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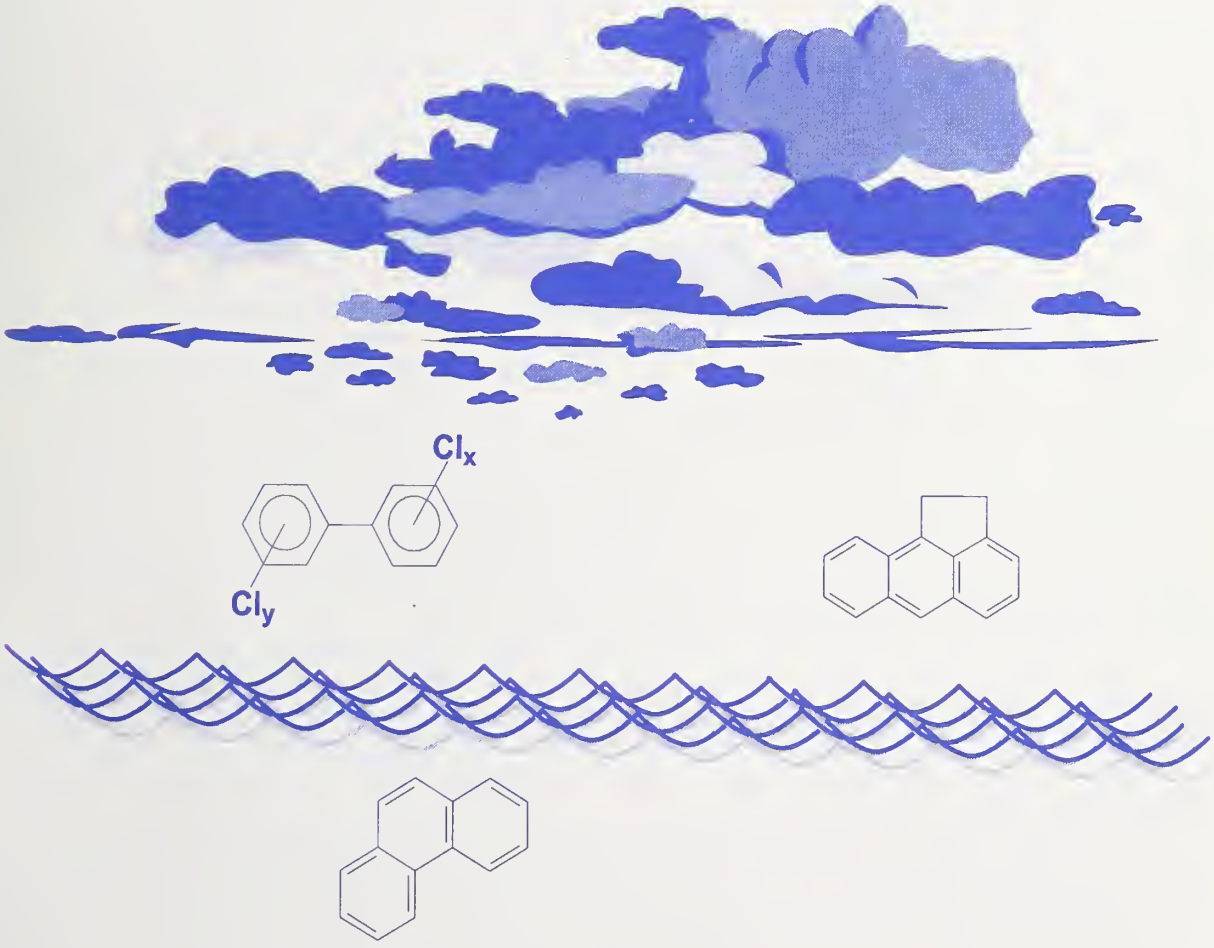
Review of Methods and Measurements of Selected Hydrophobic Organic Contaminant Aqueous Solubilities, Vapor Pressures, and Air-Water Partition Coefficients

Holly A. Bamford, Joel E. Baker, and Dianne L. Poster



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ABSTRACT

Aqueous solubilities, vapor pressures, and Henry's law constants for a wide range of organic contaminants of environmental interest are presented. Specifically, a discussion of methods used to measure these physical constants and resulting measurements are provided in an effort to examine the scope of physical constants reported in the scientific literature. Physical constants reviewed include those for 40 PAHs, 14 chlorinated aliphatics, 149 PCBs, 12 chlorinated benzenes, 16 dioxins, 63 furans, and 29 agrochemicals ($\sum$ = 323 compounds) and overall a total of 1605 values are listed. These data were compiled to initiate the incorporation of physical constant literature values of these compounds into the National Institute of Standards and Technology's (NIST) Chemical and Science Technology Laboratory (CSTL) database program.

Key Words: air-water partitioning, aqueous solubility, Henry's law constants, organic contaminants, vapor pressure

1. INTRODUCTION

A wide range of industrially synthesized organic contaminants are measurable in the environment by current sampling and analytical chemistry methods and are of environmental concern. Many of these compounds persist and migrate within and between local, regional, and even global environmental compartments for long periods of time. In addition, many have a tendency to bioaccumulate in aquatic or terrestrial food chains, exhibit toxicity at minute levels, and are probable human carcinogens. Polychlorinated biphenyl congeners (PCBs) and polychlorinated dibenzofurans and polychlorinated dibenzo-*p*-dioxins ("dioxins") are familiar examples, which are widely known to be linked with fish consumption advisories in areas such as the Great Lakes. Not-so-familiar examples are polycyclic aromatic compounds which include as a subgroup polycyclic aromatic hydrocarbons (PAHs). Many PAHs are highly persistent in the environment and are potent cancer-causing and mutagenic agents; benzo[*a*]pyrene is an example. Other examples include agricultural chemicals (pesticides, herbicides, and fungicides) that exhibit various degrees of persistence in the environment.

PCBs are a class of chlorinated compounds that were widely used in industrial applications such as electrical insulation. PCBs were produced in the United States from 1929 until about 1978 when concern over adverse environmental effects led to a ban on their manufacture under the Toxic Substances Control Act of 1976 (TSCA) (Woodyard and King, 1992). However, during this period world production of PCBs was approximately 1.5 million metric tons with about 650,000 metric tons generated in the United States (De Voogt and Brinkman, 1989). It has been estimated that 20 percent to 30 percent of this amount entered the environment as contamination (Webster and Commoner, 1994). Approximately 200,000 metric tons of PCBs are still in use in the United States in capacitors, transformers, and other electrical equipment (Amend and Lederman, 1992).

Anthropogenic dioxins, dibenzofurans, and PAHs exist in the environment due to current-uses of materials related to the production of these compounds. Dioxins are by-products of combustion of chlorine laden organic material and of chlorine bleaching in paper industries and dibenzofurans are produced by numerous combustion processes (Hites, 1990; Brzuzy and Hites, 1996). Similarly, PAHs are by-products of the burning of organic materials such as fossil fuels, refuse, and wood. Natural sources of combustion, such as forest fires and volcanos, and biosynthesis (sediment diagenesis, tar pits) also produce PAHs but these are minor relative to anthropogenic sources (Meyers and Hites, 1982; Bjørseth and Ramdahl, 1985).

The global use and widespread detection of agricultural chemicals in the environment have increased significantly over the last several decades (Montgomery 1993 and references within). Many heavily used compounds exhibit environmental residence times long enough to adversely impact soils, groundwater, aquatic ecosystems, and to some extent air quality. Obvious sources of these compounds include agricultural farming operations and commercial and residential landscaping practices. Not-so-obvious sources include non-point source areas and fugitive emissions.

1.1 Objective of this review. The environmental transport (migration) and fate (persistence) of organic contaminants and their tendency to bioaccumulate and exhibit toxicity are significantly

influenced by their chemical and physical properties. In order to fully understand local, regional, and global environmental pollution and their relation to human and environmental ecosystem health effects associated with exposure to organic contaminants, reliable organic contaminant chemical and physical property data are essential (Mackay et al., 1992). Unfortunately, gathering accurate organic contaminant physical property data is often difficult. Physical constant values reported in scientific papers as results from experimental measurements often vary by several orders of magnitude. Moreover, many different types of methods are used to obtain measurements and it is unclear if the lack of precision for reported values is related somehow to the wide range of methods used. This report provides a discussion of methods used to measure physical constants of organic environmental contaminants and measurements of physical constants from these methods are provided in an effort to examine the scope of physical constants reported in the scientific literature.

Physical constants reviewed include aqueous solubility, vapor pressure, and Henry's law constants (air-water partition coefficients) for 40 PAHs, 14 chlorinated aliphatics, 149 PCBs, 12 chlorinated benzenes, 16 dioxins, 63 furans, and 29 agrochemicals ($\sum = 323$ compounds). A total of 1605 values are given in this report. These data were compiled to initiate the incorporation of physical constant literature values of these compounds into the National Institute of Standards and Technology's (NIST) Chemical and Science Technology Laboratory (CSTL) database program. Specifically, methods and values are presented. As this report is focused on a review and discussion of the methods and currently available measured physical/chemical property data for organic contaminants of environmental concern, specification of discrete values to include in NIST's CSTL database program is deferred until evaluation of the current data is complete. In particular, results from studies currently in progress which are designed to develop estimation methods based upon molecular properties of the compounds in order to critically evaluate the current review of physical property data of organic contaminants will be used for this task. Our intent is to evaluate much of the current data using measurement data as a baseline to recommend values for the NIST database program. As demonstrated by the range of the values reported here, critical evaluation of these data is necessary to facilitate accurate use. Values span several orders of magnitude and users are left with their own intuition as to which literature value to use for their application. Several orders of magnitude can alter environmental fate assessments of chemicals, sometimes drastically. Hence, our aim is to critically evaluate much of the data reported here using our measurement data so best possible values may be recommended for inclusion in the database program described above. Other approaches for evaluating the physicochemical property values reported here may also be considered. For example, Heller et al. (1994) recently developed an expert system for evaluating the efficacy of reported methodology for determining aqueous solubility. In this work, the basic philosophy is that sound methods provide "good" data and Heller et al. developed a system for the evaluation of measured physicochemical property values using this concept. A method such as this may be considered for evaluating the current data set.

A recently published review by Mackay et al. (1992) provides a large collection of physical-chemical properties and a review of the environmental fate for organic chemicals. In addition, Mackay et al. (1992) provide a detailed discussion on the current state of quantitative structure-property relationships (QSPR). Estimates of physical properties calculated using correlative or quantitative structure-property relationships are not included in this report. This is a fast-growing area of

research directed to the development of relationships which describe physical-chemical properties of environmental concern based on a compound's chemical structure. The paucity of directly measured values has fueled the growth of this research field. Yalkowsky (1993) offer a comparative evaluation of methods available for the estimation of the aqueous solubility of complex organic compounds including PAHs, aliphatic alcohols, monosubsitituted benzenes, monofunctional aliphatics, and agrochemicals, such as malathion, chlorpyrifos, and chlordane. Sutter and Jurs (1996) offer a more recent look at aqueous solubility predictions for 140 organic compounds.

Reported values in the present work are largely from searches of articles listed by Mackay et al. (1992) and Staudinger and Roberts (1996), as well as data reported by Montgomery (1993). Methods used to measure physical constants of agrochemicals were not specifically reported by Montgomery (1993) and as a result are not listed here. The years of literature reviewed by Mackay et al. (1992) range from 1931 to the time of publication. A review of more recently published physical property measurement work relative to Mackay et al. (1992), Staudinger and Roberts (1996), and Montgomery (1993) was conducted for the current work. In particular, articles listed in *Water Resources Abstracts* (ca. 1980 - present), *Current Contents* (1980 - 1995) and *Science Citation Index* (1994 - 1997) were reviewed. A total of 135 articles were reviewed. Reported physical constants and the methods used to derive these are presented. Many of the 135 articles did not contain original physical property data. Rather, data was taken from the original papers that described the measurement work. Section 5.1. lists references that contain physical property data resulting from measurement work and these were used as sources for the data listed in Tables 2-8, with the exception of the agrochemical data given by Montgomery (1993) which are listed here without specific methods of measurement. Papers that listed, used, or propagated measurement data are listed in Section 5.2, although data reported in these papers were not extracted and included in Tables 2-8.

2. PHYSICAL AND CHEMICAL PROPERTIES

2.1 Aqueous solubility. During this work, it was found that aqueous solubility (mg/L) measurements, the concentration of a substance's saturated solution at a given temperature and pressure, were generally listed as either the result of an equilibration method of measurement or as the result of an analytical method of determination. Hence, in the aqueous solubility physical constant table solubility methods are identified by two numbers, the first being the method of equilibration followed by the method of instrumental determination. Calculated data, however, (*e.g.,* calculated from a fit of the parameter to a function of a variable such as temperature) is also provided and in this case there is only one number listed for the method identification (Method ID). Estimation of the aqueous solubilities of organic compounds are given by Yalkowsky and Valvani (1979) and more recently, Yalkowsky (1993).

Two common methods of equilibration include the shake flask method, in which an excess amount of solute chemical is added to water and then shaken gently or stirred on a stirring plate until equilibrium is achieved (Booth and Everson, 1948, Mackay et al., 1992), and the generator column method, in which an inert solid support (*e.g.,* glass beads) is coated with the analyte, packed in an open tubular column, and water is run through at a precise flow rate to achieve equilibrium. It has

been generally accepted that the generation column method is the most accurate technique of solubility determination for sparingly soluble solid hydrophobic compounds as described by May et al. (1978 a,b). Danielsson and Zhang (1996) provide a short overview of these methods in terms of working principles, although their discussion is on the determination of *n*-octanol-water partition constants rather than aqueous solubility.

Methods of instrumental determination of the saturated solution and several historical references to these include (Mackay et al., 1992): ultraviolet spectrometry (Andrews and Keffer, 1950a,b; Bohon and Claussen 1951), gas chromatography (McAuliffe 1966), fluorescence spectrophotometry (Mackay and Shiu, 1977), interferometry (Gross and Saylor, 1931), liquid chromatography (May et al., 1978a,b), and nephelometric methods (Davis and Parke, 1942; Davis et al., 1942; Hollifield 1979). Wauchope and Getzen (1972) document the temperature dependence of solubility for several PAHs. Table 1.a. provides a listing of the identification numbers for the aqueous solubility methods of determination that are given in Tables 2-8.

2.2 Vapor pressure. Like aqueous solubility, the vapor pressure (Pa) of a compound, the pressure exerted by a vapor in dynamic equilibrium with its liquid at a given temperature, is a "saturation" property. Unlike aqueous solubility, vapor pressure measurements can be made directly through the use of a pressure gauge (*e.g.,* a diaphragm gauge), or by indirect methods based on evaporation rate measurements or chromatographic retention times. Common methods for measurement and historical references of vapor pressure are (Mackay et al., 1992): calculated (from boiling points - Mackay et al., 1982), pressure gauge (Sears and Hopke, 1947; Ambrose et al., 1975; Osborn and Douslin, 1975), comparative ebulliometry (Ambrose 1981), effusion (Balson, 1947), gas saturation or transpiration (Spencer and Cliath, 1970), liquid chromatography (Sonnefeld et al., 1983), and capillary gas chromatography (Hamliton 1980; Bidleman 1984). Estimation methods for PCBs are presented by Burkhard et al. (1985). Table 1.b provides a listing of identification numbers for vapor pressure methods of determination. The last column in the vapor pressure physical constant tables, titled "phase", indicates what phase or state the solute was in during the experimental determination of its vapor pressure. For example, many measurements of vapor pressure are for supercooled liquid compounds.

2.3 Henry's law constant. The Henry's law constant is the air-water equilibrium partition coefficient for compounds in dilute aqueous solutions. It is defined as the ratio of the concentration in the gas phase to the concentration in the dissolved phase. As an equilibrium constant, the Henry's law constant is a key parameter with respect to a compound's fate and transport in the environment by providing estimates of air-water partitioning. Air-water partitioning in the enviornment can be on a small scale (*e.g.,* partitioning of atmospheric gases to raindrops) or on a large scale (*e.g.,* partitioning of atmospheric gases to surface waters).

Henry's law constants can be presented in various ways based on different sets of associated units. Henry's law constants are typically reported as $H = Pi / Cw$ where Pi is the partial pressure of the compound (Pa), Cw is the compound dissolved concentration in water (mol / m^3), and H is in units of Pa m^3 / mol. It is also found in a "dimensionless" form which is expressed as $H' = (Pi / Cw) / (RT)$ where R is the ideal gas constant (8.314 Pa m^3 / mole K) and T is temperature (K). Hence, to convert

a reported "dimensionless" H' value to units of Pa m^3 / mol one can multiply H' by *RT*. We report Henry's law constants in units of Pa m^3/mol.

Like vapor pressure, the Henry's law constant requires only one method of measurement to obtain data for each compound; however, it is more difficult to determine because it is derived from concentration measurements made in two different phases, air and water. Therefore, many methods have been developed that take measurements from one phase and by mass balance the concentration of the solute in the other phase is determined. Currently, methods of determination for the Henry's law constant are calculated, gas stripping, equilibrium partitioning in closed system (EPICS), wetted-wall column, and the variable headspace method (Table 1.c).

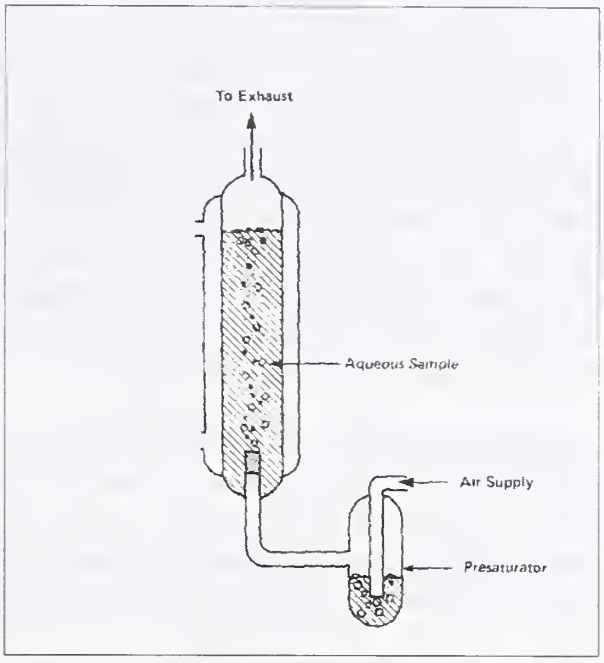

Figure 1. General schematic of a gas stripping apparatus for measuring Henry's law constants (Mackay et al., 1979; Adapted from Ashworth et al., 1988).

Calculated methods for the determination of a compound's Henry's law constant involve the use of either calculated or measured vapor pressure and aqueous solubility data. Other calculated methods include the use of structure relationships but these are commonly constrained by temperature limitations. Computer models, making use of a compound's structure and bonding to help determine its Henry's law constant, have also been developed and used (Nirmalakhandan and Spreece, 1988; Russell et al., 1992; Staudinger and Roberts, 1996), but are also variable limited in terms of environmental parameters such as temperature, salinity, and pressure.

There are generally two approaches for the direct determination of a compound's Henry's law constant. One is the dynamic equilibrium approach and the other is the static equilibrium approach. The dynamic equilibrium approach employs a particular equilibrium air-water partitioning technique. Examples are gas stripping and concurrent flow methods. The gas stripping technique, first developed by Mackay et al. (1979), can be used to determine a compound's Henry's law constant through the measurement of the rate loss of a compound from water to air by stripping it from the water phase with a gas using a bubble column apparatus (fig. 1). Other workers have recently employed this technique for the determination of Henry's law constants for a wide range of environmental organic pollutants (Ashworth et al., 1988; Kucklick et al., 1991; ten Hulscher et al., 1992; Alaee, 1996). Hassett and Millicic (1985) and Yin and Hassett (1986) have developed a similar system for measuring Henry's law constants in natural waters.

The concurrent flow technique, also called the "wetted-wall" technique, uses a vertical column to equilibrate an organic solute between a thin layer of water and a concurrent flow of gas (Fendinger

and Glotfelty, 1988, 1990; Brunner et al., 1990; Meylan and Howard, 1991; Rice et al., 1997, fig. 2). Fendinger and Glotfelty (1988) demonstrated that the wetted-wall technique yielded more reliable Henry's law constants than can be calculated from published vapor pressure and solubility data. Briefly, the concentration of the solute is determined in both the gas and aqueous phase and the Henry's law constant is calculated as the dimensionless ratio of these concentrations.

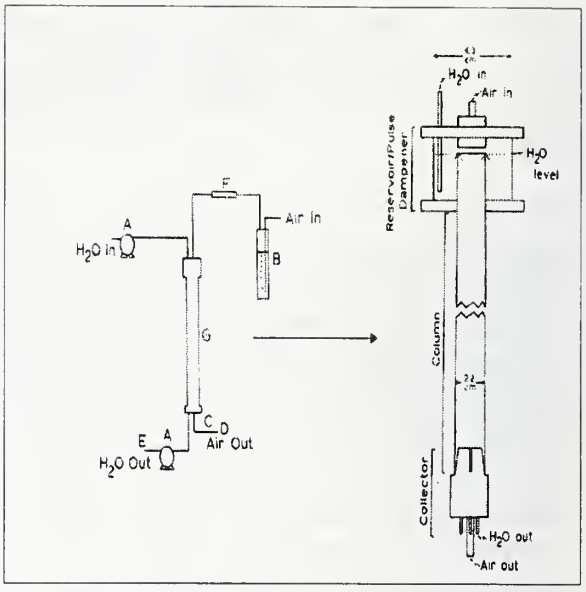

Figure 2. Schematic diagram of the wetted-wall column system by Fendinger and Glotfelty, 1988. System components are (A) valveless metering pumps, (B) impinger to saturate incoming air with water, (C) Chromosorb 102 vapor trap, (D) air outlet to bubble flow meter, (E) solid-phase extraction cartridge, (F) optional analyte vapor source, and (G) wetted-wall column (exploded view of wetted-wall column to the right).

An alternative air-water equilibrium approach for determining air-water Henry's law constants involves the use of a fog chamber (fig. 3). Air-water equilibrium of a compound is obtained with the fog chamber by aspirating water laden with solute into one end of a glass chamber and collecting droplets either *via* drain or in cyclone collectors at the other end of the chamber (Fendinger et al., 1989). This apparatus was designed to measure Henry's law constants at a greater sensitivity than achieved with the wetted-wall technique and to provide independent confirmation of Henry's law constants obtained with the wetted-wall technique. A comparison of Henry's law constants measured with the wetted-wall technique and fog chamber was presented by Fendinger et al. (1989). Differences between Henry's law constants determined by the two techniques for six pesticides were less than 30 percent.

For the static equilibrium approach, air-water partitioning of a compound is determined under equilibrium conditions in a closed system (equilibrium partitioning in closed system: EPICS). Equal amounts of a compound are placed into different bottles containing variable gas-to-water ratios and the Henry's law constant is calculated from the measurement of the concentration ratio (Lincoff and Gossett, 1984; Gossett, 1987; Tancrede and Yanagisawa, 1990; Dewulf et al., 1995). An alternative static equilibrium approach is the dynamic headspace technique (Yin and Hassett, 1986; Robbins, 1993; Hansen et al., 1993) (fig. 4). This technique does not require the exact concentration of the compound to be known but rather the equilibrium headspace peak areas are measured by gas chromatography from bottles containing different headspace-to-liquid volume ratios. Using a plot of these data gives the Henry's law constant and valid results can be generated by analyzing a wide range of headspace-to-liquid volume ratios. This method is most satisfactory for compounds with Henry's law constants greater than 100 Pa m^3/mol. These compounds are highly volatile and are expected to be lost rapidly to the gas phase. For compounds with Henry's law constants in the range of 25 Pa m^3/mol to 100 Pa m^3/mol, head space analysis is still possible but extensive purging may

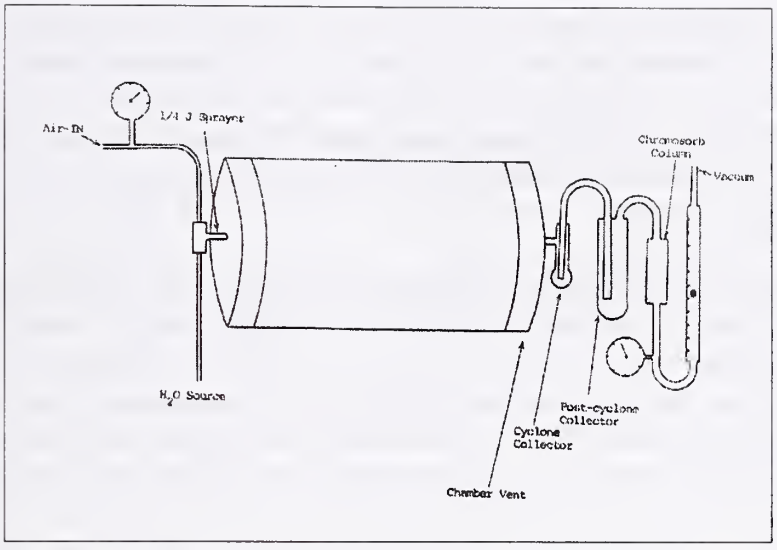

Figure 3. Diagram of fog chamber developed and used for determinations of pesticide Henry's law constants by Fendinger et al. (1989).

be required since volatilization is not very rapid. Head space analysis is rarely feasible for compounds with Henry's law constants less than 25 Pa m^3 / mol (Suntio et al., 1988). Henry's law constants for organic compounds of environmental concern are strongly influenced by a variety of environmental parameters, most importantly temperature. A change in 10 °C can lead to almost a doubling of the Henry's law constants for PAHs (Alaee et al., 1996). However, the influence of pH, compound hydration and concentration, and the presence of complex mixtures, dissolved salts,

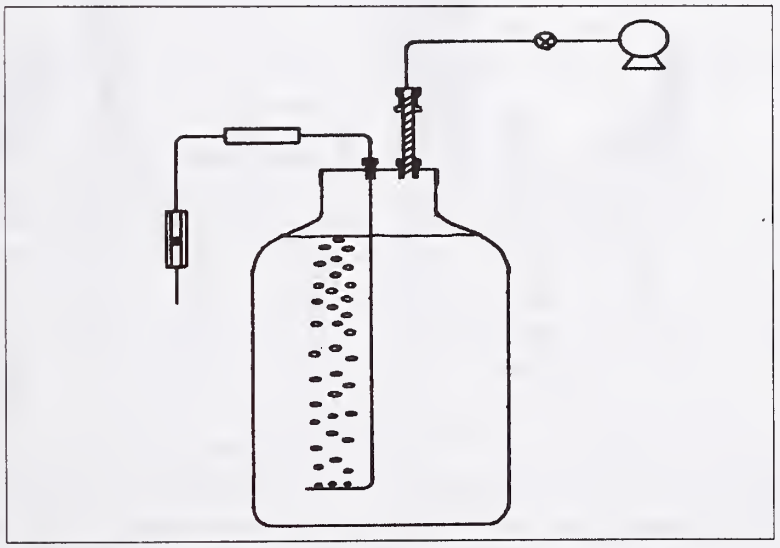

Figure 4. Dynamic headspace gas-partitioning apparatus developed and used by Yin and Hassett (1986) to measure fugacity and freely dissolved mirex in water.

suspended solids, dissolved organic matter, and surfactants can also have an influence on a compounds Henry's law constant and the evaluation of this influence remains severely limited. Staudinger and Roberts (1996) review these effects extensively for a wide range of chemicals, including carboxylic acids, alcohols, phenols, and thiols. We are currently investigating the effects of temperature on the Henry's law constant for PAHs and will use these data to critically evaluate much of the currently reviewed data.

