	160.2	235.6		(1.25)
1,3,5-Tri-	162.5	245.0		(0.00)
1,2,3,4-Tetra-	173.6	267.4		(1.90)
1,2,3,5-Tetra-	176.0	277.6		(0.65)
1,2,4,5-Tetra-	175.7	277.6		(0.00)
Penta-	189.2	314.1		(0.88)
Hexa-	202.6	347.8		(0.00)

( ) only one value reported

TABLE XIII:
SUMMARY OF THE PURE COMPONENT PROPERTIES FOR THE CHLOROBENZENES

CHLOROBENZENE	BOILING POINT (°C)	MELTING POINT (°C)	ENTHALPY OF MELTING (kJ/m)	ENTROPY OF MELTING (J/deg·mol)	VAPOR PRESSURE (atm)
Mono-	131.5	-45.5	.	.	1.62E-2
1,2-Di-	179.5	-17.1	12.9	(50.5)	2.10E-3
1,3-Di-	172.8	-24.6	(12.6)	(50.8)	3.02E-3
1,4-Di-	173.8	53.1	18.5	57.2	1.19E-3
1,2,3-Tri-	218.3	52.6	(18.5)	(56.9)	4.00E-4
1,2,4-Tri-	213.5	17.2	.	.	4.52E-4
1,3,5-Tri-	208.2	63.4	(18.8)	(56.1)	7.62E-4
1,2,3,4-Tetra-	254.0	47.3	(17.0)	(53.1)	6.96E-5
1,2,3,5-Tetra-	246.0	52.2	(19.0)	(58.6)	1.38E-4
1,2,4,5-Tetra-	243.0	139.4	(24.1)	(58.6)	5.34E-5
Penta-	277.0	85.1	18.4	(57.9)	4.78E-5
Hexa-	321.0	228.5	20.6	(44.8)	1.14E-6

( ) only one value reported

TABLE XIV:
SUMMARY OF THE AQUEOUS SOLUTION PROPERTIES FOR THE CHLOROBENZENES

CHLOROBENZENE	LOG(SOL) (m/l)	LOG(K_{OW})	LOG(K_{OC}) (ml/g)	LOG(HENRY) (atm·l/mole)
Mono-	-2.41	3.02	2.60	[0.54]
1,2-Di-	-3.02	3.44	2.92	[0.21]
1,3-Di-	-3.06	3.49	3.23	[0.41]
1,4-Di-	-3.32	3.44	3.22	[0.30]
1,2,3-Tri-	-4.04	4.11	(3.87)	[0.22]
1,2,4-Tri-	-3.65	3.97	3.83	[0.22]
1,3,5-Tri-	-4.54	4.17	3.23	[0.83]
1,2,3,4-Tetra-	-4.65	4.55	3.76	(-0.16)
1,2,3,5-Tetra-	-4.82	4.59	(4.25)	(0.20)
1,2,4,5-Tetra-	-5.34	4.60	(3.20)	(0.00)
Penta-	-5.74	5.12	(4.11)	(-0.15)
Hexa-	-7.52	5.41	3.92	[-0.24]

( ) only one value reported
[ ] average of wide scattered data

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