2.4 Additional information. Physical constant data for a variety of temperatures are reported in the literature. As physical/chemical property data for organic solutes are typically temperature dependent, the temperature at which a measurement was made is listed for each compound (when available) in the physical constant data tables (Tables 2 - 8). In addition, if the compound was in a phase other than liquid, it is noted in the last column of each table. Units for aqueous solubility, vapor pressure, and Henry's law constant data are mg/L, Pa, and Pa m^3/mol, respectively.

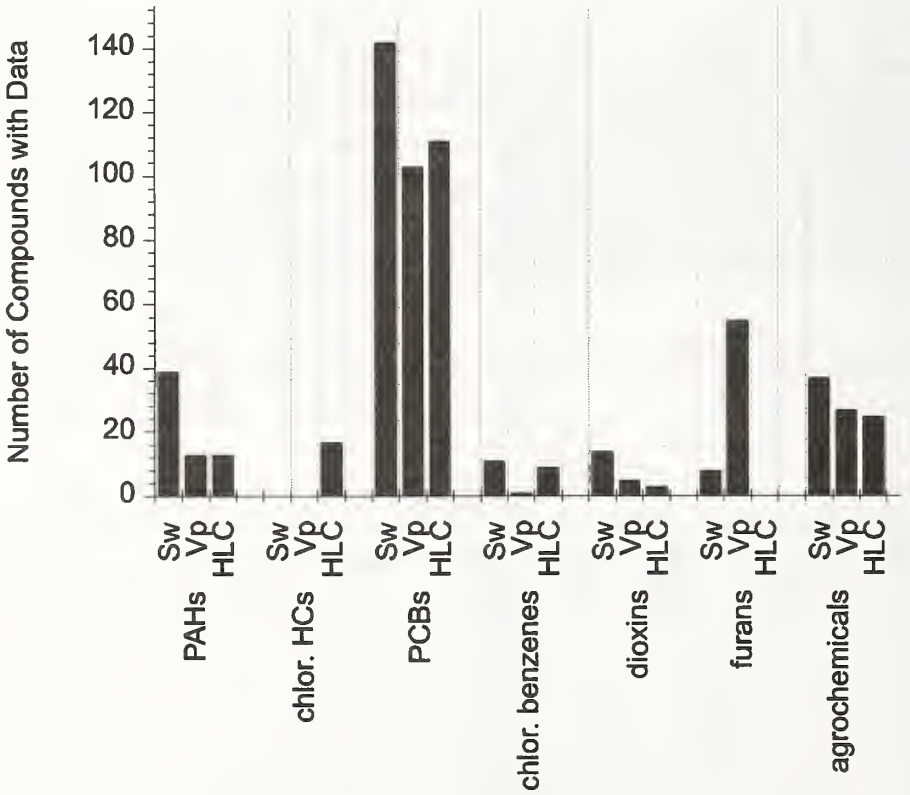

Figure 5. Number of compounds with data reported in Tables 2-8. Chemical groups, such as PAHs, are listed and include within them individual compounds, such as benzo[*a*]pyrene. See Tables 2-8 for a listing of all compounds within a group. Sw, Vp, and HLC represent aqueous solubility, vapor pressure, and Henry's law constant, respectively.

Upon examination of the data in Tables 2-8, it is evident that there is a lack of data for a wide range of compounds within the chemical groups reviewed. For example, there is a large amount of data reported for PCBs but significantly less for other classes of compounds such as PAHs (fig. 5). In general, chemical groups that have a large number of compounds in which physical properties have been determined are those that have physical properties that are less difficult to measure by current analytical techniques. For example, many PCBs are very volatile and this enables vapor pressure measurements to be made with little difficulty. In contrast, many of the compounds within the chemical groups listed in Figure 5 are hydrophobic, thereby making measurements of their solubility and Henry's law constant difficult. However, there are also a larger number of individual PCB congeners within the chemical group "PCBs" relative to other types of compounds, such as PAHs. Also, several of the chemical groups, such as PAHs, dioxins, and furans, have received little attention in terms of environmental fate and toxicological studies until recently. Hence, the physical properties necessary for understanding the environmental fate of these compounds have not been extensively studied. Despite the paucity of physical property data, which are strongly needed for the accurate assessment of the environment fate of these compounds, researchers often use data from a class of compounds other than that being investigated to use for their application, usually *via* an estimation or modeling exercise. For example, directly measured Henry's law constants as a function of temperature are not available for many PAHs but temperature dependent Henry's law constants have been estimated using a relationship that describes the temperature dependence of PCB Henry's law constants (Baker and Eisenreich, 1990, Tateya et al., 1988). In addition, many physical property data reported in the literature are the result of measurements or calculations near 25 °C and unfortunately these conditions are not applicable for many environmental systems since temperature is one of the most significant factors influencing the environmental fate of organic compounds. Knowing what effect temperature has on a compound's Henry's law constant will not only assist in accurately characterizing where the compound may accumulate in the environment, but will also further the exactness of calculating a compound's rate of transfer between and within environmental compartments (e.g., atmosphere, oceans) (Mackay and Yeun, 1983; Baker and Eisenreich, 1990, Staudinger and Roberts, 1996, Diamond et al., 1996). Therefore, studies that are designed to address the effects of temperature on the air-water partitioning of organic compounds are considered essential for evaluation of the data presented in this report.

In summary, the data presented in Tables 2-8 are evolutionary in terms of the NIST database program, largely because our intent is to evaluate the current data set using measurement data as a baseline so that the best possible values of a wide range of compounds may be recommended for the NIST database program. In particular, physical property measurements at temperatures other than 20 °C or 25 °C may be useful for critically evaluating the current data set. Results from studies which are designed to develop estimation methods based upon molecular properties of the compounds in order to critically evaluate the current review of physical property data of organic contaminants will be used for this task and these efforts are currently underway.

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4. DATA TABLES

Table 1. Method identification numbers

Table 1.a. Identification numbers for aqueous solubility methods of determination

METHODS OF EQUILIBRIUM	METHOD IDENTIFICATION NUMBER
calculated	1
shake flask	2
thin-layer coating	4
generator column	4
METHODS OF DETERMINATION	**METHOD IDENTIFICATION**
fluorescence spectrophotometry	5
interferometry	6
liquid chromatography	7
nephelometric methods	8
generator column	9
other	10
data handbook, reported	11

Table 1.b. Identification numbers for vapor pressure methods of determination

METHOD	METHOD IDENTIFICATION NUMBER
calculated	1
pressure gauge	2
comparative ebulliometry	3
effusion methods	4
gas saturation or transpiration methods	5
liquid chromatography	6
capillary gas chromatography	7
data handbook, reported	8

Table 1.c. Identification numbers for Henry's law constant methods of determination.

METHOD	METHOD IDENTIFICATION NUMBER
calculated	1
gas stripping	2
EPICS (equilibrium partitioning in closed system)	3
wetted-wall column	4
variable headspace method	5
other	6
data handbook, reported	7
fog chamber	8

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.a. Aqueous solubility data, mg / L, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1	120-12-7	Anthracene	178.24	3,7	5.2	1.27E-02	1	
2	120-12-7	Anthracene	178.24	1	5.2	1.27E-02	1	
3	120-12-7	Anthracene	178.24	3,7	10	1.75E-02	1	
4	120-12-7	Anthracene	178.24	1	10	1.74E-02	1	
5	120-12-7	Anthracene	178.24	3,7	14.1	2.22E-02	1	
6	120-12-7	Anthracene	178.24	1	14.1	2.23E-02	1	
7	120-12-7	Anthracene	178.24	3,7	18.3	2.91E-02	1	
8	120-12-7	Anthracene	178.24	1	18.3	2.90E-02	1	
9	120-12-7	Anthracene	178.24	3,7	22.4	3.72E-02	1	
10	120-12-7	Anthracene	178.24	1	22.4	3.75E-02	1	
11	120-12-7	Anthracene	178.24	3,7	24.6	4.34E-02	1	
12	120-12-7	Anthracene	178.24	1	24.6	4.31E-02	1	
13	120-12-7	Anthracene	178.24	1	25	4.42E-02	1	
14	120-12-7	Anthracene	178.24	1	25	4.42E-02	1	
15	120-12-7	Anthracene	178.24	2,7	25	7.30E-02	2	
16	120-12-7	Anthracene	178.24	2,5	25	7.50E-02	5	
17	120-12-7	Anthracene	178.24	10	27	7.50E-02	7	
18	120-12-7	Anthracene	178.24	3,7	28.7	5.57E-02	1	
19	120-12-7	Anthracene	178.24	1	28.7	5.59E-02	1	
20	120-12-7	Anthracene	178.24	2,5	35.4	1.23E-01	6	
21	120-12-7	Anthracene	178.24	2,5	39.3	1.59E-01	6	
22	120-12-7	Anthracene	178.24	2,5	44.7	2.14E-01	6	
23	120-12-7	Anthracene	178.24	2,5	47.5	2.49E-01	6	
24	120-12-7	Anthracene	178.24	2,5	50.1	2.88E-01	6	
25	120-12-7	Anthracene	178.24	2,5	54.7	3.72E-01	6	
26	120-12-7	Anthracene	178.24	2,5	59.2	4.81E-01	6	
27	120-12-7	Anthracene	178.24	2,5	64.5	6.60E-01	6	
28	120-12-7	Anthracene	178.24	2,5	65.1	6.80E-01	6	
29	120-12-7	Anthracene	178.24	2,5	69.8	9.00E-01	6	
30	120-12-7	Anthracene	178.24	2,5	70.7	9.50E-01	6	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.a. Aqueous solubility data, mg / L, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
27	120-12-7	Anthracene	178.24	2,5	71.9	1.02E+00	6	
28	120-12-7	Anthracene	178.24	2,5	74.7	1.21E+00	6	
29	56-55-3	Benz[*a*]anthracene	228.28	2,7	25	1.40E-02	2	
30	56-55-3	Benz[*a*]anthracene	228.28	2,5	25	1.00E-02	5	
31	56-55-3	Benz[*a*]anthracene	228.28	10	27	1.10E-02	7	
32	71-43-2	Benzene	78.11	2,5	25	1.86E+03	5	
33	71-43-2	Benzene	78.11	2,5	5.2	1.81E+03	4	
34	71-43-2	Benzene	78.11	2,5	10	1.80E+03	4	
35	71-43-2	Benzene	78.11	2,5	14.9	1.78E+03	4	
36	71-43-2	Benzene	78.11	2,5	21	1.79E+03	4	
37	71-43-2	Benzene	78.11	2,5	25	1.79E+03	4	
38	71-43-2	Benzene	78.11	2,5	30.2	1.84E+03	4	
39	71-43-2	Benzene	78.11	2,5	34.9	1.89E+03	4	
40	71-43-2	Benzene	78.11	2,5	42.8	1.99E+03	4	
41	71-43-2	Benzene	78.11	2,9	25	2.24E-04	8	uM
42	205-99-2	Benzo[*b*]fluoranthene	252.3	7	25	2.15E-05	29	Pa, supercooled
43	207-08-9	Benzo[*k*]fluoranthene	252.3	7	25	2.12E-05	29	Pa, supercooled
44	238-84-3	1,2-Benzoflourene	216.29	2,7	25	4.50E-02	2	
45	243-17-4	2,3-Benzoflourene	216.29	2,7	25	2.00E-03	2	
46	203-12-3	Benzo[*ghi*]perylene	276	2,7	25	2.60E-04	2	
47	50-32-8	Benzo[*a*]pyrene	252.32	2,5	25	7.32E-03	3	
48	50-32-8	Benzo[*a*]pyrene	252.32	2,7	25	3.80E-03	2	
49	50-32-8	Benzo[*a*]pyrene	252.32	2,5	25	4.79E-03	3	
50	50-32-8	Benzo[*a*]pyrene	252.32	10	27	4.00E-03	7	
51	92-52-4	Biphenyl	154.21	2,7	25	7.00E+00	2	
52	92-52-4	Biphenyl	154.21	2,9	25	3.91E-01	8	uM
53	92-52-4	Biphenyl	154.21	4,9	25	6.71E+00	21	
54	92-52-4	Biphenyl	154.21	2,6	25	7.40E+00	28	
55	104-51-8	*n* -Butylbenzene	134.2	2,5	25	5.00E+01	5	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.a. Aqueous solubility data, mg / L, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
56	218-01-9	Chrysene	228.3	2,7	25	2.00E-03	2	
57	218-01-9	Chrysene	228.3	2,5	25	6.00E-03	5	
58	218-01-9	Chrysene	228.3	10	27	1.50E-03	7	
59	191-07-1	Coronene	300.36	2,7	25	1.40E-04	2	
60	53-70-3	1,2,5,6-Dibenzanthracene	278.36	2,5	25	6.00E-04	5	
61	53-70-3	1,2,5,6-Dibenzanthracene	278.36	10	27	5.00E-04	7	
62	58-70-3	1,2,7,8-Dibenzanthracene	278.36	10	27	1.20E-02	7	
63	781-43-1	9,10-Dimethylanthracene	206.3	2,7	25	5.60E-02	2	
64	575-41-7	1,3-Dimethylnaphthalene	156.23	2,7	25	8.00E+00	2	
65	571-58-4	1,4-Dimethylnaphthalene	156.23	2,7	25	1.14E+01	2	
66	571-61-9	1,5-Dimethylnaphthalene	156.23	2,7	25	3.38E+00	2	
67	571-61-9	1,5-Dimethylnaphthalene	156.23	2,6	25	2.81E+00	28	
68	581-40-8	2,3-Dimethylnaphthalene	156.23	2,7	25	3.00E+00	2	
69	581-40-8	2,3-Dimethylnaphthalene	156.23	2,6	25	2.03E+00	28	
70	581-40-2	2,6-Dimethylnaphthalene	156.23	2,7	25	2.00E+00	2	
71	581-40-2	2,6-Dimethylnaphthalene	156.23	2,6	25	1.30E+00	28	
72	100-41-4	Ethylbenzene	106.2	2,5	25	1.75E+02	5	
73	1127-76-0	1-Ethylnaphthalene	156.23	2,7	25	1.07E+01	2	
74	206-44-0	Fluoranthene	202	2,7	25	2.60E-01	2	
75	206-44-0	Fluoranthene	202	2,5	25	2.65E-01	5	
76	206-44-0	Fluoranthene	202	10	27	2.40E-01	7	
77	86-73-7	Fluorene	166.23	2,7	25	1.98E+00	2	
78	86-73-7	Fluorene	166.23	2,5	24.6	1.86E+00	6	
79	86-73-7	Fluorene	166.23	2,5	29.9	2.37E+00	6	
80	86-73-7	Fluorene	166.23	2,5	30.3	2.41E+00	6	
81	86-73-7	Fluorene	166.23	2,5	38.4	3.53E+00	6	
82	86-73-7	Fluorene	166.23	2,5	40.1	3.84E+00	6	
83	86-73-7	Fluorene	166.23	2,5	47.5	5.54E+00	6	
84	86-73-7	Fluorene	166.23	2,5	50.1	6.32E+00	6	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.a. Aqueous solubility data, mg / L, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
85	86-73-7	Fluorene	166.23	2,5	50.2	6.35E+00	6	
86	86-73-7	Fluorene	166.23	2,5	54.7	8.02E+00	6	
87	86-73-7	Fluorene	166.23	2,5	59.2	1.02E+01	6	
88	86-73-7	Fluorene	166.23	2,5	60.5	1.09E+01	6	
89	86-73-7	Fluorene	166.23	2,5	65.1	1.41E+01	6	
90	86-73-7	Fluorene	166.23	2,5	70.7	1.93E+01	6	
91	86-73-7	Fluorene	166.23	2,5	71.9	2.06E+01	6	
92	86-73-7	Fluorene	166.23	2,5	73.4	2.25E+01	6	
93	613-12-7	2-Methylanthracene	192.26	2,7	25	3.90E-02	2	
94	613-12-7	2-Methylanthracene	192.26	3,9	31.1	3.21E+01	1	
95	613-12-7	2-Methylanthracene	192.26	1	31.1	3.18E-02	1	
96	613-12-7	2-Methylanthracene	192.26	3,9	27	2.42E-02	1	
97	613-12-7	2-Methylanthracene	192.26	1	27	2.42E-02	1	
98	613-12-7	2-Methylanthracene	192.26	3,9	23.1	1.91E-02	1	
99	613-12-7	2-Methylanthracene	192.26	1	23.1	1.89E-02	1	
100	613-12-7	2-Methylanthracene	192.26	3,9	18.3	1.45E-02	1	
101	613-12-7	2-Methylanthracene	192.26	1	18.3	1.44E-02	1	
102	613-12-7	2-Methylanthracene	192.26	3,9	13.9	1.11E-02	1	
103	613-12-7	2-Methylanthracene	192.26	1	13.9	1.12E-02	1	
104	613-12-7	2-Methylanthracene	192.26	3,9	10. 8	9.43E-03	1	
105	613-12-7	2-Methylanthracene	192.26	1	10.8	9.53E-03	1	
106	613-12-7	2-Methylanthracene	192.26	3,9	9.1	8.48E-03	1	
107	613-12-7	2-Methylanthracene	192.26	1	9.1	8.57E-03	1	
108	613-12-7	2-Methylanthracene	192.26	3,9	6.3	7.06E-03	1	
109	613-12-7	2-Methylanthracene	192.26	1	6.3	7.00E-03	1	
110	779-02-2	9-Methylanthracene	192.26	2,7	25	2.61E-01	2	
111		5-Methylbenz[*a*]pyrene	266	10	27	8.00E-04	7	
112	56-49-5	3-Methylchloanthrene		2,7	25	2.90E-03	2	
113	90-12-0	1-Methylnaphthalene	142.2	2,7	25	2.85E+01	2	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.a. Aqueous solubility data, mg / L, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
114	90-12-0	1-Methylnaphthalene	142.2	2,6	25	2.57E+01	28	
115	91-57-6	2-Methylnaphthalene	142.19	2,7	25	2.54E+01	2	
116	91-57-6	2-Methylnaphthalene	142.19	2,6	25	2.45E+01	28	
117	832-69-6	1-Methylphenanthrene	192.26	3,9	29.9	3.55E-01	1	
118	832-69-6	1-Methylphenanthrene	192.26	1	29.9	3.56E-01	1	
119	832-69-6	1-Methylphenanthrene	192.26	3,9	26.9	3.04E-01	1	
120	832-69-6	1-Methylphenanthrene	192.26	1	26.9	3.00E-01	1	
121	832-69-6	1-Methylphenanthrene	192.26	3,9	24.1	2.55E-01	1	
122	832-69-6	1-Methylphenanthrene	192.26	1	24.1	2.56E-01	1	
123	832-69-6	1-Methylphenanthrene	192.26	3,9	19.2	1.93E-01	1	
124	832-69-6	1-Methylphenanthrene	192.26	1	19.2	1.95E-01	1	
125	832-69-6	1-Methylphenanthrene	192.26	3,9	14	1.47E-01	1	
126	832-69-6	1-Methylphenanthrene	192.26	1	14	1.47E-01	1	
127	832-69-6	1-Methylphenanthrene	192.26	3,9	8.9	1.14E-01	1	
128	832-69-6	1-Methylphenanthrene	192.26	1	8.9	1.11E-01	1	
129	832-69-6	1-Methylphenanthrene	192.26	3,9	6.6	9.52E-02	1	
130	832-69-6	1-Methylphenanthrene	192.26	1	6.6	9.69E-02	1	
131	92-24-0	Naphthacene	228.28	2,7	25	5.70E-04	2	
132	92-24-0	Naphthacene	228.28	2,5	25	1.50E-03	5	
133	92-24-0	Naphthacene	228.28	10	27	1.00E-03	7	
134	91-20-3	Naphthalene	128.18	2,7	25	3.17E+01	2	
135	91-20-3	Naphthalene	128.18	2,6	25	3.11E+01	28	
136	91-20-3	Naphthalene	128.18	2,5	25	1.25E+01	5	
137	91-20-3	Naphthalene	128.18	2,5	22.2	2.83E+01	6	
138	91-20-3	Naphthalene	128.18	2,5	24.5	3.07E+01	6	
139	91-20-3	Naphthalene	128.18	2,5	29.9	3.73E+01	6	
140	91-20-3	Naphthalene	128.18	2,5	30.3	3.78E+01	6	
141	91-20-3	Naphthalene	128.18	2,5	34.5	4.43E+01	6	
142	91-20-3	Naphthalene	128.18	2,5	39.3	5.33E+01	6	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.a. Aqueous solubility data, mg / L, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
143	91-20-3	Naphthalene	128.18	2,5	40.1	5.50E+01	6	
144	91-20-3	Naphthalene	128.18	2,5	44.7	6.62E+01	6	
145	91-20-3	Naphthalene	128.18	2,5	50.2	8.31E+01	6	
146	91-20-3	Naphthalene	128.18	2,5	55.6	1.05E+02	6	
147	91-20-3	Naphthalene	128.18	2,5	64.5	1.56E+02	6	
148	91-20-3	Naphthalene	128.18	2,5	73.4	2.39E+02	6	
149	91-20-3	Naphthalene	128.18	2,5	0	1.30E+01	4	
150	91-20-3	Naphthalene	128.18	2,5	0.4	1.30E+01	4	
151	91-20-3	Naphthalene	128.18	2,5	0.5	1.30E+01	4	
152	91-20-3	Naphthalene	128.18	2,5	0.9	1.40E+01	4	
153	91-20-3	Naphthalene	128.18	2,5	1.9	1.50E+01	4	
154	91-20-3	Naphthalene	128.18	2,5	9.4	2.00E+01	4	
155	91-20-3	Naphthalene	128.18	2,5	10	1.90E+01	4	
156	91-20-3	Naphthalene	128.18	2,5	14.9	2.30E+01	4	
157	91-20-3	Naphthalene	128.18	2,5	15.9	2.40E+01	4	
158	91-20-3	Naphthalene	128.18	2,5	19.3	2.80E+01	4	
159	91-20-3	Naphthalene	128.18	2,5	25	3.44E+01	4	
160	91-20-3	Naphthalene	128.18	2,5	30.1	4.30E+01	4	
161	91-20-3	Naphthalene	128.18	2,5	30.2	4.40E+01	4	
162	91-20-3	Naphthalene	128.18	2,5	35.2	5.40E+01	4	
163	91-20-3	Naphthalene	128.18	2,5	36	5.50E+01	4	
164	91-20-3	Naphthalene	128.18	2,5	42.8	7.30E+01	4	
165	198-55-0	Perylene	252	2,7	25	4.00E-04	2	
166	85-01-8	Phenanthrene	178.24	2,5	25	1.60E+03	5	
167	85-01-8	Phenanthrene	178.24	2,7	25	1.29E+00	2	
168	85-01-8	Phenanthrene	178.24	2,6	25	1.07E+00	28	
169	85-01-8	Phenanthrene	178.24	2,5	24.6	1.16E+00	6	
170	85-01-8	Phenanthrene	178.24	2,5	29.9	1.49E+00	6	
171	85-01-8	Phenanthrene	178.24	2,5	30.3	1.52E+00	6	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.a. Aqueous solubility data, mg / L, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
172	85-01-8	Phenanthrene	178.24	2,5	38.4	2.27E+00	6	
173	85-01-8	Phenanthrene	178.24	2,5	40.1	2.47E+00	6	
174	85-01-8	Phenanthrene	178.24	2,5	47.5	3.63E+00	6	
175	85-01-8	Phenanthrene	178.24	2,5	50.1	4.16E+00	6	
176	85-01-8	Phenanthrene	178.24	2,5	50.2	4.19E+00	6	
177	85-01-8	Phenanthrene	178.24	2,5	54.7	5.34E+00	6	
178	85-01-8	Phenanthrene	178.24	2,5	59.2	6.85E+00	6	
179	85-01-8	Phenanthrene	178.24	2,5	60.5	7.40E+00	6	
180	85-01-8	Phenanthrene	178.24	2,5	65.1	9.60E+00	6	
181	85-01-8	Phenanthrene	178.24	2,5	70.7	1.33E+01	6	
182	85-01-8	Phenanthrene	178.24	2,5	71.9	1.42E+01	6	
183	85-01-8	Phenanthrene	178.24	2,5	73.4	1.56E+01	6	
184	85-01-8	Phenanthrene	178.24	3,9	29.9	1.28E+00	1	
185	85-01-8	Phenanthrene	178.24	1	29	1.27E+00	1	
186	85-01-8	Phenanthrene	178.24	1	25	1.00E+00	1	
187	85-01-8	Phenanthrene	178.24	3,9	24.3	9.95E-01	1	
188	85-01-8	Phenanthrene	178.24	1	24.3	9.68E-01	1	
189	85-01-8	Phenanthrene	178.24	3,9	21	8.16E-01	1	
190	85-01-8	Phenanthrene	178.24	1	21	8.16E-01	1	
191	85-01-8	Phenanthrene	178.24	3,9	15	6.01E-01	1	
192	85-01-8	Phenanthrene	178.24	1	15	5.95E-01	1	
193	85-01-8	Phenanthrene	178.24	3,9	12.5	5.12E-01	1	
194	85-01-8	Phenanthrene	178.24	1	12.5	5.23E-01	1	
195	85-01-8	Phenanthrene	178.24	3,9	10	4.68E-01	1	
196	85-01-8	Phenanthrene	178.24	1	10	4.61E-01	1	
197	85-01-8	Phenanthrene	178.24	3,9	8.5	4.23E-01	1	
198	85-01-8	Phenanthrene	178.24	1	8.5	4.30E-01	1	
199	85-01-8	Phenanthrene	178.24	10	27	1.60E+00	7	
200	129-00-0	Pyrene	202.26	2,7	25	1.35E-01	2	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.a. Aqueous solubility data, mg / L, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
201	129-00-0	Pyrene	202.26	2,5	22.2	1.30E-01	6	
202	129-00-0	Pyrene	202.26	2,5	34.5	2.35E-01	6	
203	129-00-0	Pyrene	202.26	2,5	44.7	3.99E-01	6	
204	129-00-0	Pyrene	202.26	2,5	50.1	5.34E-01	6	
205	129-00-0	Pyrene	202.26	2,5	55.6	7.30E-01	6	
206	129-00-0	Pyrene	202.26	2,5	56	7.40E-01	6	
207	129-00-0	Pyrene	202.26	2,5	60.7	9.70E-01	6	
208	129-00-0	Pyrene	202.26	2,5	65.2	1.27E+00	6	
209	129-00-0	Pyrene	202.26	2,5	71.9	1.90E+00	6	
210	129-00-0	Pyrene	202.26	2,5	74.7	2.26E+00	6	
211	129-00-0	Pyrene	202.26	2,5	25	1.75E-01	5	
212	129-00-0	Pyrene	202.26	10	27	1.65E-01	7	
213	108-88-3	Toluene	92	2,5	25	5.00E+02	5	
214	108-88-3	Toluene	92	11	16	4.70E+02	45	
215	108-88-3	Toluene	92	11	20	5.15E+02	45	
216	2131-41-1	1,4,5-Trimethylnaphthalene	170	2,7	25	2.10E+00	2	
217	217-59-4	Triphenylene	288.3	2,7	25	4.30E-02	2	
218	217-59-4	Triphenylene	288.3	10	27	3.80E-02	7	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.b. Vapor pressure data, Pa, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
219	120-12-7	Anthracene	178.24	7	25	6.37E-02	14	
220	120-12-7	Anthracene	178.24	7	25	6.74E-02	29	supercooled
221	56-55-3	Benz[*a*]anthracene	228.28	7	25	3.00E-04	14	
222	56-55-3	Benz[*a*]anthracene	228.28	6	25	2.80E-05	17	
223	56-55-3	Benz[*a*]anthracene	228.28	7	25	2.56E-04	29	supercooled
224	50-32-8	Benzo[*a*]pyrene	252.3	7	25	1.49E-05	14	
225	192-97-2	Benzo[*e*]pyrene	252.3	7	25	1.38E-05	29	supercooled
226	92-52-4	Biphenyl	154.21	5	5.2	1.06E-01	15	
227	92-52-4	Biphenyl	154.21	5	14.9	3.61E-01	15	
228	92-52-4	Biphenyl	154.21	5	24.7	1.15E+00	15	
229	92-52-4	Biphenyl	154.21	5	25	1.19E+00	15	
230	92-52-4	Biphenyl	154.21	7	25	2.85E+00	29	supercooled
231	218-01-9	Chrysene	228.3	7	25	2.34E-04	29	supercooled
232	206-44-0	Fluoranthene	202	7	25	6.67E-03	14	
233	206-44-0	Fluoranthene	202	7	25	7.10E-03	29	supercooled
234	206-44-0	Fluoranthene	202	6	25	1.23E-03	17	
235	86-73-7	Fluorene	166.23	7	25	3.80E-01	14	
236	86-73-7	Fluorene	166.23	6	25	8.00E-02	17	
237	86-73-7	Fluorene	166.23	7	25	4.17E-01	29	supercooled
238	90-12-0	1-Methylnaphthalene	142.2	7	25	5.92E+00	14	
239	91-20-3	Naphthalene	128.18	7	25	2.82E+01	14	
240	91-20-3	Naphthalene	128.18	6	25	1.04E+01	17	
241	91-20-3	Naphthalene	128.18	7	25	1.83E+01	29	supercooled
242	85-01-8	Phenanthrene	178.24	7	25	6.88E-02	14	
243	85-01-8	Phenanthrene	178.24	6	25	1.61E-02	17	
244	85-01-8	Phenanthrene	178.24	7	25	7.19E-02	29	supercooled
245	129-00-0	Pyrene	202.26	7	25	4.89E-03	14	
246	129-00-0	Pyrene	202.26	6	25	6.00E-04	17	
247	129-00-0	Pyrene	202.26	7	25	4.55E-03	29	supercooled

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.b. Vapor pressure data, Pa, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
248	108-88-3	Toluene	92	8	6.4	1.33E+03	45	
249	108-88-3	Toluene	92	8	20	2.93E+03	45	
250	108-88-3	Toluene	92	8	31.8	5.33E+03	45	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.c. Henry's law constant data, Pa m^3 / mol, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
251	120-12-7	Anthracene	178.24	4	25	1.96E+00	33	
252	120-12-7	Anthracene	178.24	2	5.4	2.76E+00	41	
253	120-12-7	Anthracene	178.24	2	10.1	3.12E+00	41	
254	120-12-7	Anthracene	178.24	2	14.8	3.44E+00	41	
255	120-12-7	Anthracene	178.24	2	20.6	3.91E+00	41	
256	120-12-7	Anthracene	178.24	2	25.0	4.94E+00	41	
257	120-12-7	Anthracene	178.24	2	30.2	8.05E+00	41	
258	120-12-7	Anthracene	178.24	2	35.3	8.94E+00	41	
259	71-43-2	Benzene	78.11	5	29	6.49E+02	30	
260	71-43-2	Benzene	78.11	5	25	5.35E+02	31	
261	71-43-2	Benzene	78.11	5	30	6.86E+02	31	
262	71-43-2	Benzene	78.11	5	40	8.90E+02	31	
263	71-43-2	Benzene	78.11	5	45	1.24E+03	31	
264	71-43-2	Benzene	78.11	5	50	1.45E+03	31	
265	71-43-2	Benzene	78.11	3	2	1.62E+01	32	
266	71-43-2	Benzene	78.11	3	6	2.08E+02	32	
267	71-43-2	Benzene	78.11	3	10	2.28E+02	32	
268	71-43-2	Benzene	78.11	3	18.2	3.66E+02	32	
269	71-43-2	Benzene	78.11	3	25	4.81E+02	32	
270	71-43-2	Benzene	78.11	3	10	3.34E+02	37	
271	71-43-2	Benzene	78.11	3	15	3.93E+02	37	
272	71-43-2	Benzene	78.11	3	20	4.58E+02	37	
273	71-43-2	Benzene	78.11	3	25	5.35E+02	37	
274	71-43-2	Benzene	78.11	3	30	7.29E+02	37	
275	71-43-2	Benzene	78.11	2	4.0	1.69E+02	41	
276	71-43-2	Benzene	78.11	2	10.0	2.28E+02	41	
277	71-43-2	Benzene	78.11	2	15.0	3.26E+02	41	
278	71-43-2	Benzene	78.11	2	20.6	4.41E+02	41	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.c. Henry's law constant data, Pa m^3 / mol, PAHs								
Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
279	71-43-2	Benzene	78.11	2	25.4	5.52E+02	41	
280	71-43-2	Benzene	78.11	2	30.1	7.44E+02	41	
281	71-43-2	Benzene	78.11	2	34.9	8.74E+02	41	
282	205-99-2	Benzo[*b*]fluoranthene	252.3	4	10	2.50E-02	36	
283	205-99-2	Benzo[*b*]fluoranthene	252.3	4	20	5.10E-02	36	
284	205-99-2	Benzo[*b*]fluoranthene	252.3	4	35	1.19E-01	36	
285	205-99-2	Benzo[*b*]fluoranthene	252.3	4	40.1	1.51E-01	36	
286	205-99-2	Benzo[*b*]fluoranthene	252.3	4	45	2.08E-01	36	
287	205-99-2	Benzo[*b*]fluoranthene	252.3	4	55	3.70E-01	36	
288	207-08-9	Benzo[*k*]fluoranthene	252.3	4	10	2.20E-02	36	
289	207-08-9	Benzo[*k*]fluoranthene	252.3	4	20	4.30E-02	36	
290	207-08-9	Benzo[*k*]fluoranthene	252.3	4	35	1.07E-01	36	
291	207-08-9	Benzo[*k*]fluoranthene	252.3	4	40.1	1.38E-01	36	
292	207-08-9	Benzo[*k*]fluoranthene	252.3	4	45	1.98E-01	36	
293	207-08-9	Benzo[*k*]fluoranthene	252.3	4	55	4.03E-01	36	
294	203-12-3	Benzo[*ghi*]perylene	276	4	10	1.90E-02	36	
295	203-12-3	Benzo[*ghi*]perylene	276	4	20	2.70E-02	36	
296	203-12-3	Benzo[*ghi*]perylene	276	4	35	5.20E-02	36	
297	203-12-3	Benzo[*ghi*]perylene	276	4	40.1	5.40E-02	36	
298	203-12-3	Benzo[*ghi*]perylene	276	4	45	6.60E-02	36	
299	203-12-3	Benzo[*ghi*]perylene	276	4	55	8.70E-02	36	
300	50-32-8	Benzo[*a*]pyrene	252.3	4	10	2.20E-02	36	
301	50-32-8	Benzo[*a*]pyrene	252.3	4	20	3.40E-02	36	
302	50-32-8	Benzo[*a*]pyrene	252.3	4	35	7.40E-02	36	
303	50-32-8	Benzo[*a*]pyrene	252.3	4	40.1	9.20E-02	36	
304	50-32-8	Benzo[*a*]pyrene	252.3	4	45	1.10E-01	36	
305	50-32-8	Benzo[*a*]pyrene	252.3	4	55	2.39E-01	36	
306	92-52-4	Biphenyl	154.21	2	25	4.13E+01	16	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.c. Henry's law constant data, Pa m^3 / mol, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
307	92-52-4	Biphenyl	154.21	4	25	1.96E+01	33	
308	206-44-0	Fluoranthene	202.3	4	10	2.60E-01	36	
309	206-44-0	Fluoranthene	202.3	4	20	6.40E-01	36	
310	206-44-0	Fluoranthene	202.3	4	35	1.63E+00	36	
311	206-44-0	Fluoranthene	202.3	4	40.1	2.38E+00	36	
312	206-44-0	Fluoranthene	202.3	4	45	5.84E+00	36	
313	206-44-0	Fluoranthene	202.3	4	55	6.23E+00	36	
314	86-73-7	Fluorene	166.23	4	25	6.44E+00	33	
315	90-12-0	1-Methylnaphthalene	142.2	4	25	6.20E+01	33	
316	91-57-6	2-Methylnaphthalene	142.19	4	25	3.22E+01	33	
317	91-20-3	Naphthalene	128.18	2	25	4.89E+01	16	
318	91-20-3	Naphthalene	128.18	4	25	7.44E+01	33	
319	91-20-3	Naphthalene	128.18	2	3.7	9.65E+00	41	
320	91-20-3	Naphthalene	128.18	2	9.4	1.54E+01	41	
321	91-20-3	Naphthalene	128.18	2	15.3	2.14E+01	41	
322	91-20-3	Naphthalene	128.18	2	15.5	2.31E+01	41	
323	91-20-3	Naphthalene	128.18	2	20.0	3.32E+01	41	
324	91-20-3	Naphthalene	128.18	2	25.0	4.26E+01	41	
325	91-20-3	Naphthalene	128.18	2	25.4	4.52E+01	41	
326	91-20-3	Naphthalene	128.18	2	30.2	5.86E+01	41	
327	91-20-3	Naphthalene	128.18	2	35.5	7.91E+01	41	
328	85-01-8	Phenanthrene	178.24	2	25.0	3.98E+00	16	
329	85-01-8	Phenanthrene	178.24	4	25.0	2.38E+00	33	
330	85-01-8	Phenanthrene	178.24	2	5.9	1.81E+00	41	
331	85-01-8	Phenanthrene	178.24	2	10.4	2.99E+00	41	
332	85-01-8	Phenanthrene	178.24	2	15.0	3.06E+00	41	
333	85-01-8	Phenanthrene	178.24	2	20.2	3.66E+00	41	
334	85-01-8	Phenanthrene	178.24	2	25.7	4.73E+00	41	

Table 2. Physical constant data for polycyclic aromatic hydrocarbons (PAHs)

Table 2.c. Henry's law constant data, Pa m^3 / mol, PAHs

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
335	85-01-8	Phenanthrene	178.24	2	30.2	5.54E+00	41	
336	85-01-8	Phenanthrene	178.24	2	34.7	7.90E+00	41	

Table 3. Physical constant data for chlorinated aliphatics

Table 3. Physical constant data for chlorinated aliphatics

Table 3.a. Henry's law constant data, Pa m^3 / mol, chlorinated aliphatics

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
337	75-27-4	Bromodichloromethane	163.83	6	20	1.60E+02	40	
338	75-27-4	Bromodichloromethane	163.83	6	30	2.60E+02	40	
339	75-27-4	Bromodichloromethane	163.83	6	40	4.00E+02	40	
340	75-25-2	Bromoform	252.8	6	20	4.00E+01	40	
341	75-25-2	Bromoform	252.8	6	30	7.00E+01	40	
342	75-25-2	Bromoform	252.8	6	40	1.20E+02	40	
343	56-23-5	Carbon tetrachloride	153.82	6	20	2.04E+03	40	
344	56-23-5	Carbon tetrachloride	153.82	6	30	3.37E+03	40	
345	56-23-5	Carbon tetrachloride	153.82	6	35	3.82E+03	40	
346	56-23-5	Carbon tetrachloride	153.82	6	40	4.52E+03	40	
347	124-48-1	Chlorodibromomethane	208.28	6	20	8.00E+01	40	
348	124-48-1	Chlorodibromomethane	208.28	6	30	1.40E+02	40	
349	124-48-1	Chlorodibromomethane	208.28	6	40	2.20E+02	40	
350	74-95-3	Dibromomethane	173.82	6	20	7.00E+01	40	
351	74-95-3	Dibromomethane	173.82	6	30	1.10E+02	40	
352	74-95-3	Dibromomethane	173.82	6	35	1.40E+02	40	
353	74-95-3	Dibromomethane	173.82	6	40	1.70E+02	40	
354	75-34-3	1,1-Dichloroethane	98.93	6	20	4.60E+02	40	
355	75-34-3	1,1-Dichloroethane	98.93	6	30	7.00E+02	40	
356	75-34-3	1,1-Dichloroethane	98.93	6	40	1.02E+03	40	
357	107-6-2	1,2-Dichloroethane	98.93	6	20	1.00E+02	40	
358	107-6-2	1,2-Dichloroethane	98.93	6	30	1.50E+02	40	
359	107-6-2	1,2-Dichloroethane	98.93	6	35	1.80E+02	40	
360	107-6-2	1,2-Dichloroethane	98.93	6	40	2.20E+02	40	
361	75-35-4	1,1-Dichloroethylene	96.93	6	20	2.29E+03	40	
362	75-35-4	1,1-Dichloroethylene	96.93	6	30	3.37E+03	40	
363	75-35-4	1,1-Dichloroethylene	96.93	6	40	4.75E+03	40	
364	156-59-2	*cis*-1,2-Dichloroethylene	96.93	6	20	3.20E+02	40	

Table 3. Physical constant data for chlorinated aliphatics

Table 3.a. Henry's law constant data, Pa m^3 / mol, chlorinated aliphatics

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
365	156-59-2	*cis* -1,2-Dichloroethylene	96.93	6	30	4.90E+02	40	
366	156-59-2	*cis* -1,2-Dichloroethylene	96.93	6	40	7.30E+02	40	
367	156-60-5	*trans* -1,2-Dichloroethylene	96.93	6	20	7.90E+02	40	
368	156-60-5	*trans* -1,2-Dichloroethylene	96.93	6	30	1.18E+03	40	
369	156-60-5	*trans* -1,2-Dichloroethylene	96.93	6	40	1.77E+03	40	
370	75-09-2	Dichloromethane	84.92	6	20	2.10E+02	40	
371	75-09-2	Dichloromethane	84.92	6	30	3.10E+02	40	
372	75-09-2	Dichloromethane	84.92	6	35	3.70E+02	40	
373	75-09-2	Dichloromethane	84.92	6	40	4.50E+02	40	
374	78-87-5	1,2-Dichloropropane	112.94	6	20	2.10E+02	40	
375	78-87-5	1,2-Dichloropropane	112.94	6	30	3.20E+02	40	
376	78-87-5	1,2-Dichloropropane	112.94	6	40	4.80E+02	40	
377	630-20-6	1,1,1,2-Tetrachloroethane	167.83	6	20	1.70E+02	40	
378	630-20-6	1,1,1,2-Tetrachloroethane	167.83	6	30	2.80E+02	40	
379	630-20-6	1,1,1,2-Tetrachloroethane	167.83	6	35	3.60E+02	40	
380	630-20-6	1,1,1,2-Tetrachloroethane	167.83	6	40	4.60E+02	40	
381	79-34-5	1,1,2,2-Tetrachloroethane	167.83	6	20	3.00E+01	40	
382	79-34-5	1,1,2,2-Tetrachloroethane	167.83	6	30	5.00E+01	40	
383	79-34-5	1,1,2,2-Tetrachloroethane	167.83	6	34	6.00E+01	40	
384	79-34-5	1,1,2,2-Tetrachloroethane	167.83	6	40	9.00E+01	40	
385	71-55-6	1,1,1-Trichloroethane	133.38	6	20	1.26E+03	40	
386	71-55-6	1,1,1-Trichloroethane	133.38	6	30	2.00E+03	40	
387	71-55-6	1,1,1-Trichloroethane	133.38	6	35	2.35E+03	40	
388	71-55-6	1,1,1-Trichloroethane	133.38	6	40	2.81E+03	40	
389	79-00-5	1,1,2-Trichloroethane	133.38	6	20	7.00E+01	40	
390	79-00-5	1,1,2-Trichloroethane	133.38	6	30	1.10E+02	40	
391	79-00-5	1,1,2-Trichloroethane	133.38	6	40	1.70E+02	40	
392	79-01-6	Trichloroethylene	131.38	6	20	7.00E+02	40	

Table 3. Physical constant data for chlorinated aliphatics

Table 3.a. Henry's law constant data, Pa m^3 / mol, chlorinated aliphatics

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
393	79-01-6	Trichloroethylene	131.38	6	30	1.14E+03	40	
394	79-01-6	Trichloroethylene	131.38	6	40	1.73E+03	40	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
395	2051-60-7	1	2-Chlorobiphenyl	188.7	1	25	5.76E+00	10	
396	2051-60-7	1	2-Chlorobiphenyl	188.7	1	25	5.76E+00	26	
397	2051-60-7	1	2-Chlorobiphenyl	188.7	4,9	25	5.06E+00	21	
398	2051-61-8	2	3-Chlorobiphenyl	188.7	1	25	4.77E+00	10	
399	2051-61-8	2	3-Chlorobiphenyl	188.7	1	25	6.22E+00	26	
400	2051-62-9	3	4-Chlorobiphenyl	188.7	1	25	7.66E-01	10	
401	2051-62-9	3	4-Chlorobiphenyl	188.7	1	25	1.87E+00	26	
402	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1	1	25	1.29E+00	10	
403	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1	4	25	1.21E+00	20	
404	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1	1	25	1.00E+00	26	
405	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1	2	20	1.12E+00	39	supercooled
406	16605-91-7	5	2,3-Dichlorobiphenyl	223.1	1	25	1.36E+00	10	
407	25569-80-6	6	2,3'-Dichlorobiphenyl	223.1	2	20	5.80E-01	39	supercooled
408	33284-50-3	7	2,4-Dichlorobiphenyl	223.1	1	25	1.07E+00	10	
409	33284-50-3	7	2,4-Dichlorobiphenyl	223.1	4	25	1.15E+00	20	
410	33284-50-3	7	2,4-Dichlorobiphenyl	223.1	1	25	2.03E+00	26	
411	33284-50-3	7	2,4-Dichlorobiphenyl	223.1	2	20	6.13E-01	39	supercooled
412	34883-43-7	8	2,4'-Dichlorobiphenyl	223.1	1	25	6.43E-01	10	
413	34883-43-7	8	2,4'-Dichlorobiphenyl	223.1	3,6	25	6.37E+02	9	
414	34883-43-7	8	2,4'-Dichlorobiphenyl	223.1	1	25	1.33E+00	26	
415	34883-43-7	8	2,4'-Dichlorobiphenyl	223.1	2	20	5.38E-01	39	supercooled
416	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	1	25	1.51E+00	10	
417	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	4	25	1.12E+00	20	
418	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	4,9	25	1.94E+00	21	
419	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	1	25	2.09E+00	26	
420	33146-45-1	10	2,6-Dichlorobiphenyl	223.1	1	25	2.57E+00	10	
421	33146-45-1	10	2,6-Dichlorobiphenyl	223.1	4,9	25	1.39E+00	21	
422	33146-45-1	10	2,6-Dichlorobiphenyl	223.1	4	25	2.40E+00	20	
423	2050-67-1	11	3,3'-Dichlorobiphenyl	223.1	1	25	7.12E-01	10	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
424	2050-67-1	11	3,3'-Dichlorobiphenyl	223.1	4	25	3.54E-01	20	
425	2974-92-7	12	3,4-Dichlorobiphenyl	223.1	1	25	3.99E-01	10	
426	2974-92-7	12	3,4-Dichlorobiphenyl	223.1	4	25	7.91E-03	20	
427	31883-41-5	14	3,5-Dichlorobiphenyl	223.1	1	25	6.47E-01	10	
428	2050-68-2	15	4,4'-Dichlorobiphenyl	223.1	1	25	2.41E-02	10	
429	2050-68-2	15	4,4'-Dichlorobiphenyl	223.1	4	25	3.63E-02	20	
430	2050-68-2	15	4,4'-Dichlorobiphenyl	223.1	1	25	1.04E-01	26	
431	2050-68-2	15	4,4'-Dichlorobiphenyl	223.1	2,6	24	6.20E-02	38	
432	38444-78-9	16	2,2',3-Trichlorobiphenyl	257.54	1	25	5.95E-01	10	
433	38444-78-9	16	2,2',3-Trichlorobiphenyl	257.54	2	20	2.93E-01	39	supercooled
434	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	1	25	4.48E-01	10	
435	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	3,6		2.48E+02	9	
436	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	4	25	5.09E-01	20	
437	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	1	25	4.07E-01	26	
438	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	2	20	2.99E-01	39	supercooled
439	38444-73-4	19	2,2',6-Trichlorobiphenyl	257.54	2	20	4.48E-04	39	supercooled
440	55702-46-0	21	2,3,4-Trichlorobiphenyl	257.54	1	25	4.82E-02	10	
441	38444-85-8	22	2,3,4'-Trichlorobiphenyl	257.54	1	25	6.95E-02	10	
442	38444-85-8	22	2,3,4'-Trichlorobiphenyl	257.54	2	20	1.42E-01	39	supercooled
443	55720-44-0	23	2,3,5-Trichlorobiphenyl	257.54	1	25	2.23E-01	10	
444	5872-45-9	24	2,3,6-Trichlorobiphenyl	257.54	2	20	1.23E-04	39	supercooled
445	38444-81-4	26	2,3',5-Trichlorobiphenyl	257.54	1	25	2.53E-01	10	
446	38444-81-4	26	2,3',5-Trichlorobiphenyl	257.54	4	25	2.51E-01	20	
447	38444-81-4	26	2,3',5-Trichlorobiphenyl	257.54	2	20	1.38E-01	39	supercooled
448	38444-76-7	27	2,3',6-Trichlorobiphenyl	257.54	2	20	3.86E-02	39	supercooled
449	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	1	25	8.86E-02	10	
450	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	4	25	1.17E-01	20	
451	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	1	25	2.66E-01	26	
452	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	2	20	1.43E-01	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
453	15862-07-4	29	2,4,5-Trichlorobiphenyl	257.54	1	25	8.34E-02	10	
454	15862-07-4	29	2,4,5-Trichlorobiphenyl	257.54	4,9	25	1.63E-01	21	
455	15862-07-4	29	2,4,5-Trichlorobiphenyl	257.54	1	25	1.93E-01	26	
456	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	4,6	4	8.04E-02	22	
457	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	1	25	2.01E-01	10	
458	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	4,9	25	2.26E-01	21	
459	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	4,6	25	1.87E-01	22	
460	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	4	25	2.43E-01	20	
461	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	4,6	40	4.35E-01	22	
462	16606-02-3	31	2,4',5-Trichlorobiphenyl	257.54	1	25	9.55E-02	10	
463	16606-02-3	31	2,4',5-Trichlorobiphenyl	257.54	2	20	1.43E-01	39	supercooled
464	38444-86-9	33	2',3,4-Trichlorobiphenyl	257.54	1	25	1.52E-01	10	
465	38444-86-9	33	2',3,4-Trichlorobiphenyl	257.54	1	25	2.91E-01	26	
466	38444-86-9	33	2',3,4-Trichlorobiphenyl	257.54	2	20	1.33E-01	39	supercooled
467	37680-68-5	34	2',3,5-Trichlorobiphenyl	257.54	1	25	2.05E-01	10	
468	38444-90-5	37	3,4,4'-Trichlorobiphenyl	257.54	1	25	2.86E-02	10	
469	38444-90-5	37	3,4,4'-Trichlorobiphenyl	257.54	1	25	1.35E-01	26	
470	38444-90-5	37	3,4,4'-Trichlorobiphenyl	257.54	2	20	7.19E-02	39	supercooled
471	16606-02-3	39	3,4',5-Trichlorobiphenyl	257.54	1	25	3.09E-02	10	
472	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99	1	25	1.29E-02	10	
473	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99	4	25	1.56E-02	20	
474	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99	1	25	2.62E-02	26	
475	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99	2	20	8.07E-02	39	supercooled
476	52663-59-9	41	2,2',3,4-Tetrachlorobiphenyl	291.99	2	20	6.48E-02	39	supercooled
477	36559-22-5	42	2,2',3,4'-Tetrachlorobiphenyl	291.99	1	25	3.33E-02	10	
478	36559-22-5	42	2,2',3,4'-Tetrachlorobiphenyl	291.99	2	20	6.08E-02	39	supercooled
479	70362-46-8	43	2,2',3,5-Tetrachlorobiphenyl	291.99	1	25	1.21E-01	26	
480	41464-39-5	44	2,2',3,5'-Tetrachlorobiphenyl	291.99	1	25	8.76E+05	10	
481	41464-39-5	44	2,2',3,5'-Tetrachlorobiphenyl	291.99	2	20	1.00E-01	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
482	41464-47-5	46	2,2',3,6'-Tetrachlorobiphenyl	291.99	1	25	2.79E-02	10	
483	41464-47-5	46	2,2',3,6'-Tetrachlorobiphenyl	291.99	2	20	1.06E-01	39	supercooled
484	2437-79-8	47	2,2',4,4'-Tetrachlorobiphenyl	291.99	1	25	4.96E-02	10	
485	2437-79-8	47	2,2',4,4'-Tetrachlorobiphenyl	291.99	1	25	1.15E-01	26	
486	41464-47-9	48	2,2',4,5-Tetrachlorobiphenyl	291.99	4,9	25	1.64E-02	21	
487	41464-47-9	48	2,2',4,5-Tetrachlorobiphenyl	291.99	2	20	3.00E-02	39	supercooled
488	41464-40-8	49	2,2',4,5'-Tetrachlorobiphenyl	291.99	1	25	4.09E-02	10	
489	41464-40-8	49	2,2',4,5'-Tetrachlorobiphenyl	291.99	2	20	7.81E-02	39	supercooled
490	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	1	25	3.33E-02	10	
491	35693-99-3	52	2,2',5,6'-Tetrachlorobiphenyl	291.99	3,6	25	4.60E+01	9	
492	35693-99-3	52	2,2',5,6'-Tetrachlorobiphenyl	291.99	4	25	1.10E-01	20	
493	35693-99-3	52	2,2',5,6'-Tetrachlorobiphenyl	291.99	1	25	4.13E-02	26	
494	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	2	20	1.13E-01	39	supercooled
495	41464-41-9	53	2,2',5,6'-Tetrachlorobiphenyl	291.99	1	25	5.20E-02	10	
496	41464-41-9	53	2,2',5,6'-Tetrachlorobiphenyl	291.99	4	25	4.76E-02	20	
497	41464-41-9	53	2,2',5,6'-Tetrachlorobiphenyl	291.99	2	20	1.09E-01	39	supercooled
498	15968-05-5	54	2,2',6,6'-Tetrachlorobiphenyl	291.99	1	25	1.44E-02	10	
499	15968-05-5	54	2,2',6,6'-Tetrachlorobiphenyl	291.99	4	25	1.19E-02	20	
500	41464-43-9	56	2,3,3',4'-Tetrachlorobiphenyl	291.99	1	25	1.15E-02	10	
501	41464-43-9	56	2,3,3',4'-Tetrachlorobiphenyl	291.99	2	20	3.89E-02	39	supercooled
502	41464-49-7	58	2,3,3',5'-Tetrachlorobiphenyl	291.99	1	25	5.58E-03	10	
503	33025-41-1	60	2,3,4,4'-Tetrachlorobiphenyl	291.99	1	25	2.74E-03	10	
504	33025-41-1	60	2,3,4,4'-Tetrachlorobiphenyl	291.99	2	20	3.89E-02	39	supercooled
505	33284-53-6	61	2,3,4,5-Tetrachlorobiphenyl	291.99	1	25	4.32E-02	10	
506	33284-53-6	61	2,3,4,5-Tetrachlorobiphenyl	291.99	4,9	25	2.09E-02	21	
507	33284-53-6	61	2,3,4,5-Tetrachlorobiphenyl	291.99	1	25	5.28E-02	26	
508	74472-34-7	63	2,3,4',5-Tetrachlorobiphenyl	291.99	1	25	7.15E-03	10	
509	74472-34-7	63	2,3,4',5-Tetrachlorobiphenyl	291.99	2	20	2.63E-02	39	supercooled
510	52663-58-8	64	2,3,4',6-Tetrachlorobiphenyl	291.99	2	20	9.37E-02	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
511	33284-54-7	65	2,3,5,6-Tetrachlorobiphenyl	291.99	1	25	1.80E-02	10	
512	33284-54-7	65	2,3,5,6-Tetrachlorobiphenyl	291.99	4	25	1.40E-02	20	
513	32598-10-0	66	2,3',4,4'-Tetrachlorobiphenyl	291.99	1	25	4.47E-03	10	
514	32598-10-0	66	2,3',4,4'-Tetrachlorobiphenyl	291.99	1	25	1.68E-02	26	
515	32598-10-0	66	2,3',4,4'-Tetrachlorobiphenyl	291.99	2	20	3.68E-02	39	supercooled
516	32598-11-1	70	2,3',4',5-Tetrachlorobiphenyl	291.99	1	25	1.11E-02	10	
517	32598-11-1	70	2,3',4',5-Tetrachlorobiphenyl	291.99	1	25	2.90E-02	26	
518	32598-11-1	70	2,3',4',5-Tetrachlorobiphenyl	291.99	2	20	3.62E-02	39	supercooled
519	41464-42-0	72	2,3',5,5'-Tetrachlorobiphenyl	291.99	1	25	1.07E-02	10	
520	32690-93-0	74	2,4,4',5-Tetrachlorobiphenyl	291.99	1	25	4.53E-03	10	
521	32690-93-0	74	2,4,4',5-Tetrachlorobiphenyl	291.99	2	20	3.06E-02	39	supercooled
522	32598-12-2	75	2,4,4',6-Tetrachlorobiphenyl	291.99	4	25	9.10E-02	20	
523	70362-48-0	76	2',3,4,5-Tetrachlorobiphenyl	291.99	2	20	5.51E-02	39	supercooled
524	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	1	25	9.78E-04	10	
525	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	4,6	4	1.46E-04	11	
526	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	4,6	20	4.35E-04	11	
527	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	4,6	25	5.69E-04	11	
528	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	4,6	32	1.18E-03	11	
529	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	4	25	5.50E-04	20	
530	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	1	25	1.74E-02	26	
531	41464-48-6	79	3,3',4,5'-Tetrachlorobiphenyl	291.99	1	25	3.59E-03	10	
532	33284-52-5	80	3,3',5,5'-Tetrachlorobiphenyl	291.99	1	25	1.21E-03	10	
533	33284-52-5	80	3,3',5,5'-Tetrachlorobiphenyl	291.99	4	25	1.24E-03	20	
534	70362-50-4	81	3,4,4',5-Tetrachlorobiphenyl	291.99	2	20	0.00E+00	39	supercooled
535	52663-62-4	82	2,2',3,3',4-Pentachlorobiphenyl	326.43	1	25	2.80E-03	10	
536	52663-62-4	82	2,2',3,3',4-Pentachlorobiphenyl	326.43	2	20	2.91E-02	39	supercooled
537	60145-20-2	83	2,2',3,3',5-Pentachlorobiphenyl	326.43	2	20	2.82E-02	39	supercooled
538	52663-60-2	84	2,2',3,3',6-Pentachlorobiphenyl	326.43	2	20	4.70E-02	39	supercooled
539	65510-45-4	85	2,2',3,4,4'-Pentachlorobiphenyl	326.43	2	20	2.19E-02	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
540	55312-69-1	86	2,2',3,4,5-Pentachlorobiphenyl	326.43	1	25	1.33E-02	26	
541	38380-02-8	87	2,2',3,4,5'-Pentachlorobiphenyl	326.43	1	25	3.53E-03	10	
542	38380-02-8	87	2,2',3,4,5'-Pentachlorobiphenyl	326.43	1	25	8.60E-03	26	
543	38380-02-8	87	2,2',3,4,5'-Pentachlorobiphenyl	326.43	2	20	2.94E-02	39	supercooled
544	68194-05-8	91	2,2',3,4',6-Pentachlorobiphenyl	326.43	2	20	3.95E-02	39	supercooled
545	38379-99-6	95	2,2',3,5',6-Pentachlorobiphenyl	326.43	1	25	1.10E-02	10	
546	38379-99-6	95	2,2',3,5',6-Pentachlorobiphenyl	326.43	2	20	5.41E-02	39	supercooled
547	41464-51-1	97	2,2',3',4,5-Pentachlorobiphenyl	326.43	1	25	8.45E-03	10	
548	41464-51-1	97	2,2',3',4,5-Pentachlorobiphenyl	326.43	2	20	2.84E-02	39	supercooled
549	60233-25-2	98	2,2',3,4,6-Pentachlorobiphenyl	326.43	1	25	1.29E-02	26	
550	38380-01-7	99	2,2',4,4',5-Pentachlorobiphenyl	326.43	2	20	2.22E-02	39	supercooled
551	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	1	25	9.40E-03	10	
552	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	3,6		1.03E+01	9	
553	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	4,6	4	6.14E-03	11	
554	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	4,6	20	1.21E-02	11	
555	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	4,6	25	1.54E-02	11	
556	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	4,6	32	2.23E-02	11	
557	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	4,9	25	1.93E-02	21	
558	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	4	25	6.74E-03	20	
559	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	1	25	1.63E-02	26	
560	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	2	20	2.63E-02	39	supercooled
561	56558-16-8	104	2,2',4,6,6'-Pentachlorobiphenyl	326.43	4	25	1.56E-02	20	
562	32598-14-4	105	2,3,3',4,4'-Pentachlorobiphenyl	326.43	1	25	1.90E-03	10	
563	70424-68-9	107	2,3,3',4',5-Pentachlorobiphenyl	326.43	2	20	1.48E-02	39	supercooled
564	38380-03-9	110	2,3,3',4',6-Pentachlorobiphenyl	326.43	2	20	2.88E-02	39	supercooled
565	74472-37-0	114	2,3,4,4',5-Pentachlorobiphenyl	326.43	1	25	2.46E-03	10	
566	74472-37-0	114	2,3,4,4',5-Pentachlorobiphenyl	326.43	2	20	1.60E-02	39	supercooled
567	18259-05-7	116	2,3,4,5,6-Pentachlorobiphenyl	326.43	1	25	4.34E-03	10	
568	18259-05-7	116	2,3,4,5,6-Pentachlorobiphenyl	326.43	4,9	25	5.48E-03	21	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
569	18259-05-7	116	2,3,4,5,6-Pentachlorobiphenyl	326.43	4	25	4.01E-03	20	
570	18259-05-7	116	2,3,4,5,6-Pentachlorobiphenyl	326.43	1	25	9.04E-03	26	
571	31508-0-6	118	2,3',4,4',5-Pentachlorobiphenyl	326.43	1	25	1.99E-03	10	
572	31508-0-6	118	2,3',4,4',5-Pentachlorobiphenyl	326.43	2	20	1.34E-02	39	supercooled
573	76842-07-4	122	2',3,3',4,5-Pentachlorobiphenyl	326.43	2	20	1.28E-02	39	supercooled
574	70424-70-3	124	2'[,3,4,5,5'-Pentachlorobiphenyl	326.43	2	20	1.58E-02	39	supercooled
575	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	1	25	2.93E-04	10	
576	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	4,9	25	2.83E-04	21	
577	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	4	25	2.30E-03	20	
578	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	1	25	1.32E-03	26	
579	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	2	20	6.70E-03	39	supercooled
580	55215-18-4	129	2,2',3,3',4,5-Hexachlorobiphenyl	360.88	4	25	5.82E-03	20	
581	55215-18-4	129	2,2',3,3',4,5-Hexachlorobiphenyl	360.88	1	25	5.81E-03	26	
582	55215-18-4	129	2,2',3,3',4,5-Hexachlorobiphenyl	360.88	2	20	1.17E-02	39	supercooled
583	52663-66-8	130	2,2',3,3',4,5'-Hexachlorobiphenyl	360.88	2	20	5.69E-03	39	supercooled
584	52663-60-2	131	2,2',3,3',4,6-Hexachlorobiphenyl	360.88	2	20	1.21E-02	39	supercooled
585	35694-4-3	133	2,2',3,3',5,5'-Hexachlorobiphenyl	360.88	1	25	4.37E-04	10	
586	35694-4-3	133	2,2',3,3',5,5'-Hexachlorobiphenyl	360.88	1	25	3.99E-03	26	
587	52704-70-8	134	2,2',3,3',5,6-Hexachlorobiphenyl	360.88	2	20	1.30E-02	39	supercooled
588	52744-13-5	135	2,2',3,3',5,6'-Hexachlorobiphenyl	360.88	2	20	1.29E-02	39	supercooled
589	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	1	25	3.79E-03	10	
590	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	4,6	4	1.10E-03	11	
591	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	4,6	20	3.25E-03	11	
592	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	4,6	25	4.51E-03	11	
593	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	4,9	25	6.03E-03	21	
594	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	4,6	32	6.68E-03	11	
595	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	2	20	2.02E-02	39	supercooled
596	35694-6-5	137	2,2',3,4,4',5-Hexachlorobiphenyl	360.88	1	25	1.71E-03	10	
597	35694-6-5	137	2,2',3,4,4',5-Hexachlorobiphenyl	360.88	2	20	8.40E-03	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
598	35065-28-2	138	2,2',3,4,4',5'-Hexachlorobiphenyl	360.88	1	25	1.52E-03	10	
599	35065-28-2	138	2,2',3,4,4',5'-Hexachlorobiphenyl	360.88	2	20	7.29E-03	39	supercooled
600	35065-28-2	140	2,2',3,4,4',5'-Hexachlorobiphenyl	360.88	1	25	3.24E-03	10	
601	52712-04-6	141	2,2',3,4,5,5'-Hexachlorobiphenyl	360.9	2	20	7.55E-03	39	supercooled
602	41411-61-4	142	2,2',3,4,5,6-Hexachlorobiphenyl	360.88	1	25	1.37E-03	10	
603	68194-14-9	144	2,2',3,4,5',6-Hexachlorobiphenyl	360.88	2	20	1.29E-02	39	supercooled
604	74472-40-5	145	2,2',3,4,6,6'-Hexachlorobiphenyl	360.88	2	20	0.00E+00	39	supercooled
605	51908-16-8	146	2,2',3,4',5,5'-Hexachlorobiphenyl	360.88	2	20	7.59E-03	39	supercooled
606	38380-04-0	149	2,2',3,4',5',6-Hexachlorobiphenyl	360.88	2	20	1.22E-02	39	supercooled
607	52663-63-5	151	2,2',3,5,5',6-Hexachlorobiphenyl	360.88	1	25	2.23E-03	10	
608	52663-63-5	151	2,2',3,5,5',6-Hexachlorobiphenyl	360.88	2	20	1.36E-02	39	supercooled
609	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	4,6	4	4.62E-03	22	
610	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	1	25	8.84E-04	10	
611	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	4,6	25	8.44E-03	22	
612	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	3,6	25	9.53E-01	9	
613	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	4	25	8.60E-04	20	
614	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	4,6	40	1.28E-02	22	
615	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	1	25	2.78E-03	26	
616	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	2	20	9.14E-03	39	supercooled
617	33979-03-2	155	2,2',4,4',6,6'-Hexachlorobiphenyl	360.88	1	25	2.27E-03	10	
618	33979-03-2	155	2,2',4,4',6,6'-Hexachlorobiphenyl	360.88	4,9	25	4.08E-04	21	
618	33979-03-2	155	2,2',4,4',6,6'-Hexachlorobiphenyl	360.88	4	25	2.30E-03	20	
619	33979-03-2	155	2,2',4,4',6,6'-Hexachlorobiphenyl	360.88	1	25	2.04E-03	26	
620	38380-08-4	156	2,,3,3',4,4',5-Hexachlorobiphenyl	360.88	2	20	5.33E-03	39	supercooled
621	74472-42-7	158	2,,3,3',4,4',6-Hexachlorobiphenyl	360.88	2	20	8.07E-03	39	supercooled
622	41411-62-5	160	2,3,3',4,5,6-Hexachlorobiphenyl	360.88	1	25	1.58E-03	10	
623	41411-63-6	166	2,3,4,4',5,6-Hexachlorobiphenyl	360.88	1	25	2.46E-04	10	
624	52663-72-6	167	2,3',4,4',5,5'-Hexachlorobiphenyl	360.88	2	20	0.00E+00	39	supercooled
625	59291-65-6	168	2,3',4,4',5',6-Hexachlorobiphenyl	360.88	1	25	9.74E-04	10	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
626	32774-16-6	169	3,3',4,4',5,5'-Hexachlorobiphenyl	360.88	1	25	4.19E-05	10	
627	35065-30-6	170	2,2',3,3',4,4',5-Heptachlorobiphenyl	395.32	1	25	1.19E-04	10	
628	35065-30-6	170	2,2',3,3',4,4',5-Heptachlorobiphenyl	395.32	2	20	3.47E-03	39	supercooled
629	52663-71-5	171	2,2',3,3',4,4',6-Heptachlorobiphenyl	395.32	4,9	25	2.17E-03	21	
630	52663-71-5	171	2,2',3,3',4,4',6-Heptachlorobiphenyl	395.32	2	20	4.12E-03	39	supercooled
631	52663-74-8	172	2,2',3,3',4,5,5'-Heptachlorobiphenyl	395.32	2	20	4.30E-03	39	supercooled
632	68194-16-1	173	2,2',3,3',4,5,6-Heptachlorobiphenyl	395.32	2	20	4.16E-03	39	supercooled
633	40186-70-7	174	2,2',3,3',4,5,6'-Heptachlorobiphenyl	395.32	1	25	3.19E-04	10	
634	40186-70-7	174	2,2',3,3',4,5,6'-Heptachlorobiphenyl	395.32	2	20	5.25E-03	39	supercooled
635	40186-70-7	175	2,2',3,3',4,5',6-Heptachlorobiphenyl	395.32	2	20	8.94E-03	39	supercooled
636	52663-65-7	176	2,2',3,3',4,6,6'-Heptachlorobiphenyl	395.32	2	20	5.85E-03	39	supercooled
637	52663-70-4	177	2,2',3,3',4',5,6-Heptachlorobiphenyl	395.32	2	20	4.82E-03	39	supercooled
638	52663-67-9	178	2,2',3,3',5,5'6-Heptachlorobiphenyl	395.32	2	20	8.84E-03	39	supercooled
639	35065-29-3	180	2,2',3,4,4',5,5'-Heptachlorobiphenyl	395.32	1	25	2.25E-04	10	
640	35065-29-3	180	2,2',3,4,4',5,5'-Heptachlorobiphenyl	395.32	2	20	3.85E-03	39	supercooled
641	74472-47-2	182	2,2',3,4,4',5,6'-Heptachlorobiphenyl	395.32	1	25	1.36E-04	10	
642	52663-69-1	183	2,2',3,4,4',5',6-Heptachlorobiphenyl	395.32	2	20	4.90E-03	39	supercooled
643	52712-05-7	185	2,2',3,4,5,5',6-Heptachlorobiphenyl	395.32	1	25	1.93E-04	10	
644	52712-05-7	185	2,2',3,4,5,5',6-Heptachlorobiphenyl	395.32	1	25	4.02E-04	26	
645	52712-05-7	185	2,2',3,4,5,5',6-Heptachlorobiphenyl	395.32	2	20	5.46E-03	39	supercooled
646	52663-68-0	187	2,2',3,4',5,5',6-Heptachlorobiphenyl	395.32	2	20	4.51E-03	39	supercooled
647	39635-31-9	189	2,3,3',4,4',5,5'-Heptachlorobiphenyl	395.32	1	25	4.47E-05	10	
648	39635-31-9	189	2,3,3',4,4',5,5'-Heptachlorobiphenyl	395.32	2	20	0.00E+00	39	supercooled
649	41411-64-7	190	2,3,3',4,4',5,6-Heptachlorobiphenyl	395.32	1	25	2.20E-04	10	
650	74472-50-7	191	2,3,3',4,4',5',6-Heptachlorobiphenyl	395.32	2	20	0.00E+00	39	supercooled
651	69782-91-8	193	2,3,3',4',5,5',6-Heptachlorobiphenyl	395.32	2	20	0.00E+00	39	supercooled
652	35694-08-7	194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	429.77	1	25	2.11E-05	10	
653	35694-08-7	194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	429.77	1	25	1.01E-04	26	
654	35694-08-7	194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	429.77	2	20	0.00E+00	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
655	52663-78-2	195	2,2',3,3',4,4',5,6-Octachlorobiphenyl	429.77	2	20	0.00E+00	39	supercooled
656	33091-17-7	197	2,2',3,3',4,4',6,6'-Octachlorobiphenyl	429.77	1	25	1.03E-04	10	
657	68194-17-2	198	2,2',3,3',4,5,5',6-Octachlorobiphenyl	429.77	2	20	0.00E+00	39	supercooled
658	2136-99-4	201	2,2',3,3',4,5',6,6'-Octachlorobiphenyl	429.77	2	20	0.00E+00	39	supercooled
659	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	1	25	4.56E-05	10	
660	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	4,6	20	1.14E-04	11	
661	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	4,6	25	1.47E-04	11	
662	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	4,9	25	3.93E-04	21	
663	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	4,6	32	2.12E-04	11	
664	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	4,6	50	7.65E-04	11	
665	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	1	25	8.80E-05	26	
666	52663-76-0	203	2,2',3,4,4',5,5',6-Octachlorobiphenyl	429.77	2	20	0.00E+00	39	supercooled
667	74472-53-0	205	2,3,3',4,4',5,5',6-Octachlorobiphenyl	429.77	2	20	0.00E+00	39	supercooled
668	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	1	25	2.66E-06	10	
669	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	4,6	25	2.54E-05	11	
670	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	4,6	32	5.08E-05	11	
671	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	4,6	40	6.56E-05	11	
672	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	4,6	50	1.31E-04	11	
673	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	1	25	1.20E-05	26	
674	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	2	20	0.00E+00	39	supercooled
675	52663-79-3	207	2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	462.21	2	20	0.00E+00	39	supercooled
676	52663-77-1	208	2,2',3,3',4,5,5',6,6'-Nanochlorobiphenyl	462.21	4,9	25	1.79E-05	21	
677	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	1	25	1.26E-07	10	
678	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	4,6	25	6.48E-07	11	
679	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	4,9	25	7.43E-06	21	
680	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	4,6	60	8.38E-06	11	
681	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	4,6	70	1.76E-05	11	
682	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	4,6	80	4.95E-05	11	
683	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	1	25	4.00E-07	26	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.a. Aqueous solubility data, mg / L, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase

[1] PCB congeners are numbered according to method proposed by Ballschmitter and Zell (1980) and later revised by Schulte and Malisch (1983) to be conducive with IUPAC guidelines. (Ballschmitter, K.; Zell, M. *Fresenius Z. Anal. Chem.* **1980,** *302,* 20-31; Schulte, E.; Malisch, R. *Fresenius Z. Anal. Chem.* **1983,** *314,* 545-551).

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.b. Vapor pressure data, Pa, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
684	2051-62-9	3	4-Chlorobiphenyl	188.7	5	4.2	1.11E-02	15	
685	2051-62-9	3	4-Chlorobiphenyl	188.7	5	15	4.93E-02	15	
686	2051-62-9	3	4-Chlorobiphenyl	188.7	5	24.9	1.72E-01	15	
687	2051-62-9	3	4-Chlorobiphenyl	188.7	5	25	1.75E-01	15	
688	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1	1	25	1.84E-01	20	solid
689	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1		20	1.50E-01	39	supercooled
690	25569-80-6	6	2,3'-Dichlorobiphenyl	223.1		20	7.89E-02	39	supercooled
691	33284-50-3	7	2,4-Dichlorobiphenyl	223.1		20	9.87E-02	39	supercooled
692	34883-43-7	8	2,4'-Dichlorobiphenyl	223.1		20	6.76E-02	39	supercooled
693	2050-67-1	11	3,3'-Dichlorobiphenyl	223.1	1	25	3.76E-02	20	solid
694	2974-92-7	12	3,4-Dichlorobiphenyl	223.1	1	25	7.36E-04	20	solid
695	2050-68-2	15	4,4'-Dichlorobiphenyl	223.1	1	25	3.28E-03	20	solid
696	38444-78-9	16	2,2',3-Trichlorobiphenyl	257.54		20	2.72E-02	39	supercooled
697	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54		20	3.47E-02	39	supercooled
698	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	1	25	7.62E-02	20	solid
699	38444-73-4	19	2,2',6-Trichlorobiphenyl	257.54		20	5.22E-02	39	supercooled
700	38444-85-8	22	2,3,4'-Trichlorobiphenyl	257.54		20	1.10E-02	39	supercooled
701	5872-45-9	24	2,3,6-Trichlorobiphenyl	257.54		20	1.64E-02	39	supercooled
702	38444-81-4	26	2,3',5-Trichlorobiphenyl	257.54		20	1.80E-02	39	supercooled
703	38444-81-4	26	2,3',5-Trichlorobiphenyl	257.54	1	25	3.23E-02	20	solid
704	38444-76-7	27	2,3',6-Trichlorobiphenyl	257.54		20	4.20E-03	39	supercooled
705	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54		20	1.47E-02	39	supercooled
706	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	1	25	1.45E-02	20	solid
707	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	1	25	6.44E-02	20	solid
708	16606-02-3	31	2,4',5-Trichlorobiphenyl	257.54		20	1.47E-02	39	supercooled
709	38444-86-9	33	2',3,4-Trichlorobiphenyl	257.54		20	1.17E-02	39	supercooled
710	38444-86-9	33	2',3,4-Trichlorobiphenyl	257.54	5	25	1.33E-02	18	
711	38444-86-9	33	2',3,4-Trichlorobiphenyl	257.54	5	30	1.73E-02	18	
712	38444-90-5	37	3,4,4'-Trichlorobiphenyl	257.54		20	4.48E-03	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.b. Vapor pressure data, Pa, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
713	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99		20	4.46E-03	39	supercooled
714	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99	1	25	1.09E-03	20	solid
715	52663-59-9	41	2,2',3,4-Tetrachlorobiphenyl	292		20	4.53E-03	39	supercooled
716	36559-22-5	42	2,2',3,4'-Tetrachlorobiphenyl	291.99		20	4.14E-03	39	supercooled
717	41464-39-5	44	2,2',3,5'-Tetrachlorobiphenyl	291.99		20	6.31E-03	39	supercooled
718	41464-47-5	46	2,2',3,6'-Tetrachlorobiphenyl	291.99		20	8.94E-03	39	supercooled
719	41464-47-9	48	2,2',4,5-Tetrachlorobiphenyl	291.99		20	2.62E-03	39	supercooled
720	41464-40-8	49	2,2',4,5'-Tetrachlorobiphenyl	291.99		20	7.33E-03	39	supercooled
721	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99		20	8.92E-03	39	supercooled
722	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	5	25	2.53E-03	18	
723	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	5	30	4.80E-03	18	
724	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	1	25	1.30E-02	20	solid
725	41464-41-9	53	2,2',5,6'-Tetrachlorobiphenyl	291.99		20	1.05E-02	39	supercooled
726	41464-41-9	53	2,2',5,6'-Tetrachlorobiphenyl	291.99	1	25	6.71E-03	20	solid
727	15968-05-5	54	2,2',6,6'-Tetrachlorobiphenyl	291.99	1	25	2.27E-03	20	solid
728	41464-43-9	56	2,3,3',4'-Tetrachlorobiphenyl	291.99		20	2.14E-03	39	supercooled
729	33025-41-1	60	2,3,4,4'-Tetrachlorobiphenyl	291.99		20	2.14E-03	39	supercooled
730	74472-34-7	63	2,3,4',5-Tetrachlorobiphenyl	291.99		20	2.60E-03	39	supercooled
731	52663-58-8	64	2,3,4',6-Tetrachlorobiphenyl	291.99		20	5.44E-03	39	supercooled
732	32598-10-0	66	2,3',4,4'-Tetrachlorobiphenyl	291.99		20	2.48E-03	39	supercooled
733	32598-11-1	70	2,3',4',5-Tetrachlorobiphenyl	291.99		20	2.33E-03	39	supercooled
734	32690-93-0	74	2,4,4',5-Tetrachlorobiphenyl	291.99		20	2.09E-03	39	supercooled
735	70362-48-0	76	2',3,4,5-Tetrachlorobiphenyl	291.99		20	2.41E-03	39	supercooled
736	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	1	25	1.82E-05	20	solid
737	70362-50-4	81	3,4,4',5-Tetrachlorobiphenyl	291.99		20	0.00E+00	39	supercooled
738	52663-62-4	82	2,2',3,3',4-Pentachlorobiphenyl	326.43		20	1.04E-03	39	supercooled
739	60145-20-2	83	2,2',3,3',5-Pentachlorobiphenyl	326.43		20	1.52E-03	39	supercooled
740	52663-60-2	84	2,2',3,3',6-Pentachlorobiphenyl	326.43		20	2.51E-03	39	supercooled
741	65510-45-4	85	2,2',3,4,4'-Pentachlorobiphenyl	326.43		20	1.10E-03	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.b. Vapor pressure data, Pa, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
742	38380-02-8	87	2,2',3,4,5'-Pentachlorobiphenyl	326.43		20	1.15E-03	39	supercooled
743	68194-05-8	91	2,2',3,4',6-Pentachlorobiphenyl	326.43		20	3.28E-03	39	supercooled
744	38379-99-6	95	2,2',3,5',6-Pentachlorobiphenyl	326.43		20	3.31E-03	39	supercooled
745	41464-51-1	97	2,2',3',4,5-Pentachlorobiphenyl	326.43		20	1.29E-03	39	supercooled
746	38380-01-7	99	2,2',4,4',5-Pentachlorobiphenyl	326.43		20	1.45E-03	39	supercooled
747	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43		20	1.44E-03	39	supercooled
748	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	5	25	9.60E-04	18	
749	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	5	30	1.73E-03	18	
750	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	1	25	5.27E-04	20	
751	56558-16-8	104	2,2',4,6,6'-Pentachlorobiphenyl	326.43	1	25	4.34E-03	20	solid
752	70424-68-9	107	2,3,3',4',5-Pentachlorobiphenyl	326.43		20	2.58E-04	39	supercooled
753	38380-03-9	110	2,3,3',4',6-Pentachlorobiphenyl	326.43		20	9.36E-04	39	supercooled
754	74472-37-0	114	2,3,4,4',5-Pentachlorobiphenyl	326.43		20	3.40E-04	39	supercooled
755	31508-0-6	118	2,3',4,4',5-Pentachlorobiphenyl	326.43		20	3.50E-04	39	supercooled
756	76842-07-4	122	2',3,3',4,5-Pentachlorobiphenyl	326.43		20	3.17E-04	39	supercooled
757	70424-70-3	124	2'[,3,4,5,5'-Pentachlorobiphenyl	326.43		20	2.57E-04	39	supercooled
758	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88		20	9.70E-05	39	supercooled
759	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	1	25	2.94E-06	20	solid
760	55215-18-4	129	2,2',3,3',4,5-Hexachlorobiphenyl	360.88		20	0.00E+00	39	supercooled
761	52663-66-8	130	2,2',3,3',4,5'-Hexachlorobiphenyl	360.88		20	1.59E-04	39	supercooled
762	52663-60-2	131	2,2',3,3',4,6-Hexachlorobiphenyl	360.88		20	2.60E-04	39	supercooled
763	52704-70-8	134	2,2',3,3',5,6-Hexachlorobiphenyl	360.88		20	3.53E-04	39	supercooled
764	52744-13-5	135	2,2',3,3',5,6'-Hexachlorobiphenyl	360.88		20	5.00E-04	39	supercooled
765	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88		20	1.26E-03	39	supercooled
766	35694-6-5	137	2,2',3,4,4',5-Hexachlorobiphenyl	360.88		20	1.48E-04	39	supercooled
767	35065-28-2	138	2,2',3,4,4',5'-Hexachlorobiphenyl	360.88		20	1.45E-04	39	supercooled
768	52712-04-6	141	2,2',3,4,5,5'-Hexachlorobiphenyl	360.88		20	2.02E-04	39	supercooled
769	68194-14-9	144	2,2',3,4,5',6-Hexachlorobiphenyl	360.88		20	5.00E-04	39	supercooled
770	74472-40-5	145	2,2',3,4,6,6'-Hexachlorobiphenyl	360.88		20	0.00E+00	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.b. Vapor pressure data, Pa, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
771	51908-16-8	146	2,2',3,4',5,5'-Hexachlorobiphenyl	360.88		20	1.85E-04	39	supercooled
772	38380-04-0	149	2,2',3,4',5',6-Hexachlorobiphenyl	360.88		20	4.90E-04	39	supercooled
773	52663-63-5	151	2,2',3,5,5',6-Hexachlorobiphenyl	360.88		20	5.89E-04	39	supercooled
774	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88		20	2.50E-04	39	supercooled
775	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	1	25	3.24E-05	20	solid
776	33979-03-2	155	2,2',4,4',6,6'-Hexachlorobiphenyl	360.88	1	25	4.80E-04	20	solid
777	38380-08-4	156	2,,3,3',4,4',5-Hexachlorobiphenyl	360.88		20	0.00E+00	39	supercooled
778	74472-42-7	158	2,,3,3',4,4',6-Hexachlorobiphenyl	360.88		20	9.60E-05	39	supercooled
779	52663-72-6	167	2,3',4,4',5,5'-Hexachlorobiphenyl	360.88		20	0.00E+00	39	supercooled
780	35065-30-6	170	2,2',3,3',4,4',5-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
781	52663-71-5	171	2,2',3,3',4,4',6-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
782	52663-74-8	172	2,2',3,3',4,5,5'-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
783	68194-16-1	173	2,2',3,3',4,5,6-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
784	40186-70-7	174	2,2',3,3',4,5,6'-Heptachlorobiphenyl	395.32		20	6.50E-05	39	supercooled
785	40186-70-7	175	2,2',3,3',4,5',6-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
786	52663-65-7	176	2,2',3,3',4,6,6'-Heptachlorobiphenyl	395.32		20	1.33E-04	39	supercooled
787	52663-70-4	177	2,2',3,3',4',5,6-Heptachlorobiphenyl	395.32		20	4.10E-05	39	supercooled
788	52663-67-9	178	2,2',3,3',5,5'6-Heptachlorobiphenyl	395.32		20	1.45E-04	39	supercooled
789	35065-29-3	180	2,2',3,4,4',5,5'-Heptachlorobiphenyl	395.32		20	3.10E-05	39	supercooled
790	52663-69-1	183	2,2',3,4,4',5',6-Heptachlorobiphenyl	395.32		20	8.50E-05	39	supercooled
791	52712-05-7	185	2,2',3,4,5,5',6-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
792	52663-68-0	187	2,2',3,4',5,5',6-Heptachlorobiphenyl	395.32		20	9.30E-05	39	supercooled
793	39635-31-9	189	2,3,3',4,4',5,5'-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
794	74472-50-7	191	2,3,3',4,4',5',6-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
795	69782-91-8	193	2,3,3',4',5,5',6-Heptachlorobiphenyl	395.32		20	0.00E+00	39	supercooled
796	35694-08-7	194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	429.77		20	0.00E+00	39	supercooled
797	52663-78-2	195	2,2',3,3',4,4',5,6-Octachlorobiphenyl	429.77		20	0.00E+00	39	supercooled
798	68194-17-2	198	2,2',3,3',4,5,5',6-Octachlorobiphenyl	429.77		20	0.00E+00	39	supercooled
799	2136-99-4	201	2,2',3,3',4,5',6,6'-Octachlorobiphenyl	429.77		20	0.00E+00	39	supercooled

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.b. Vapor pressure data, Pa, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
800	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	5	29	4.95E-05	15	
801	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	5	25	2.90E-10	15	
802	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	5	39.9	2.24E-04	15	
803	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	5	50	5.83E-04	15	
804	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	5	61.2	2.65E-03	15	
805	52663-76-0	203	2,2',3,4,4',5,5',6-Octachlorobiphenyl	429.77		20	0.00E+00	39	supercooled
806	74472-53-0	205	2,3,3',4,4',5,5',6-Octachlorobiphenyl	429.77		20	0.00E+00	39	supercooled
807	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21		20	0.00E+00	39	supercooled
808	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	4	89.8	3.36E-04	15	
809	52663-79-3	207	2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	462.21		20	0.00E+00	39	supercooled
810	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	5	25	5.30E-08	15	
811	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	5	50.7	2.69E-06	15	
812	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	5	64.9	1.68E-05	15	
813	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	5	72.3	4.00E-05	15	
814	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	5	80.5	1.43E-04	15	
815	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	5	85.2	1.88E-04	15	

[1] PCB congeners are numbered according to method proposed by Ballschmitter and Zell (1980) and later revised by Schulte and Malisch (1983) to be conducive with IUPAC guidelines. (Ballschmitter, K.; Zell, M. *Fresenius Z. Anal. Chem.* **1980,** *302,* 20-31; Schulte, E.; Malisch, R. *Fresenius Z. Anal. Chem.* **1983,** *314,* 545-551).

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.c. Henry's law constant data, Pa m^3 / mol, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
816	2051-60-7	1	2-Chlorobiphenyl	188.7	1	25	3.02E+01	10	
817	2051-61-8	2	3-Chlorobiphenyl	188.7	1	25	2.90E+01	10	
818	2051-62-9	3	4-Chlorobiphenyl	188.7	1	25	2.78E+01	10	
819	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1	1	25	3.33E+01	10	
820	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1	2	25	3.41E+01	20;27	
821	13029-08-8	4	2,2'-Dichlorobiphenyl	223.1	4	25	2.48E+01	33	
822	16605-91-7	5	2,3-Dichlorobiphenyl	223.1	1	25	2.42E+01	10	
823	25569-80-6	6	2,3'-Dichlorobiphenyl	223.1	1	25	3.31E+01	10	
824	25569-80-6	6	2,3'-Dichlorobiphenyl	223.1	6	25	2.50E+01	35	
825	33284-50-3	7	2,4-Dichlorobiphenyl	223.1	1	25	3.82E+01	10	
826	34883-43-7	8	2,4'-Dichlorobiphenyl	223.1	1	25	3.07E+01	10	
827	34883-43-7	8	2,4'-Dichlorobiphenyl	223.1	2	23	9.60E+01	50	distilled water
828	34883-43-7	8	2,4'-Dichlorobiphenyl	223.1	2	23	1.95E+02	50	seawater
827	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	1	25	3.28E+01	10	
828	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	2	25	3.93E+01	20;27	
829	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	4	10.4	1.61E+01	36	
830	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	4	20	2.96E+01	36	
831	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	4	30.1	5.82E+01	36	
832	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	4	34.9	8.22E+01	36	
833	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	4	42.1	1.23E+02	36	
834	34883-39-1	9	2,5-Dichlorobiphenyl	223.1	4	47.9	1.65E+02	36	
835	33146-45-1	10	2,6-Dichlorobiphenyl	223.1	1	25	4.30E+01	10	
836	2050-67-1	11	3,3'-Dichlorobiphenyl	223.1	1	25	2.94E+01	10	
837	2050-67-1	11	3,3'-Dichlorobiphenyl	223.1	2	25	2.36E+01	20;27	
838	2974-92-7	12	3,4-Dichlorobiphenyl	223.1	1	25	2.37E+01	10	
839	2974-92-7	12	3,4-Dichlorobiphenyl	223.1	2	25	2.08E+01	20;27	
840	2974-92-7	12	3,4-Dichlorobiphenyl	223.1	6	25	1.40E+01	35	
841	31883-41-5	14	3,5-Dichlorobiphenyl	223.1	1	25	4.27E+01	10	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.c. Henry's law constant data, Pa m^3 / mol, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
842	2050-68-2	15	4,4'-Dichlorobiphenyl	223.1	1	25	2.27E+01	10	
843	2050-68-2	15	4,4'-Dichlorobiphenyl	223.1	2	25	2.02E+01	20;27	
844	2050-68-2	15	4,4'-Dichlorobiphenyl	223.1	4	25	9.67E+00	33	
845	38444-78-9	16	2,2',3-Trichlorobiphenyl	257.54	1	25	2.54E+01	10	
846	38444-78-9	16	2,2',3-Trichlorobiphenyl	257.54	2	23	8.13E+01	50	distilled water
847	38444-78-9	16	2,2',3-Trichlorobiphenyl	257.54	2	23	3.20E+02	50	seawater
848	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	1	25	3.24E+01	10	
849	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	6	25	2.50E+01	35	
850	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	2	23	1.01E+02	50	distilled water
851	37680-65-2	18	2,2',5-Trichlorobiphenyl	257.54	2	23	2.71E+02	50	seawater
850	38444-73-4	19	2,2',6-Trichlorobiphenyl	257.54	6	25	2.30E+01	35	
851	55702-46-0	21	2,3,4-Trichlorobiphenyl	257.54	1	25	2.30E+01	10	
852	38444-85-8	22	2,3,4'-Trichlorobiphenyl	257.54	1	25	1.94E+01	10	
853	55720-44-0	23	2,3,5'-Trichlorobiphenyl	257.54	1	25	3.22E+01	10	
854	5872-45-9	24	2,3,6-Trichlorobiphenyl	257.54	6	25	2.20E+01	35	
855	38444-81-4	26	2,3',5-Trichlorobiphenyl	257.54	1	25	3.02E+01	10	
856	38444-81-4	26	2,3',5-Trichlorobiphenyl	257.54	2	25	3.29E+01	20;27	
857	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	1	25	2.90E+01	10	
858	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	2	25	3.20E+01	20;27	
859	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	6	25	2.00E+01	35	
860	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	4	10.4	8.70E+00	36	
861	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	4	20	2.12E+01	36	
862	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	4	30.1	4.74E+01	36	
863	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	4	34.9	5.03E+01	36	
864	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	4	42.1	7.08E+01	36	
865	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	4	47.9	1.21E+02	36	
866	7012-37-5	28	2,4,4'-Trichlorobiphenyl	257.54	4	48.4	1.22E+02	36	
867	15862-07-4	29	2,4,5-Trichlorobiphenyl	257.54	1	25	3.00E+01	10	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.c. Henry's law constant data, Pa m^3 / mol, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
868	15862-07-4	29	2,4,5-Trichlorobiphenyl	257.54	6	25	2.00E+01	35	
869	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	1	25	5.80E+01	10	
870	35693-92-6	30	2,4,6-Trichlorobiphenyl	257.54	2	25	6.58E+01	20;27	
871	16606-02-3	31	2,4',5-Trichlorobiphenyl	257.54	1	25	2.78E+01	10	
872	16606-02-3	31	2,4',5-Trichlorobiphenyl	257.54	6	25	1.90E+01	35	
873	38444-86-9	33	2',3,4-Trichlorobiphenyl	257.54	1	25	3.95E+01	18	
874	38444-86-9	33	2',3,4-Trichlorobiphenyl	257.54	1	25	2.42E+01	10	
875	37680-68-5	34	2',3,5-Trichlorobiphenyl	257.54	1	25	4.27E+01	10	
876	38444-90-5	37	3,4,4'-Trichlorobiphenyl	257.54	2	23	8.37E+01	50	distilled water
877	38444-90-5	37	3,4,4'-Trichlorobiphenyl	257.54	2	23	4.68E+02	50	seawater
878	38444-90-5	37	3,4,4'-Trichlorobiphenyl	257.54	1	25	1.54E+01	10	
879	38444-90-5	37	3,4,4'-Trichlorobiphenyl	257.54	6	25	1.00E+01	35	
880	16606-02-3	39	3,4',5-Trichlorobiphenyl	257.54	1	25	3.03E+01	10	
881	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99	1	25	1.84E+01	10	
882	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99	2	25	2.05E+01	20;27	
883	38444-93-8	40	2,2',3,3'-Tetrachlorobiphenyl	291.99	6	25	1.00E+01	35	
884	36559-22-5	42	2,2',3,4'-Tetrachlorobiphenyl	291.99	1	25	2.59E+01	10	
885	41464-39-5	44	2,2',3,5'-Tetrachlorobiphenyl	291.99	2	23	7.88E+01	50	distilled water
886	41464-39-5	44	2,2',3,5'-Tetrachlorobiphenyl	291.99	2	23	5.42E+02	50	seawater
887	41464-39-5	44	2,2',3,5'-Tetrachlorobiphenyl	291.99	1	25	2.33E+01	10	
888	41464-47-5	46	2,2',3,6'-Tetrachlorobiphenyl	291.99	1	25	3.42E+01	10	
889	2437-79-8	47	2,2',4,4'-Tetrachlorobiphenyl	291.99	1	25	3.73E+01	10	
890	2437-79-8	47	2,2',4,4'-Tetrachlorobiphenyl	291.99	6	25	1.90E+01	35	
891	41464-40-8	49	2,2',4,5'-Tetrachlorobiphenyl	291.99	1	25	3.58E+01	10	
892	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	4	10.4	8.60E+00	36	
893	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	4	20	1.64E+01	36	
894	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	2	23	9.36E+01	50	distilled water
895	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	2	23	4.92E+02	50	seawater

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.c. Henry's law constant data, Pa m^3 / mol, polychlorinated biphenyls (PCBs)									
Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
896	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	1	25	3.14E+01	18	
897	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	1	25	3.23E+01	10	
898	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	2	25	3.47E+01	20;27	
899	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	6	25	2.00E+01	35	
900	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	4	30.1	3.74E+01	36	
901	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	4	34.9	3.88E+01	36	
902	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	4	42.1	6.87E+01	36	
903	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	4	47.9	1.09E+02	36	
904	35693-99-3	52	2,2',5,5'-Tetrachlorobiphenyl	291.99	4	48.4	1.21E+02	36	
905	41464-41-9	53	2,2',5,6'-Tetrachlorobiphenyl	291.99	1	25	4.37E+01	10	
906	41464-41-9	53	2,2',5,6'-Tetrachlorobiphenyl	291.99	2	25	4.11E+01	20;27	
907	15968-05-5	54	2,2',6,6'-Tetrachlorobiphenyl	291.99	1	25	5.80E+01	10	
908	15968-05-5	54	2,2',6,6'-Tetrachlorobiphenyl	291.99	2	25	5.57E+01	20;27	
909	15968-05-5	54	2,2',6,6'-Tetrachlorobiphenyl	291.99	6	25	2.00E+01	35	
910	41464-43-9	56	2,3,3',4'-Tetrachlorobiphenyl	291.99	1	25	1.53E+01	10	
911	41464-49-7	58	2,3,3',5'-Tetrachlorobiphenyl	291.99	1	25	2.53E+01	10	
912	33025-41-1	60	2,3,4,4'-Tetrachlorobiphenyl	291.99	2	23	8.37E+01	50	distilled water
913	33025-41-1	60	2,3,4,4'-Tetrachlorobiphenyl	291.99	2	23	4.68E+02	50	seawater
914	33025-41-1	60	2,3,4,4'-Tetrachlorobiphenyl	291.99	1	25	1.59E+01	10	
915	33284-53-6	61	2,3,4,5-Tetrachlorobiphenyl	291.99	1	25	3.40E+01	10	
916	54230-22-7	62	2,3,4,6-Tetrachlorobiphenyl	292	6	25	2.10E+01	35	
917	74472-34-7	63	2,3,4',5-Tetrachlorobiphenyl	291.99	1	25	2.45E+01	10	
918	33284-54-7	65	2,3,5,6-Tetrachlorobiphenyl	291.99	1	25	2.41E+01	10	
919	32598-10-0	66	2,3',4,4'-Tetrachlorobiphenyl	291.99	1	25	2.10E+01	10	
920	72575-53-8	67	2,3',4,5-Tetrachlorobiphenyl	292	6	25	1.00E+01	35	
921	32598-11-1	70	2,3',4',5-Tetrachlorobiphenyl	291.99	1	25	2.23E+01	10	
922	32598-11-1	70	2,3',4',5-Tetrachlorobiphenyl	291.99	6	25	1.00E+01	35	
923	41464-42-0	72	2,3',5,5'-Tetrachlorobiphenyl	291.99	1	25	3.67E+01	10	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.c. Henry's law constant data, Pa m^3 / mol, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
924	32690-93-0	74	2,4,4',5-Tetrachlorobiphenyl	291.99	1	25	2.17E+01	10	
925	32690-93-0	74	2,4,4',5-Tetrachlorobiphenyl	291.99	6	25	1.00E+01	35	
926	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	1	25	1.03E+01	10	
927	32598-13-3	77	3,3',4,4'-Tetrachlorobiphenyl	291.99	2	25	9.52E+00	20;27	
928	41464-48-6	79	3,3',4,5'-Tetrachlorobiphenyl	291.99	1	25	2.00E+01	10	
929	33284-52-5	80	3,3',5,5'-Tetrachlorobiphenyl	291.99	1	25	3.80E+01	10	
930	52663-62-4	82	2,2',3,3',4-Pentachlorobiphenyl	326.43	1	25	1.48E+01	10	
931	38380-02-8	87	2,2',3,4,5'-Pentachlorobiphenyl	326.43	1	25	1.86E+01	10	
932	38379-99-6	95	2,2',3,5',6-Pentachlorobiphenyl	326.43	1	25	3.04E+01	10	
933	41464-51-1	97	2,2',3',4,5-Pentachlorobiphenyl	326.43	1	25	1.82E+01	10	
934	41464-51-1	97	2,2',3',4,5-Pentachlorobiphenyl	326.43	6	25	7.40E+00	35	
935	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	1	25	1.11E+01	18	
936	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	1	25	2.48E+01	10	
937	37680-73-2	101	2,2',4,5,5'-Pentachlorobiphenyl	326.43	2	25	2.54E+01	20;27	
938	56558-16-8	104	2,2',4,6,6'-Pentachlorobiphenyl	326.43	2	25	9.09E+01	20;27	
939	32598-14-4	105	2,3,3',4,4'-Pentachlorobiphenyl	326.43	1	25	1.01E+01	10	
940	74472-37-0	114	2,3,4,4',5-Pentachlorobiphenyl	326.43	1	25	1.45E+01	10	
941	18259-05-7	116	2,3,4,5,6-Pentachlorobiphenyl	326.43	1	25	2.99E+01	10	
942	31508-0-6	118	2,3',4,4',5-Pentachlorobiphenyl	326.43	1	25	1.27E+01	10	
943	68194-12-7	120	2,3',4,5,5'-Pentachlorobiphenyl	326.43	6	25	5.60E+00	35	
944	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	1	25	1.05E+01	10	
945	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	2	25	3.06E+00	20;27	
946	38380-07-3	128	2,2',3,3',4,4'-Hexachlorobiphenyl	360.88	6	25	1.30E+00	35	
947	55215-18-4	129	2,2',3,3',4,5-Hexachlorobiphenyl	360.88	6	25	2.90E+00	35	
948	52663-66-8	130	2,2',3,3',4,5'-Hexachlorobiphenyl	360.88	6	25	3.70E+00	35	
949	38380-05-1	132	2,2',3,3',4,6'-Hexachlorobiphenyl	360.88	6	25	4.40E+00	35	
950	35694-4-3	133	2,2',3,3',5,5'-Hexachlorobiphenyl	360.88	1	25	2.06E+01	10	
951	52704-70-8	134	2,2',3,3',5,6-Hexachlorobiphenyl	360.88	6	25	4.90E+00	35	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.c. Henry's law constant data, Pa m^3 / mol, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
952	52744-13-5	135	2,2',3,3',5,6'-Hexachlorobiphenyl	360.88	6	25	5.60E+00	35	
953	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	1	25	3.26E+01	10	
954	38411-22-2	136	2,2',3,3',6,6',-Hexachlorobiphenyl	360.88	6	25	8.80E+00	35	
955	35694-6-5	137	2,2',3,4,4',5-Hexachlorobiphenyl	360.88	1	25	1.87E+01	10	
956	35065-28-2	138	2,2',3,4,4',5'-Hexachlorobiphenyl	360.88	1	25	1.32E+01	10	
957	35065-28-2	138	2,2',3,4,4',5'-Hexachlorobiphenyl	360.88	6	25	2.10E+00	35	
958	35065-28-2	140	2,2',3,4,4',5'-Hexachlorobiphenyl	360.88	1	25	3.11E+01	10	
959	52712-04-6	141	2,2',3,4,5,5'-Hexachlorobiphenyl	360.9	6	25	2.30E+00	35	
960	41411-61-4	142	2,2',3,4,5,6-Hexachlorobiphenyl	360.88	1	25	3.18E+01	10	
961	41908-16-8	146	2,2',3,4',5,5'-Hexachlorobiphenyl	360.88	6	25	2.50E+00	35	
962	68194-13-8	147	2,2',3,4',5,6-Hexachlorobiphenyl	360.88	6	25	5.10E+00	35	
963	52663-63-5	151	2,2',3,5,5',6-Hexachlorobiphenyl	360.88	1	25	2.87E+01	10	
964	52663-63-5	151	2,2',3,5,5',6-Hexachlorobiphenyl	360.88	6	25	5.90E+00	35	
965	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	1	25	1.66E+01	10	
966	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	2	25	1.34E+01	20;27	
967	35065-27-1	153	2,2',4,4',5,5'-Hexachlorobiphenyl	360.88	6	25	2.40E+00	35	
968	33979-03-2	155	2,2',4,4',6,6'-Hexachlorobiphenyl	360.88	1	25	8.52E+01	10	
969	33979-03-2	155	2,2',4,4',6,6'-Hexachlorobiphenyl	360.88	2	25	7.65E+01	20;27	
970	39635-35-3	159	2,3,3',4,5.5'-Hexachlorobiphenyl	360.88	6	25	4.70E+00	35	
971	41411-62-5	160	2,3,3',4,5,6-Hexachlorobiphenyl	360.88	1	25	2.20E+00	10	
972	41411-62-5	160	2,3,3',4,5,6-Hexachlorobiphenyl	360.88	6	25	2.16E+01	35	
973	74472-44-9	163	2,3,3',4',5,6-Hexachlorobiphenyl	360.88	6	25	1.50E+00	35	
974	74472-46-1	165	2,3,3',5,5',6-Hexachlorobiphenyl	360.88	6	25	2.90E+00	35	
975	41411-63-6	166	2,3,4,4',5,6-Hexachlorobiphenyl	360.88	1	25	1.86E+01	10	
976	59291-65-6	168	2,3',4,4',5',6-Hexachlorobiphenyl	360.88	1	25	2.80E+01	10	
977	32774-16-6	169	3,3',4,4',5,5'-Hexachlorobiphenyl	360.88	1	25	6.60E+00	10	
978	35065-30-6	170	2,2',3,3',4,4',5-Heptachlorobiphenyl	395.32	1	25	8.85E+00	10	
979	35065-30-6	170	2,2',3,3',4,4',5-Heptachlorobiphenyl	395.32	6	25	9.00E-01	35	

Table 4. Physical constant data for polychlorinated biphenyls (PCBs)

Table 4.c. Henry's law constant data, Pa m^3 / mol, polychlorinated biphenyls (PCBs)

Entry #	CAS #	IUPAC #[1]	Common Name	Molecular Wt. (amu)	Method ID	Temp °C	Value	Ref. #	Phase
980	52663-74-8	172	2,2',3,3',4,5,5'-Heptachlorobiphenyl	395.32	6	25	1.30E+00	35	supercooled
981	68194-16-1	173	2,2',3,3',4,5,6-Heptachlorobiphenyl	395.32	6	25	1.40E+00	35	
982	40186-70-7	174	2,2',3,3',4,5,6'-Heptachlorobiphenyl	395.32	1	25	1.71E+01	10	
983	40186-70-7	174	2,2',3,3',4,5,6'-Heptachlorobiphenyl	395.32	6	25	1.40E+00	35	
984	52663-67-9	178	2,2',3,3',5,5'6-Heptachlorobiphenyl	395.32	6	25	2.30E+00	35	
985	52663-64-6	179	2,2',3,3',5,6,6'-Heptachlorobiphenyl	395.32	6	25	2.40E+00	35	
986	35065-29-3	180	2,2',3,4,4',5,5'-Heptachlorobiphenyl	395.32	1	25	1.09E+01	10	
987	74472-47-2	182	2,2',3,4,4',5,6'-Heptachlorobiphenyl	395.32	1	25	2.61E+01	10	
988	52712-05-7	185	2,2',3,4,5,5',6-Heptachlorobiphenyl	395.32	1	25	2.17E+01	10	
989	52712-05-7	185	2,2',3,4,5,5',6-Heptachlorobiphenyl	395.32	6	25	1.60E+00	35	
990	39635-31-9	189	2,3,3',4,4',5,5'-Heptachlorobiphenyl	395.32	1	25	6.74E+00	10	
991	41411-64-7	190	2,3,3',4,4',5,6-Heptachlorobiphenyl	395.32	1	25	1.14E+01	10	
992	35694-08-7	194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	429.77	1	25	6.79E+00	10	
993	35694-08-7	194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	429.77	6	25	1.00E+00	35	
994	52663-78-2	195	2,2',3,3',4,4',5,6-Octachlorobiphenyl	429.77	6	25	1.10E+00	35	
995	42740-50-1	196	2,2',3,3',4,4',5,6'-Octachlorobiphenyl	429.77	6	25	1.00E+00	35	
996	33091-17-7	197	2,2',3,3',4,4',6,6'-Octachlorobiphenyl	429.77	1	25	2.57E+01	10	
997	68194-17-2	198	2,2',3,3',4,5,5',6-Octachlorobiphenyl	429.77	6	25	1.40E+00	35	
998	52663-75-9	199	2,2',3,3',4,5,5',6'-Octachlorobiphenyl	429.77	6	25	1.00E+00	35	
999	2136-99-4	201	2,2',3,3',4,5',6,6'-Octachlorobiphenyl	429.77	6	25	1.70E+00	35	
1000	2136-99-4	202	2,2',3,3',5,5',6,6',-Octachlorobiphenyl	429.77	1	25	2.26E+01	10	
1001	40186-72-9	206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	462.21	1	25	8.85E+00	10	
1002	2051-24-3	209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	498.66	1	25	1.14E+01	10	

[1] PCB congeners are numbered according to method proposed by Ballschmitter and Zell (1980) and later revised by Schulte and Malisch (1983) to be conducive with IUPAC guidelines. (Ballschmitter, K.; Zell, M. *Fresenius Z. Anal. Chem.* **1980,** *302,* 20-31; Schulte, E.; Malisch, R. *Fresenius Z. Anal. Chem.* **1983,** *314,* 545-551).

Table 5. Physical constant data for chlorinated benzenes

Table 5. Physical constant data for chlorinated benzenes

Table 5.a. Aqueous solubility data, mg / L, chlorinated benzenes

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1003	108-90-7	Chlorobenzene	112.56	4,9	25	2.95E+02	21	
1004	95-50-1	*o* -dichlorobenzene	147.01	4,9	25	9.23E+01	21	
1005	541-73-1	*m* -dichlorobenzene	147.01	4,9	25	1.25E+02	21	
1006	106-46-7	*p* -dichlorobenzene	147.01	4,9	25	3.09E+01	21	
1007	87-61-6	1,2,3-trichlorobenzene	181.45	4,9	25	1.23E+01	21	
1008	120-82-1	1,2,4-trichlorobenzene	181.45	4,9	25	4.61E+01	21	
1009	108-70-3	1,2,5-trichlorobenzene	181.45	4,9	25	4.12E+00	21	
1010	634-66-2	1,2,3,4-tetrachlorobenzene	215.9	4,9	25	1.22E+01	21	
1011	634-90-2	1,2,3,5-tetrachlorobenzene	215.9	4,9	25	2.89E+00	21	
1012	95-94-3	1,2,4,5-tetrachlorobenzene	215.9	4,9	25	2.35E+00	21	
1013	608-93-5	pentachlorobenzene	250.34	4,9	25	8.31E-01	21	

Table 5.b. Vapor pressure data, Pa, chlorinated benzenes

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1014	634-66-2	1,2,3,4-tetrachlorobenzene	215.9	7	25	3.49E+00	14	

Table 5.c. Henry's law constant data, Pa m^3 / mol, chlorinated benzenes

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1015	108-90-7	Chlorobenzene	112.56	2	25	3.82E+02	16	
1016	108-90-7	Chlorobenzene	112.56	3	10	2.47E+02	37	
1017	108-90-7	Chlorobenzene	112.56	3	15	2.85E+02	37	

Table 5. Physical constant data for chlorinated benzenes

Table 5.c. Henry's law constant data, Pa m^3 / mol, chlorinated benzenes								
Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1018	108-90-7	Chlorobenzene	112.56	3	20	3.46E+02	37	
1019	108-90-7	Chlorobenzene	112.56	3	25	3.65E+02	37	
1020	108-90-7	Chlorobenzene	112.56	3	30	4.79E+02	37	
1021	95-50-1	*o* -dichlorobenzene	147.01	3	10	1.65E+02	37	
1022	95-50-1	*o* -dichlorobenzene	147.01	3	15	1.45E+02	37	
1023	95-50-1	*o* -dichlorobenzene	147.01	3	20	1.70E+02	37	
1024	95-50-1	*o* -dichlorobenzene	147.01	3	25	1.59E+02	37	
1025	95-50-1	*o* -dichlorobenzene	147.01	3	30	2.40E+02	37	
1026	541-73-1	*m* -dichlorobenzene	147.01	3	10	2.24E+02	37	
1027	541-73-1	*m* -dichlorobenzene	147.01	3	15	2.34E+02	37	
1028	541-73-1	*m* -dichlorobenzene	147.01	3	20	2.98E+02	37	
1029	541-73-1	*m* -dichlorobenzene	147.01	3	25	2.88E+02	37	
1030	541-73-1	*m* -dichlorobenzene	147.01	3	30	4.25E+02	37	
1031	106-46-7	*p* -dichlorobenzene	147.01	3	10	2.15E+02	37	
1032	106-46-7	*p* -dichlorobenzene	147.01	3	15	2.19E+02	37	
1033	106-46-7	*p* -dichlorobenzene	147.01	3	20	2.62E+02	37	
1034	106-46-7	*p* -dichlorobenzene	147.01	3	25	3.20E+02	37	
1035	106-46-7	*p* -dichlorobenzene	147.01	3	30	3.92E+02	37	
1036	87-61-6	1,2,3-trichlorobenzene	181.45	4	25	7.20E+01	36	
1037	120-82-1	1,2,4-trichlorobenzene	181.45	4	25	1.01E+02	36	
1038	108-70-3	1,3,5-trichlorobenzene	181.45	4	25	1.92E+02	36	
1039	634-66-2	1,2,3,4-tetrachlorobenzene	215.9	4	14.8	4.85E+01	36	
1040	634-66-2	1,2,3,4-tetrachlorobenzene	215.9	4	20.1	5.20E+01	36	
1041	634-66-2	1,2,3,4-tetrachlorobenzene	215.9	4	22.1	6.81E+01	36	
1042	634-66-2	1,2,3,4-tetrachlorobenzene	215.9	4	24.2	7.09E+01	36	
1043	634-66-2	1,2,3,4-tetrachlorobenzene	215.9	4	34.8	1.28E+02	36	
1044	634-66-2	1,2,3,4-tetrachlorobenzene	215.9	4	50.5	2.76E+02	36	

Table 5. Physical constant data for chlorinated benzenes

Table 5.c. Henry's law constant data, Pa m^3 / mol, chlorinated benzenes.

Entry #	CAS #	Common Name	Molecular Weight	Method I.D.	Temp °C	Value	Ref. #	Phase
1045	634-90-2	1,2,3,5-tetrachlorobenzene	215.9	4	25	9.90E+01	36	
1046	608-93-5	pentachlorobenzene	250.34	4	14.8	3.74E+01	36	
1047	608-93-5	pentachlorobenzene	250.34	4	20.1	4.94E+01	36	
1048	608-93-5	pentachlorobenzene	250.34	4	22.1	6.81E+01	36	
1049	608-93-5	pentachlorobenzene	250.34	4	24.2	6.67E+01	36	
1050	608-93-5	pentachlorobenzene	250.34	4	34.8	1.24E+02	36	
1051	608-93-5	pentachlorobenzene	250.34	4	50.5	2.76E+02	36	

Table 6. Physical constant data for polychlorinated dibenzo-*p*-dioxins

Table 6. Physical constant data for polyclorinated dibenzo-*p*-dioxins

Table 6.a. Aqueous solubility data, mg / L, polychlorinated dibenzo-*p*-dioxins

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1052	262-12-4	Dibenzo-*p*-dioxin	184	4,6	4.1	2.12E-01	22	
1053	262-12-4	Dibenzo-*p*-dioxin	184	4,6	25	9.00E-01	22	
1054	262-12-4	Dibenzo-*p*-dioxin	184	4,6	40	2.39E+00	22	
1055	262-12-4	Dibenzo-*p*-dioxin	184	4,6	25	8.42E-01	23	
1056	39227-53-7	1-chloro-	218.5	4,6	25	4.17E-01	23	
1057	39227-54-8	2-Chloro-	218.5	4,6	3.9	1.33E-01	22	
1058	39227-54-8	2-Chloro-	218.5	4,6	25	3.19E-01	22	
1059	39227-54-8	2-Chloro-	218.5	4,6	25	2.78E-01	23	
1060	39227-54-8	2-Chloro-	218.5	4,6	39	7.49E-01	22	
1061	39227-54-8	2-Chloro-	218.5	4,6	25	7.49E-01	22	
1062	29446-15-9	2,3-Dichloro-	253	4,6	25	1.49E-02	23	
1063	33857-26-0	2,7-Dichloro-	253	4,6	25	3.75E-03	23	
1064	33857-26-0	2,7-Dichloro-	253	4,6	25	2.24E-03	34	
1065	38964-22-6	2,8-Dichloro-	253	4,6	25	1.67E-02	23	
1066	39227-58-2	1,2,4-Trichloro-	287.5	4,6	25	8.41E-03	23	
1067	39227-58-2	1,2,4-Trichloro-	287.5	4,6	25	6.95E-03	34	
1068	30746-58-8	1,2,3,4-Tetrachloro-	322	4,6	4	1.13E-04	22	
1069	30746-58-8	1,2,3,4-Tetrachloro-	322	4,6	25	4.70E-04	22	
1070	30746-58-8	1,2,3,4-Tetrachloro-	322	4,6	25	6.30E-04	23	
1071	30746-58-8	1,2,3,4-Tetrachloro-	322	4,6	40	1.17E-03	22	
1072	30746-58-8	1,2,3,4-Tetrachloro-	322	4,6	25	3.88E-04	34	
1073	67028-18-6	1,2,3,7-Tetrachloro-	322	3,9	20	4.30E-04	19	
1074	67028-18-6	1,2,3,7-Tetrachloro-	322	3,9	40	1.27E-03	19	
1075	30746-58-8	1,3,6,8-Tetrachloro-	322	3,9	20	3.20E-04	19	
1076	30746-58-8	1,3,6,8-Tetrachloro-	322	3,9	40	3.90E-04	19	
1077	39227-61-7	1,2,3,4,7-Pentachloro-	356.4	3,9	20	1.20E-04	19	
1078	39227-61-7	1,2,3,4,7-Pentachloro-	356.4	3,9	40	4.60E-04	19	
1079	39227-26-8	1,2,3,4,7,8-Hexachloro-	391	3,9	20	4.40E-06	19	

Table 6. Physical constant data for polyclorinated dibenzo-*p* -dioxins

Table 6.a. Aqueous solubility data, mg / L, polychlorinated dibenzo-*p* -dioxins, continued

Entry #	CAS #	Common Name	Molecular Weight	Method I.D.	Temp °C	Value	Ref. #	Phase
1080	39227-26-8	1,2,3,4,7,8-Hexachloro-	391	3,9	40	1.90E-05	19	
1081	35822-46-9	1,2,3,4,6,7,8-Heptachloro-	425.2	3,9	20	2.40E-06	19	
1082	35822-46-9	1,2,3,4,6,7,8-Heptachloro-	425.2	3,9	40	6.30E-06	19	
1083	3268-87-9	Octachloro-	460	3,9	20	4.00E-07	19	
1084	3268-87-9	Octachloro-	460	3,9	40	2.00E-06	19	
1085	3268-87-9	Octachloro-	460	4,6	40	3.10E-07	22	
1086	3268-87-9	Octachloro-	460	4,6	60	1.82E-06	22	
1087	3268-87-9	Octachloro-	460	4,6	80	7.87E-07	22	

Table 6.b. Vapor pressure data, Pa, polychlorinated dibenzo-*p* -dioxins

Entry #	CAS #	Common Name	Molecular Weight	Method I.D.	Temp °C	Value	Ref. #	Phase
1088	30746-58-8	1,2,3,4-Tetrachloro-	322	7	25	1.04E-04	24	supercooled
1089	40321-76-4	1,2,3,7,8-Pentachloro-	356.4	7	25	1.75E-05	24	supercooled
1090	39227-26-8	1,2,3,4,7,8-Hexachloro-	391	7	25	3.96E-06	24	supercooled
1091	35822-46-9	1,2,3,4,6,7,8-Heptachloro-	425.2	7	25	1.02E-06	24	supercooled
1092	3268-87-9	Octachloro-	460	7	25	2.77E-07	24	supercooled

Table 6.c. Henry's law constant data, Pa m^3 / mol, polychlorinated dibenzo-*p* -dioxins

Entry #	CAS #	Common Name	Molecular Weight	Method I.D.	Temp °C	Value	Ref. #	Phase
1093	33857-26-0	2,7-Dichloro-	253	6	25	5.96E+00	34	
1094	39227-58-2	1,2,4-Trichloro-	287.5	6	25	3.64E+00	34	
1095	30746-58-8	1,2,3,4-Tetrachloro-	322	6	25	2.02E+00	34	

Table 7. Physical constant data for polychlorinated dibenzofurans

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.a. Aqueous solubility data, mg / L, polychlorinated dibenzofurans

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1096	132-64-9	Dibenzofuran	168.21	4,6	4	1.65E+00	22	
1097	132-64-9	Dibenzofuran	168.21	2,9	25	5.96E-01	8	uM
1098	132-64-9	Dibenzofuran	168.21	4,6	25	4.22E+00	22	
1099	132-64-9	Dibenzofuran	168.21	4,6	39.8	6.96E+00	22	
1100	5409-83-6	2,8-Dichlorodibenzofuran	237.05	4,6	4.5	3.84E-03	22	
1101	5409-83-6	2,8-Dichlorodibenzofuran	237.05	4,6	25	1.45E-02	22	
1102	5409-83-6	2,8-Dichlorodibenzofuran	237.05	4,6	39.5	3.39E-02	22	
1103	51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	305.89	4,6	22.7	4.19E-04	12	
1104	51207-31-4	2,3,4,7,8-Pentachlorodibenzofuran	340.31	4,6	22.7	2.35E-04	12	
1105	70658-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	374.73	4,6	22.7	8.24E-06	12	
1106	75117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	374.73	4,6	22.7	1.77E-05	12	
1107	67462-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	409.15	4,6	22.7	1.35E-06	12	
1108	39001-02-0	Octachlorodibenzofuran	443.57	4,6	39.5	3.85E-06	22	
1109	39001-02-0	Octachlorodibenzofuran	443.57	4,6	58.6	1.40E-05	22	
1110	39001-02-0	Octachlorodibenzofuran	443.57	4,6	80	6.08E-06	22	

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1111	51230-49-0	2-Chlorodibenzofuran	202.63	1	25	9.60E-03	13	
1112	51230-49-0	2-Chlorodibenzofuran	202.63	1	50	1.90E-01	13	
1113	51230-49-0	2-Chlorodibenzofuran	202.63	1	75	2.40E+00	13	
1114	51230-49-0	2-Chlorodibenzofuran	202.63	1	100	2.20E+01	13	
1115	51230-49-0	2-Chlorodibenzofuran	202.63	1	125	1.50E+02	13	
1116	25074-67-3	3-Chlorodibenzofuran	202.63	1	25	9.70E-03	13	
1117	25074-67-3	3-Chlorodibenzofuran	202.63	1	50	1.90E-01	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1118	25074-67-3	3-Chlorodibenzofuran	202.63	1	75	2.40E+00	13	
1119	25074-67-3	3-Chlorodibenzofuran	202.63	1	100	2.20E+01	13	
1120	25074-67-3	3-Chlorodibenzofuran	202.63	1	125	1.50E+02	13	
1121	64126-86-9	2,3-Dichlorodibenzofuran	237.05	1	25	6.50E-04	13	
1122	64126-86-9	2,3-Dichlorodibenzofuran	237.05	1	50	1.70E-02	13	
1123	64126-86-9	2,3-Dichlorodibenzofuran	237.05	1	75	2.90E-01	13	
1124	64126-86-9	2,3-Dichlorodibenzofuran	237.05	1	100	3.20E+00	13	
1125	64126-86-9	2,3-Dichlorodibenzofuran	237.05	1	125	2.70E+01	13	
1126	5409-83-6	2,8-Dichlorodibenzofuran	237.05	1	25	3.90E-04	13	
1127	5409-83-6	2,8-Dichlorodibenzofuran	237.05	1	50	9.10E-03	13	
1128	5409-83-6	2,8-Dichlorodibenzofuran	237.05	1	75	1.40E-01	13	
1129	5409-83-6	2,8-Dichlorodibenzofuran	237.05	1	100	1.40E+00	13	
1130	5409-83-6	2,8-Dichlorodibenzofuran	237.05	1	125	1.10E+01	13	
1131	57117-32-5	2,3,8-Trichlorodibenzofuran	271.47	1	25	3.00E-05	13	
1132	57117-32-5	2,3,8-Trichlorodibenzofuran	271.47	1	50	9.90E-04	13	
1133	57117-32-5	2,3,8-Trichlorodibenzofuran	271.47	1	75	2.00E-02	13	
1134	57117-32-5	2,3,8-Trichlorodibenzofuran	271.47	1	100	2.60E-01	13	
1135	57117-32-5	2,3,8-Trichlorodibenzofuran	271.47	1	125	2.50E+00	13	
1136	58802-14-5	2,4,6-Trichlorodibenzofuran	271.47	1	25	8.20E-05	13	
1137	58802-14-5	2,4,6-Trichlorodibenzofuran	271.47	1	50	3.10E-03	13	
1138	58802-14-5	2,4,6-Trichlorodibenzofuran	271.47	1	75	6.80E-02	13	
1139	58802-14-5	2,4,6-Trichlorodibenzofuran	271.47	1	100	1.00E+00	13	
1140	58802-14-5	2,4,6-Trichlorodibenzofuran	271.47	1	125	1.00E+01	13	
1141	24478-72-6	1,2,3,4-Tetrachlorodibenzofuran	305.89	1	25	4.10E-06	13	
1142	24478-72-6	1,2,3,4-Tetrachlorodibenzofuran	305.89	1	50	1.90E-04	13	
1143	24478-72-6	1,2,3,4-Tetrachlorodibenzofuran	305.89	1	75	5.10E-03	13	
1144	24478-72-6	1,2,3,4-Tetrachlorodibenzofuran	305.89	1	100	8.70E-02	13	
1145	24478-72-6	1,2,3,4-Tetrachlorodibenzofuran	305.89	1	125	1.00E+00	13	
1146	83704-22-7	1,2,3,7-Tetrachlorodibenzofuran	305.89	1	25	4.20E-06	13	

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1147	83704-22-7	1,2,3,7-Tetrachlorodibenzofuran	305.89	1	50	1.90E-04	13	
1148	83704-22-7	1,2,3,7-Tetrachlorodibenzofuran	305.89	1	75	5.20E-03	13	
1149	83704-22-7	1,2,3,7-Tetrachlorodibenzofuran	305.89	1	100	8.90E-02	13	
1150	83704-22-7	1,2,3,7-Tetrachlorodibenzofuran	305.89	1	125	1.10E+00	13	
1151	62615-08-1	1,2,3,8-Tetrachlorodibenzofuran	305.89	1	25	2.80E-06	13	
1152	62615-08-1	1,2,3,8-Tetrachlorodibenzofuran	305.89	1	50	1.20E-04	13	
1153	62615-08-1	1,2,3,8-Tetrachlorodibenzofuran	305.89	1	75	3.10E-03	13	
1154	62615-08-1	1,2,3,8-Tetrachlorodibenzofuran	305.89	1	100	5.20E-02	13	
1155	62615-08-1	1,2,3,8-Tetrachlorodibenzofuran	305.89	1	125	6.00E-01	13	
1156	64126-87-0	1,2,4,8-Tetrachlorodibenzofuran	305.89	1	25	3.00E-06	13	
1157	64126-87-0	1,2,4,8-Tetrachlorodibenzofuran	305.89	1	50	1.30E-04	13	
1158	64126-87-0	1,2,4,8-Tetrachlorodibenzofuran	305.89	1	75	3.40E-03	13	
1159	64126-87-0	1,2,4,8-Tetrachlorodibenzofuran	305.89	1	100	5.70E-02	13	
1160	64126-87-0	1,2,4,8-Tetrachlorodibenzofuran	305.89	1	125	6.70E-01	13	
1161	83704-25-0	1,2,6,7-Tetrachlorodibenzofuran	305.89	1	25	2.70E-06	13	
1162	83704-25-0	1,2,6,7-Tetrachlorodibenzofuran	305.89	1	50	1.20E-04	13	
1163	83704-25-0	1,2,6,7-Tetrachlorodibenzofuran	305.89	1	75	3.00E-03	13	
1164	83704-25-0	1,2,6,7-Tetrachlorodibenzofuran	305.89	1	100	5.00E-02	13	
1165	83704-25-0	1,2,6,7-Tetrachlorodibenzofuran	305.89	1	125	5.80E-01	13	
1166	58802-20-3	1,2,7,8-Tetrachlorodibenzofuran	305.89	1	25	2.40E-06	13	
1167	58802-20-3	1,2,7,8-Tetrachlorodibenzofuran	305.89	1	50	1.00E-04	13	
1168	58802-20-3	1,2,7,8-Tetrachlorodibenzofuran	305.89	1	75	2.60E-03	13	
1169	58802-20-3	1,2,7,8-Tetrachlorodibenzofuran	305.89	1	100	4.20E-02	13	
1170	58802-20-3	1,2,7,8-Tetrachlorodibenzofuran	305.89	1	125	4.90E-01	13	
1171	83604-26-1	1,2,7,9-Tetrachlorodibenzofuran	305.89	1	25	3.30E-06	13	
1172	83604-26-1	1,2,7,9-Tetrachlorodibenzofuran	305.89	1	50	1.50E-04	13	
1173	83604-26-1	1,2,7,9-Tetrachlorodibenzofuran	305.89	1	75	3.80E-03	13	
1174	83604-26-1	1,2,7,9-Tetrachlorodibenzofuran	305.89	1	100	6.50E-02	13	
1175	83604-26-1	1,2,7,9-Tetrachlorodibenzofuran	305.89	1	125	7.60E-01	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1176	57117-36-9	1,3,6,7-Tetrachlorodibenzofuran	305.89	1	25	3.70E-06	13	
1177	57117-36-9	1,3,6,7-Tetrachlorodibenzofuran	305.89	1	50	1.70E-04	13	
1178	57117-36-9	1,3,6,7-Tetrachlorodibenzofuran	305.89	1	75	4.40E-03	13	
1179	57117-36-9	1,3,6,7-Tetrachlorodibenzofuran	305.89	1	100	7.50E-02	13	
1180	57117-36-9	1,3,6,7-Tetrachlorodibenzofuran	305.89	1	125	8.90E-01	13	
1181	71998-72-6	1,3,6,8-Tetrachlorodibenzofuran	305.89	1	25	3.60E-06	13	
1182	71998-72-6	1,3,6,8-Tetrachlorodibenzofuran	305.89	1	50	1.60E-04	13	
1183	71998-72-6	1,3,6,8-Tetrachlorodibenzofuran	305.89	1	75	4.30E-03	13	
1184	71998-72-6	1,3,6,8-Tetrachlorodibenzofuran	305.89	1	100	7.40E-02	13	
1185	71998-72-6	1,3,6,8-Tetrachlorodibenzofuran	305.89	1	125	8.80E-01	13	
1186	67560-17-4	1,3,7,9-Tetrachlorodibenzofuran	305.89	1	25	2.50E-06	13	
1187	67560-17-4	1,3,7,9-Tetrachlorodibenzofuran	305.89	1	50	1.10E-04	13	
1188	67560-17-4	1,3,7,9-Tetrachlorodibenzofuran	305.89	1	75	2.70E-03	13	
1189	67560-17-4	1,3,7,9-Tetrachlorodibenzofuran	305.89	1	100	4.50E-02	13	
1190	67560-17-4	1,3,7,9-Tetrachlorodibenzofuran	305.89	1	125	5.10E-01	13	
1191	66794-59-0	1,4,6,7-Tetrachlorodibenzofuran	305.89	1	25	3.50E-06	13	
1192	66794-59-0	1,4,6,7-Tetrachlorodibenzofuran	305.89	1	50	1.56E-04	13	
1193	66794-59-0	1,4,6,7-Tetrachlorodibenzofuran	305.89	1	75	4.10E-03	13	
1194	66794-59-0	1,4,6,7-Tetrachlorodibenzofuran	305.89	1	100	7.00E-02	13	
1195	66794-59-0	1,4,6,7-Tetrachlorodibenzofuran	305.89	1	125	8.30E-01	13	
1196	83704-30-7	2,3,4,6-Tetrachlorodibenzofuran	305.89	1	25	5.30E-06	13	
1197	83704-30-7	2,3,4,6-Tetrachlorodibenzofuran	305.89	1	50	2.50E-04	13	
1198	83704-30-7	2,3,4,6-Tetrachlorodibenzofuran	305.89	1	75	6.90E-03	13	
1199	83704-30-7	2,3,4,6-Tetrachlorodibenzofuran	305.89	1	100	1.20E-01	13	
1200	83704-30-7	2,3,4,6-Tetrachlorodibenzofuran	305.89	1	125	1.50E+00	13	
1201	83704-31-8	2,3,4,7-Tetrachlorodibenzofuran	305.89	1	25	3.90E-06	13	
1202	83704-31-8	2,3,4,7-Tetrachlorodibenzofuran	305.89	1	50	1.80E-04	13	
1203	83704-31-8	2,3,4,7-Tetrachlorodibenzofuran	305.89	1	75	4.70E-03	13	
1204	83704-31-8	2,3,4,7-Tetrachlorodibenzofuran	305.89	1	100	8.10E-02	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1205	83704-31-8	2,3,4,7-Tetrachlorodibenzofuran	305.89	1	125	9.60E-01	13	
1206	83704-32-9	2,3,4,8-Tetrachlorodibenzofuran	305.89	1	25	3.70E-06	13	
1207	83704-32-9	2,3,4,8-Tetrachlorodibenzofuran	305.89	1	50	1.70E-04	13	
1208	83704-32-9	2,3,4,8-Tetrachlorodibenzofuran	305.89	1	75	4.40E-03	13	
1209	83704-32-9	2,3,4,8-Tetrachlorodibenzofuran	305.89	1	100	7.50E-02	13	
1210	83704-32-9	2,3,4,8-Tetrachlorodibenzofuran	305.89	1	125	8.90E-01	13	
1211	57117-39-2	2,3,6,7-Tetrachlorodibenzofuran	305.89	1	25	2.80E-06	13	
1212	57117-39-2	2,3,6,7-Tetrachlorodibenzofuran	305.89	1	50	1.30E-04	13	
1213	57117-39-2	2,3,6,7-Tetrachlorodibenzofuran	305.89	1	75	3.20E-03	13	
1214	57117-39-2	2,3,6,7-Tetrachlorodibenzofuran	305.89	1	100	5.40E-02	13	
1215	57117-39-2	2,3,6,7-Tetrachlorodibenzofuran	305.89	1	125	6.30E-01	13	
1216	57117-37-0	2,3,6,8-Tetrachlorodibenzofuran	305.89	1	25	2.60E-06	13	
1217	57117-37-0	2,3,6,8-Tetrachlorodibenzofuran	305.89	1	50	1.10E-04	13	
1218	57117-37-0	2,3,6,8-Tetrachlorodibenzofuran	305.89	1	75	2.90E-03	13	
1219	57117-37-0	2,3,6,8-Tetrachlorodibenzofuran	305.89	1	100	4.80E-02	13	
1220	57117-37-0	2,3,6,8-Tetrachlorodibenzofuran	305.89	1	125	5.50E-01	13	
1221	51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	305.89	1	25	2.67E-04	13	
1222	51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	305.89	7	25	1.23E-04	24	
1223	51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	305.89	6	50	8.50E-05	13	
1224	51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	305.89	6	75	2.10E-03	13	
1225	51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	305.89	6	100	3.30E-02	13	
1226	51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	305.89	6	125	3.80E-01	13	
1227	57117-38-1	2,4,6,7-Tetrachlorodibenzofuran	305.89	1	25	4.40E-06	13	
1228	57117-38-1	2,4,6,7-Tetrachlorodibenzofuran	305.89	1	50	2.10E-04	13	
1229	57117-38-1	2,4,6,7-Tetrachlorodibenzofuran	305.89	1	75	5.50E-03	13	
1230	57117-38-1	2,4,6,7-Tetrachlorodibenzofuran	305.89	1	100	9.50E-02	13	
1231	57117-38-1	2,4,6,7-Tetrachlorodibenzofuran	305.89	1	125	1.20E+00	13	
1232	58802-19-0	2,4,6,8-Tetrachlorodibenzofuran	305.89	1	25	2.70E-06	13	
1233	58802-19-0	2,4,6,8-Tetrachlorodibenzofuran	305.89	1	50	1.20E-04	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1234	58802-19-0	2,4,6,8-Tetrachlorodibenzofuran	305.89	1	75	3.10E-03	13	
1235	58802-19-0	2,4,6,8-Tetrachlorodibenzofuran	305.89	1	100	5.10E-02	13	
1236	58802-19-0	2,4,6,8-Tetrachlorodibenzofuran	305.89	1	125	5.90E-01	13	
1237	83704-47-6	1,2,3,4,6-Pentachlorodibenzofuran	340.31	1	25	3.60E-07	13	
1238	83704-47-6	1,2,3,4,6-Pentachlorodibenzofuran	340.31	1	50	2.10E-05	13	
1239	83704-47-6	1,2,3,4,6-Pentachlorodibenzofuran	340.31	1	75	6.90E-04	13	
1240	83704-47-6	1,2,3,4,6-Pentachlorodibenzofuran	340.31	1	100	1.40E-02	13	
1241	83704-47-6	1,2,3,4,6-Pentachlorodibenzofuran	340.31	1	125	2.00E-01	13	
1242	67517-48-0	1,2,3,4,8-Pentachlorodibenzofuran	340.31	1	25	4.80E-07	13	
1243	67517-48-0	1,2,3,4,8-Pentachlorodibenzofuran	340.31	1	50	2.90E-05	13	
1244	67517-48-0	1,2,3,4,8-Pentachlorodibenzofuran	340.31	1	75	9.80E-04	13	
1245	67517-48-0	1,2,3,4,8-Pentachlorodibenzofuran	340.31	1	100	2.00E-02	13	
1246	67517-48-0	1,2,3,4,8-Pentachlorodibenzofuran	340.31	1	125	2.90E-01	13	
1247	57117-42-7	1,2,3,6,7-Pentachlorodibenzofuran	340.31	1	25	3.00E-07	13	
1248	57117-42-7	1,2,3,6,7-Pentachlorodibenzofuran	340.31	1	50	1.70E-05	13	
1249	57117-42-7	1,2,3,6,7-Pentachlorodibenzofuran	340.31	1	75	5.60E-04	13	
1250	57117-42-7	1,2,3,6,7-Pentachlorodibenzofuran	340.31	1	100	1.10E-02	13	
1251	57117-42-7	1,2,3,6,7-Pentachlorodibenzofuran	340.31	1	125	1.60E-01	13	
1252	57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	340.31	1	25	2.30E-07	13	
1253	57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	340.31	7	25	3.64E-05	24	
1254	57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	340.31	1	50	1.30E-05	13	
1255	57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	340.31	1	75	4.00E-04	13	
1256	57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	340.31	1	100	8.00E-03	13	
1257	57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	340.31	1	125	1.10E-01	13	
1258	83704-50-1	1,2,4,6,7-Pentachlorodibenzofuran	340.31	1	25	4.70E-07	13	
1259	83704-50-1	1,2,4,6,7-Pentachlorodibenzofuran	340.31	1	50	2.80E-05	13	
1260	83704-50-1	1,2,4,6,7-Pentachlorodibenzofuran	340.31	1	75	9.50E-04	13	
1261	83704-50-1	1,2,4,6,7-Pentachlorodibenzofuran	340.31	1	100	2.00E-02	13	
1262	83704-50-1	1,2,4,6,7-Pentachlorodibenzofuran	340.31	1	125	2.80E-01	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1263	69698-57-3	1,2,4,6,8-Pentachlorodibenzofuran	340.31	1	25	3.10E-07	13	
1264	69698-57-3	1,2,4,6,8-Pentachlorodibenzofuran	340.31	1	50	1.80E-05	13	
1265	69698-57-3	1,2,4,6,8-Pentachlorodibenzofuran	340.31	1	75	5.80E-04	13	
1266	69698-57-3	1,2,4,6,8-Pentachlorodibenzofuran	340.31	1	100	1.20E-02	13	
1267	69698-57-3	1,2,4,6,8-Pentachlorodibenzofuran	340.31	1	125	1.60E-01	13	
1268	58802-15-6	1,2,4,7,8-Pentachlorodibenzofuran	340.31	1	25	2.00E-07	13	
1269	58802-15-6	1,2,4,7,8-Pentachlorodibenzofuran	340.31	1	50	1.10E-05	13	
1270	58802-15-6	1,2,4,7,8-Pentachlorodibenzofuran	340.31	1	75	3.40E-04	13	
1271	58802-15-6	1,2,4,7,8-Pentachlorodibenzofuran	340.31	1	100	6.70E-03	13	
1272	58802-15-6	1,2,4,7,8-Pentachlorodibenzofuran	340.31	1	125	9.10E-02	13	
1273	71998-74-8	1,2,4,7,9-Pentachlorodibenzofuran	340.31	1	25	3.50E-07	13	
1274	71998-74-8	1,2,4,7,9-Pentachlorodibenzofuran	340.31	1	50	2.00E-05	13	
1275	71998-74-8	1,2,4,7,9-Pentachlorodibenzofuran	340.31	1	75	6.70E-04	13	
1276	71998-74-8	1,2,4,7,9-Pentachlorodibenzofuran	340.31	1	100	1.40E-02	13	
1277	71998-74-8	1,2,4,7,9-Pentachlorodibenzofuran	340.31	1	125	1.90E-01	13	
1278	69433-00-7	1,2,6,7,8-Pentachlorodibenzofuran	340.31	1	25	2.50E-07	13	
1279	69433-00-7	1,2,6,7,8-Pentachlorodibenzofuran	340.31	1	50	1.40E-05	13	
1280	69433-00-7	1,2,6,7,8-Pentachlorodibenzofuran	340.31	1	75	4.40E-04	13	
1281	69433-00-7	1,2,6,7,8-Pentachlorodibenzofuran	340.31	1	100	8.80E-03	13	
1282	69433-00-7	1,2,6,7,8-Pentachlorodibenzofuran	340.31	1	125	1.20E-01	13	
1283	83704-36-3	1,3,4,6,7-Pentachlorodibenzofuran	340.31	1	25	3.60E-07	13	
1284	83704-36-3	1,3,4,6,7-Pentachlorodibenzofuran	340.31	1	50	2.10E-05	13	
1285	83704-36-3	1,3,4,6,7-Pentachlorodibenzofuran	340.31	1	75	6.80E-04	13	
1286	83704-36-3	1,3,4,6,7-Pentachlorodibenzofuran	340.31	1	100	1.40E-02	13	
1287	83704-36-3	1,3,4,6,7-Pentachlorodibenzofuran	340.31	1	125	2.00E-01	13	
1288	58802-16-7	1,3,4,7,8-Pentachlorodibenzofuran	340.31	1	25	5.70E-07	13	
1289	58802-16-7	1,3,4,7,8-Pentachlorodibenzofuran	340.31	1	50	3.50E-05	13	
1290	58802-16-7	1,3,4,7,8-Pentachlorodibenzofuran	340.31	1	75	1.20E-03	13	
1291	58802-16-7	1,3,4,7,8-Pentachlorodibenzofuran	340.31	1	100	2.50E-02	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1292	58802-16-7	1,3,4,7,8-Pentachlorodibenzofuran	340.31	1	125	3.60E-01	13	
1293	57117-43-8	2,3,4,6,7-Pentachlorodibenzofuran	340.31	1	25	3.20E-07	13	
1294	57117-43-8	2,3,4,6,7-Pentachlorodibenzofuran	340.31	1	50	1.90E-05	13	
1295	57117-43-8	2,3,4,6,7-Pentachlorodibenzofuran	340.31	1	75	6.10E-04	13	
1296	57117-43-8	2,3,4,6,7-Pentachlorodibenzofuran	340.31	1	100	1.20E-02	13	
1297	57117-43-8	2,3,4,6,7-Pentachlorodibenzofuran	340.31	1	125	1.70E-01	13	
1298	67481-22-5	2,3,4,6,8-Pentachlorodibenzofuran	340.31	1	25	2.50E-07	13	
1299	67481-22-5	2,3,4,6,8-Pentachlorodibenzofuran	340.31	1	50	1.40E-05	13	
1300	67481-22-5	2,3,4,6,8-Pentachlorodibenzofuran	340.31	1	75	4.50E-04	13	
1301	67481-22-5	2,3,4,6,8-Pentachlorodibenzofuran	340.31	1	100	8.90E-03	13	
1302	67481-22-5	2,3,4,6,8-Pentachlorodibenzofuran	340.31	1	125	1.20E-01	13	
1303	51207-31-4	2,3,4,7,8-Pentachlorodibenzofuran	340.31	1	25	3.50E-07	13	
1304	51207-31-4	2,3,4,7,8-Pentachlorodibenzofuran	340.31	7	25	2.17E-05	24	
1305	51207-31-4	2,3,4,7,8-Pentachlorodibenzofuran	340.31	1	50	2.10E-05	13	
1306	51207-31-4	2,3,4,7,8-Pentachlorodibenzofuran	340.31	1	75	6.70E-04	13	
1307	51207-31-4	2,3,4,7,8-Pentachlorodibenzofuran	340.31	1	100	1.40E-02	13	
1308	51207-31-4	2,3,4,7,8-Pentachlorodibenzofuran	340.31	1	125	1.90E-01	13	
1309	79060-60-9	1,2,3,4,6,7-Hexachlorodibenzofuran	374.73	1	25	3.20E-08	13	
1310	79060-60-9	1,2,3,4,6,7-Hexachlorodibenzofuran	374.73	1	50	2.30E-06	13	
1311	79060-60-9	1,2,3,4,6,7-Hexachlorodibenzofuran	374.73	1	75	9.00E-05	13	
1312	79060-60-9	1,2,3,4,6,7-Hexachlorodibenzofuran	374.73	1	100	2.20E-03	13	
1313	79060-60-9	1,2,3,4,6,7-Hexachlorodibenzofuran	374.73	1	125	3.50E-02	13	
1314	69698-60-8	1,2,3,4,6,8-Hexachlorodibenzofuran	374.73	1	25	2.90E-08	13	
1315	69698-60-8	1,2,3,4,6,8-Hexachlorodibenzofuran	374.73	1	50	2.10E-06	13	
1316	69698-60-8	1,2,3,4,6,8-Hexachlorodibenzofuran	374.73	1	75	8.10E-05	13	
1317	69698-60-8	1,2,3,4,6,8-Hexachlorodibenzofuran	374.73	1	100	1.90E-03	13	
1318	69698-60-8	1,2,3,4,6,8-Hexachlorodibenzofuran	374.73	1	125	3.10E-02	13	
1319	91538-83-9	1,2,3,4,6,9-Hexachlorodibenzofuran	374.73	1	25	5.50E-08	13	
1320	91538-83-9	1,2,3,4,6,9-Hexachlorodibenzofuran	374.73	1	50	4.20E-06	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1321	91538-83-9	1,2,3,4,6,9-Hexachlorodibenzofuran	374.73	1	75	1.70E-04	13	
1322	91538-83-9	1,2,3,4,6,9-Hexachlorodibenzofuran	374.73	1	100	4.20E-03	13	
1323	91538-83-9	1,2,3,4,6,9-Hexachlorodibenzofuran	374.73	1	125	7.00E-02	13	
1324	70658-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	374.73	1	25	3.20E-08	13	
1325	70658-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	374.73	1	50	2.40E-06	13	
1326	70658-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	374.73	1	75	9.30E-05	13	
1327	70658-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	374.73	1	100	2.20E-03	13	
1328	70658-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	374.73	1	125	3.60E-02	13	
1329	91538-84-0	1,2,3,4,7,9-Hexachlorodibenzofuran	374.73	1	25	3.80E-08	13	
1330	91538-84-0	1,2,3,4,7,9-Hexachlorodibenzofuran	374.73	1	50	2.80E-06	13	
1331	91538-84-0	1,2,3,4,7,9-Hexachlorodibenzofuran	374.73	1	75	1.10E-04	13	
1332	91538-84-0	1,2,3,4,7,9-Hexachlorodibenzofuran	374.73	1	100	2.70E-03	13	
1333	91538-84-0	1,2,3,4,7,9-Hexachlorodibenzofuran	374.73	1	125	4.40E-02	13	
1334	57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	374.73	1	25	2.90E-08	13	
1335	57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	374.73	1	50	2.10E-06	13	
1336	57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	374.73	1	75	8.50E-05	13	
1337	57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	374.73	1	100	2.00E-03	13	
1338	57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	374.73	1	125	3.10E-02	13	
1339	75198-38-8	1,2,3,6,8,9-Hexachlorodibenzofuran	374.73	1	25	4.50E-08	13	
1340	75198-38-8	1,2,3,6,8,9-Hexachlorodibenzofuran	374.73	1	50	3.40E-06	13	
1341	75198-38-8	1,2,3,6,8,9-Hexachlorodibenzofuran	374.73	1	75	1.40E-04	13	
1342	75198-38-8	1,2,3,6,8,9-Hexachlorodibenzofuran	374.73	1	100	3.30E-03	13	
1343	75198-38-8	1,2,3,6,8,9-Hexachlorodibenzofuran	374.73	1	125	5.50E-02	13	
1344	67562-40-7	1,2,4,6,7,8-Hexachlorodibenzofuran	374.73	1	25	3.50E-08	13	
1345	67562-40-7	1,2,4,6,7,8-Hexachlorodibenzofuran	374.73	1	50	2.60E-06	13	
1346	67562-40-7	1,2,4,6,7,8-Hexachlorodibenzofuran	374.73	1	75	1.00E-04	13	
1347	67562-40-7	1,2,4,6,7,8-Hexachlorodibenzofuran	374.73	1	100	2.40E-03	13	
1348	67562-40-7	1,2,4,6,7,8-Hexachlorodibenzofuran	374.73	1	125	4.00E-02	13	
1349	75627-02-0	1,2,4,6,7,9-Hexachlorodibenzofuran	374.73	1	25	7.60E-08	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1350	75627-02-0	1,2,4,6,7,9-Hexachlorodibenzofuran	374.73	1	50	5.90E-06	13	
1351	75627-02-0	1,2,4,6,7,9-Hexachlorodibenzofuran	374.73	1	75	2.50E-04	13	
1352	75627-02-0	1,2,4,6,7,9-Hexachlorodibenzofuran	374.73	1	100	6.20E-03	13	
1353	75627-02-0	1,2,4,6,7,9-Hexachlorodibenzofuran	374.73	1	125	1.00E-01	13	
1354	69698-59-5	1,2,4,6,8,9-Hexachlorodibenzofuran	374.73	1	25	2.40E-08	13	
1355	69698-59-5	1,2,4,6,8,9-Hexachlorodibenzofuran	374.73	1	50	1.70E-06	13	
1356	69698-59-5	1,2,4,6,8,9-Hexachlorodibenzofuran	374.73	1	75	6.40E-05	13	
1357	69698-59-5	1,2,4,6,8,9-Hexachlorodibenzofuran	374.73	1	100	1.50E-03	13	
1358	69698-59-5	1,2,4,6,8,9-Hexachlorodibenzofuran	374.73	1	125	2.40E-02	13	
1359	71998-75-9	1,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	25	3.10E-08	13	
1360	71998-75-9	1,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	50	2.20E-06	13	
1361	71998-75-9	1,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	75	8.70E-05	13	
1362	71998-75-9	1,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	100	2.10E-03	13	
1363	71998-75-9	1,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	125	3.40E-02	13	
1364	60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	25	2.60E-08	13	
1365	60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	50	1.90E-06	13	
1366	60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	75	7.30E-05	13	
1367	60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	100	1.70E-03	13	
1368	60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	374.73	1	125	2.80E-02	13	
1369	67462-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	409.15	1	25	4.70E-09	13	
1370	67462-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	409.15	1	50	4.30E-07	13	
1371	67462-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	409.15	1	75	2.00E-05	13	
1372	67462-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	409.15	1	100	5.80E-04	13	
1373	67462-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	409.15	1	125	1.20E-02	13	
1374	67462-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	409.15	7	25	2.24E-06	24	
1375	69698-58-4	1,2,3,4,6,8,9-Heptachlorodibenzofuran	409.15	1	25	7.70E-09	13	
1376	69698-58-4	1,2,3,4,6,8,9-Heptachlorodibenzofuran	409.15	1	50	7.20E-07	13	
1377	69698-58-4	1,2,3,4,6,8,9-Heptachlorodibenzofuran	409.15	1	75	3.60E-05	13	
1378	69698-58-4	1,2,3,4,6,8,9-Heptachlorodibenzofuran	409.15	1	100	1.00E-03	13	

Table 7. Physical property data for polychlorinated dibenzofurans

Table 7.b. Vapor pressure data, Pa, polychlorinated dibenzofurans, continued								
Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1379	69698-58-4	1,2,3,4,6,8,9-Heptachlorodibenzofuran	409.15	1	125	2.00E-02	13	
1380	55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	409.15	1	25	6.20E-09	13	
1381	55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	409.15	7	25	1.31E-06	24	
1382	55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	409.15	1	50	5.80E-07	13	
1383	55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	409.15	1	75	2.80E-05	13	
1384	55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	409.15	1	100	8.00E-04	13	
1385	55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	409.15	1	125	1.50E-02	13	

Table 8. Physical constant data for agrochemicals

Table 8. Physical constant data for agrochemicals

Table 8.a. Aqueous solubility data, mg / L, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1386	15972-60-8	alachlor	269.77	11	25	2.42E+02	42	
1387	309-00-2	aldrin	364.93	11	20	2.00E-02	46	
1388	959-98-8	α-endosulfan (endosulfan-I)	406.92	11	25	5.30E-01	42	
1389	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	11	20	1.63E+00	42	
1390	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	11	not rep.	1.40E+00	45	saltwater
1391	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	11	20	1.00E+00	46	
1392	319-85-7	β-hexachlorocyclohexane (HCH)	290.83	11	25	2.40E-01	42	
1393	319-85-7	β-hexachlorocyclohexane (HCH)	290.83	11	20	1.00E-01	46	
1394	5103-74-2	*cis* -chlordane	409.78	11	20-25	5.10E-02	42	
1395	2921-88-2	chloropyrifos	350.59	11	10	4.50E-01	42	
1396	2921-88-2	chloropyrifos	350.59	11	20	7.30E-01	42	
1397	2921-88-2	chloropyrifos	350.59	11	30	1.30E+00	42	
1398	53-19-0	*o,p'*-DDD	320.05	11	20	1.00E-01	46	
1399	72-54-8	*p,p'*-DDD	320.05	11	20	5.00E-02	46	
1400	3424-82-6	*o,p'*-DDE	319.03	11	20	1.00E-01	46	
1401	72-55-9	*p,p'*-DDE	319.03	11	20	4.00E-02	46	
1402	333-41-5	diazinon	304.35	11	10	7.11E+01	42	
1403	333-41-5	diazinon	304.35	11	20	5.35E+01	42	
1404	333-41-5	diazinon	304.35	11	30	4.37E+01	42	
1405	60-57-1	dieldrin	380.91	11	not rep.	1.00E-01	45	
1406	60-57-1	dieldrin	380.91	11	10	8.00E-02	42	
1407	60-57-1	dieldrin	380.91	11	20	1.40E-01	42	
1408	60-57-1	dieldrin	380.91	11	30	2.00E-01	42	
1409	72-20-8	endrin	380.93	11	20	2.30E-01	46	
1410	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	11	20	6.50E+00	46	
1411	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	11	24	1.70E+01	42	
1412	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	11	24	1.70E+01	45	
1413	76-44-8	heptachlor	373.32	11	25	1.80E-01	42	

Table 8. Physical constant data for agrochemicals

Table 8.a. Aqueous solubility data, mg / L, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1414	76-44-8	heptachlor	373.32	11	20	1.00E-01	46	
1415	1024-57-3	heptachlor epoxide	389.3	11	25	2.75E-01	42	
1416	118-74-1	hexachlorobenzene (HCB)	284.8	11	20	4.00E-02	46	
1417	118-74-1	hexachlorobenzene (HCB)	284.8	11	20	4.00E-02	42	
1418	118-74-1	hexachlorobenzene (HCB)	284.8	11	24	1.10E-01	45	
1419	118-74-1	hexachlorobenzene (HCB)	284.8	4,9	25	4.70E-02	21	
1420	2385-85-5	mirex	545.59	11	20	6.50E-05	46	
1421	1582-09-8	trifluralin	335.29	11	27	4.00E+00	42	

Table 8. Physical constant data for agrochemicals

Table 8.b. Vapor pressure data, Pa, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1422	15972-60-8	alachlor	269.77	11	25	4.13E-03	42	
1423	309-00-2	aldrin	364.93	8	20	3.08E-03	42	
1424	309-00-2	aldrin	364.93	8	20	5.00E-03	46	
1425	309-00-2	aldrin	364.92	8	20	3.08E-03	42	
1426	309-00-2	aldrin	364.92	7	25	2.29E-02	14	
1427	309-00-2	aldrin	364.92	7	25	3.33E-02	14	
1428	5103-74-2	*cis* -chlordane	409.78	1,8	23	1.11E-02	42	
1429	5103-74-2	*cis* -chlordane	409.78	7	25	4.80E-03	51	
1430	5103-71-9	*trans* -chlordane	409.78	7	25	6.70E-03	51	
1431	2921-88-2	chloropyrifos	350.59	8	25	2.49E-03	42	
1432	2921-88-2	chloropyrifos	350.59	7	25	6.70E-03	51	
1433	53-19-0	*o,p'*-DDD	320.00	8	20	2.00E-04	46	
1434	72-54-8	*p,p'*-DDD	320.05	8	20	1.00E-04	46	
1435	72-54-8	*p,p'*-DDD	320.05	8	25	6.20E-04	42	
1436	72-54-8	*p,p'*-DDD	320.05	7	25	1.60E-03	14	
1437	72-54-8	*p,p'*-DDD	320.05	7	25	6.20E-04	14	
1438	3424-82-6	*o,p'*-DDE	319.03	8	20	8.00E-04	46	
1439	72-55-9	*p,p'*-DDE	319.03	8	20	1.00E-03	46	
1440	72-55-9	*p,p'*-DDE	319.03	8	25	2.10E-03	42	
1441	72-55-9	*p,p'*-DDE	319.03	7	25	2.70E-03	14	
1442	72-55-9	*p,p'*-DDE	319.03	7	25	2.10E-03	14	
1443	789-02-6	*o,p'*-DDT	354.49	7	25	1.60E-03	14	
1444	789-02-6	*o,p'*-DDT	354.49	7	25	1.30E-03	14	
1445	50-29-3	*p,p'*-DDT	354.49	7	25	8.30E-04	14	
1446	50-29-3	*p,p'*-DDT	354.49	7	25	4.70E-04	14	
1447	333-41-5	diazinon	304.35	8	20	1.13E-02	42	
1448	333-41-5	diazinon	304.35	8	20	1.13E-02	42	
1449	333-41-5	diazinon	304.35	7	25	2.00E-02	51	
1450	60-57-1	dieldrin	380.91	8	20	2.37E-05	42	

Table 8. Physical constant data for agrochemicals

Table 8.b. Vapor pressure data, Pa, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1451	60-57-1	dieldrin	380.91	8	20	5.00E-04	46	
1452	60-57-1	dieldrin	380.91	8	25	2.39E-05	45	
1453	60-57-1	dieldrin	380.91	7	25	5.32E-03	14	
1454	60-57-1	dieldrin	380.91	7	25	5.97E-03	14	
1455	959-98-8	α-endosulfan (endosulfan-I)	406.92	8	25	1.33E-03	42	
1456	959-98-8	α-endosulfan (endosulfan-I)	406.92	7	25	6.10E-03	51	
1457	33213-65-9	β-endosulfan (endosulfan-II)	406.92	7	25	3.20E-03	51	
1458	1031-07-8	endosulfan sulfate	422.92	7	25	1.30E-03	51	
1459	72-20-8	endrin	380.92	8	20	2.00E-05	46	
1460	72-20-8	endrin	380.92	8	25	9.33E-05	42	
1461	76-44-8	heptachlor	373.32	8	20	4.00E-02	42	
1462	76-44-8	heptachlor	373.32	8	20	3.00E-02	46	
1463	76-44-8	heptachlor	373.32	8	25	3.99E-02	45	
1464	76-44-8	heptachlor	373.32	7	25	3.10E-02	51	
1465	1024-57-3	heptachlor epoxide	389.3	8	20	3.47E-04	42	
1466	118-74-1	hexachlorobenzene (HCB)	284.8	8	20	1.45E-03	42	
1467	118-74-1	hexachlorobenzene (HCB)	284.8	8	20	1.00E-03	46	
1468	118-74-1	hexachlorobenzene (HCB)	284.8	8	not rep.	1.45E-03	45	
1469	118-74-1	hexachlorobenzene (HCB)	284.8	7	25	1.22E-01	14	
1470	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	8	20	3.33E-03	42	
1471	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	8	20	3.00E-03	46	
1472	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	7	25	2.30E-01	51	
1473	319-85-7	β-hexachlorocyclohexane (HCH)	290.83	8	20	3.73E-05	42	
1474	319-85-7	β-hexachlorocyclohexane (HCH)	290.83	8	20	4.00E-05	46	
1475	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	8	20	1.25E-03	42	
1476	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	8	20	3.00E-03	46	
1477	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	7	25	1.07E-01	14	
1478	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	7	25	6.54E-02	14	
1479	2385-85-5	mirex	545.59	8	20	1.00E-04	46	

Table 8. Physical constant data for agrochemicals

Table 8.b. Vapor pressure data, Pa, agrochemicals								
Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1480	2385-85-5	mirex	545.59	7	25	2.80E-04	51	
1481	5103-73-1	*cis* -nonachlor	443.75	7	25	1.60E-03	51	
1482	39765-80-5	*trans* -nonachlor	443.75	7	25	3.70E-03	51	
1483	1582-09-8	trifluralin	335.29	11	25	1.47E-02	42	

Table 8. Physical constant data for agrochemicals

Table 8.c. Henry's law constant data, Pa m^3 / mol, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1484	15972-60-8	alachlor	269.77	4	23	8.37E-04	49	
1485	15972-60-8	alachlor	269.77	8	23	1.23E-03	48	drain, 22-24 C
1486	15972-60-8	alachlor	269.77	8	23	9.85E-04	48	cyclone, 22-24 C
1487	15972-60-8	alachlor	269.77	1,7	25	6.20E-03	42	
1488	309-00-2	aldrin	364.92	1,7	20	9.12E+01	46	
1489	309-00-2	aldrin	364.92	7	25	5.03E+01	42	
1490	5103-74-2	*cis* -chlordane	409.78	2	23	8.86E+01	50	distilled water
1491	5103-74-2	*cis* -chlordane	409.78	2	23	4.19E+02	50	seawater
1492	5103-71-9	*trans* -chlordane	409.78	8	23	5.42E+00	48	drain, 22-24 C
1493	5103-71-9	*trans* -chlordane	409.78	8	23	5.91E+00	48	cyclone, 22-24 C
1494	5103-71-9	*trans* -chlordane	409.78	4	23	8.37E+00	48	
1495	5103-71-9	*trans* -chlordane	409.78	2	23	1.35E+02	50	distilled water
1496	5103-71-9	*trans* -chlordane	409.78	2	23	5.66E+02	50	seawater
1497	2921-88-2	chlorpyrifos	350.59	4	8.3	3.30E-01	47	sub. Arctic water[1,6]
1498	2921-88-2	chlorpyrifos	350.59	4	8.3	2.76E-01	47	sml Arctic water[2,6]
1499	2921-88-2	chlorpyrifos	350.59	4	8.3	3.28E-01	47	sub. Arctic water[3,6]
1500	2921-88-2	chlorpyrifos	350.59	4	8.3	2.85E-01	47	sml Arctic water[4,6]
1501	2921-88-2	chlorpyrifos	350.59	4	8.3	2.18E-01	47	Arctic ice[5,6]
1502	2921-88-2	chlorpyrifos	350.59	4	20	4.14E-01	47	sub. Arctic water[1,6]
1503	2921-88-2	chlorpyrifos	350.59	4	20	3.56E-01	47	sml Arctic water[2,6]
1504	2921-88-2	chlorpyrifos	350.59	4	20	4.24E-01	47	sub. Arctic water[3,6]
1505	2921-88-2	chlorpyrifos	350.59	4	20	3.68E-01	47	sml Arctic water[4,6]
1506	2921-88-2	chlorpyrifos	350.59	4	20	2.68E-01	47	Arctic ice[5,6]
1507	2921-88-2	chlorpyrifos	350.59	4	43.5	8.69E-01	47	sub. Arctic water[1,6]
1508	2921-88-2	chlorpyrifos	350.59	4	43.5	7.98E-01	47	sml Arctic water[2,6]
1509	2921-88-2	chlorpyrifos	350.59	4	43.5	7.82E-01	47	sub. Arctic water[3,6]
1510	2921-88-2	chlorpyrifos	350.59	4	43.5	7.50E-01	47	sml Arctic water[4,6]
1511	2921-88-2	chlorpyrifos	350.59	4	43.5	6.16E-01	47	Arctic ice[5,6]

Table 8. Physical constant data for agrochemicals

Table 8.c. Henry's law constant data, Pa m^3 / mol, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1512	2921-88-2	chlorpyrifos	350.59	4	25	4.21E-01	33	distilled water
1513	2921-88-2	chlorpyrifos	350.59	4	20	4.92E-01	47	33.3% saltwater
1514	2921-88-2	chlorpyrifos	350.59	4	20	3.17E-01	47	distilled water
1517	53-19-0	*o,p'*-DDD	320.00	1,7	20	6.40E-01	46	
1518	72-54-8	*p,p'*-DDD	320.05	1,7	20	6.40E-01	46	
1519	72-54-8	*p,p'*-DDD	320.05	1,7	23	2.18E+00	42	
1520	3424-82-6	*o,p'*-DDE	319.03	1,7	20	2.54E+00	46	
1521	72-55-9	*p,p'*-DDE	319.03	1,7	20	7.95E+00	46	
1522	72-55-9	*p,p'*-DDE	319.03	2	23	1.23E+02	50	distilled water
1523	72-55-9	*p,p'*-DDE	319.03	2	23	3.69E+02	50	seawater
1524	50-29-3	*p,p'*-DDT	354.49	7	23	1.30E+00	42	
1525	333-41-5	diazinon	304.35	8	23	1.38E-02	48	drain, 22-24 C
1526	333-41-5	diazinon	304.35	8	23	1.01E-02	48	cyclone, 22-24 C
1527	333-41-5	diazinon	304.35	4	23	1.13E-02	49	
1528	60-57-1	dieldrin	380.91	1,7	20	1.12E+00	46	
1529	60-57-1	dieldrin	380.91	7	25	5.88E+00	42	
1530	959-98-8	α-endosulfan (endosulfan-I)	406.92	4	20	1.29E+01	47	33.3% saltwater
1531	959-98-8	α-endosulfan (endosulfan-I)	406.92	4	20	6.63E+00	47	distilled water
1532	959-98-8	α-endosulfan (endosulfan-I)	406.92	7	25	1.02E+01	42	
1533	33213-65-9	β-endosulfan (endosulfan-II)	406.92	4	20	2.12E+00	47	33.3% saltwater
1534	33213-65-9	β-endosulfan (endosulfan-II)	406.92	4	20	8.77E-01	47	distilled water
1535	72-20-8	endrin	380.92	7	not rep.	5.07E-02	42	
1536	72-20-8	endrin	380.92	1,7	20	3.30E-02	46	
1537	76-44-8	heptachlor	373.32	7	not rep.	2.33E+02	42	
1538	76-44-8	heptachlor	373.32	1,7	20	1.12E+02	46	
1539	1024-57-3	heptachlor epoxide	389.3	7	25	3.24E+00	42	
1540	118-74-1	hexachlorobenzene (HCB)	284.8	4	14.8	2.36E+01	36	
1541	118-74-1	hexachlorobenzene (HCB)	284.8	7	20	7.19E+02	42	

Table 8. Physical constant data for agrochemicals

Table 8.c. Henry's law constant data, Pa m^3 / mol, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1542	118-74-1	hexachlorobenzene (HCB)	284.8	1,7	20	7.12E+00	46	
1543	118-74-1	hexachlorobenzene (HCB)	284.8	4	20.1	3.00E+01	36	
1544	118-74-1	hexachlorobenzene (HCB)	284.8	4	22.1	4.66E+01	36	
1545	118-74-1	hexachlorobenzene (HCB)	284.8	2	23	1.33E+02	50	distilled water
1546	118-74-1	hexachlorobenzene (HCB)	284.8	2	23	1.72E+02	50	seawater
1547	118-74-1	hexachlorobenzene (HCB)	284.8	4	24.2	5.25E+01	36	
1548	118-74-1	hexachlorobenzene (HCB)	284.8	5	26	2.62E+04	30	
1549	118-74-1	hexachlorobenzene (HCB)	284.8	4	34.8	8.83E+01	36	
1550	118-74-1	hexachlorobenzene (HCB)	284.8	4	50.5	2.17E+02	36	
1551	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	0.5	1.40E-01	44	
1552	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	0.5	1.40E-01	44	seawater
1553	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	10	2.55E-01	44	
1554	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	10	2.57E-01	44	seawater
1555	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	1,7	20	5.37E-01	42	
1556	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	1,7	20	8.70E-01	46	
1557	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	23	6.77E-01	44	
1558	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	23	7.10E-01	44	seawater
1559	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	23	2.36E+00	50	distilled water
1560	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	23	1.08E+00	50	seawater
1561	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	35	1.34E+00	44	
1562	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	35	2.10E+00	44	seawater
1563	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	45	3.27E+00	44	
1564	319-84-6	α-hexachlorocyclohexane (HCH)	290.83	2	45	5.99E+00	44	seawater
1565	319-85-7	β-hexachlorocyclohexane (HCH)	290.83	1,7	20	1.20E-01	46	
1566	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	0.5	7.21E-02	44	
1567	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	0.5	6.27E-02	44	seawater
1568	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	10	1.26E-01	44	
1569	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	10	1.37E-01	44	seawater

Table 8. Physical constant data for agrochemicals

Table 8.c. Henry's law constant data, Pa m^3 / mol, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1570	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	1,7	20	1.30E-01	46	
1571	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	23	3.39E-01	44	
1572	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	23	3.63E-01	44	seawater
1573	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	7	23	2.46E-02	42	
1574	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	4	23	2.02E-01	49	
1575	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	8	23	1.99E-01	48	drain, 22-24 C
1576	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	8	23	2.09E-01	48	cyclone, 22-24 C
1577	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	35	6.24E-01	44	
1578	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	35	9.96E-01	44	seawater
1579	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	45	1.17E+00	44	
1580	58-89-9	γ-hexachlorocyclohexane (HCH)	290.83	2	45	2.57E+00	44	seawater
1581	2385-85-5	mirex	545.59	1,7	20	8.39E+02	46	
1582	2385-85-5	mirex	545.59	5	22	5.23E+01	43	
1584	298-00-0	methyl parathion	263.23	4	20	3.83E-03	47	distilled water
1585	298-00-0	methyl parathion	263.23	4	25	6.20E-03	33	
1586	51218-45-2	metolachlor	283.81	4	20	7.82E-03	47	distilled water
1587	1582-09-8	trifluralin	335.29	4	8.3	8.26E+00	47	sml Arctic water[2,6]
1588	1582-09-8	trifluralin	335.29	4	8.3	8.61E+00	47	sub. Arctic water[3,6]
1589	1582-09-8	trifluralin	335.29	4	8.3	7.72E+00	47	sml Arctic water[4,6]
1590	1582-09-8	trifluralin	335.29	4	8.3	6.79E+00	47	Arctic ice[5,6]
1591	1582-09-8	trifluralin	335.29	4	20	1.31E+01	47	sub. Arctic water[1,6]
1592	1582-09-8	trifluralin	335.29	4	20	1.28E+01	47	sml Arctic water[2,6]
1593	1582-09-8	trifluralin	335.29	4	20	1.23E+01	47	sub. Arctic water[3,6]
1594	1582-09-8	trifluralin	335.29	4	20	1.20E+01	47	sml Arctic water[4,6]
1595	1582-09-8	trifluralin	335.29	4	20	9.94E+00	47	Arctic ice[5,6]
1596	1582-09-8	trifluralin	335.29	4	43.5	1.97E+01	47	sub. Arctic water[1,6]
1597	1582-09-8	trifluralin	335.29	4	43.5	1.96E+01	47	sml Arctic water[2,6]
1598	1582-09-8	trifluralin	335.29	4	43.5	1.97E+01	47	sub. Arctic water[3,6]

Table 8.c. Henry's law constant data, Pa m^3 / mol, agrochemicals

Entry #	CAS #	Common Name	Molecular Wt. (amu)	Method I.D.	Temp °C	Value	Ref. #	Phase
1599	1582-09-8	trifluralin	335.29	4	43.5	1.94E+01	47	sml Arctic water[4,6]
1600	1582-09-8	trifluralin	335.29	4	43.5	1.58E+01	47	Arctic ice[5,6]
1601	1582-09-8	trifluralin	335.29	4	20	1.51E+01	47	33.3% saltwater
1602	1582-09-8	trifluralin	335.29	4	20	1.04E+01	47	distilled water
1603	1582-09-8	trifluralin	335.29	4	23	5.91E+00	48	distilled water
1604	1582-09-8	trifluralin	335.29	8	23	4.68E+00	48	drain, 22-24 C
1605	1582-09-8	trifluralin	335.29	8	23	5.66E+00	48	cyclone, 22-24 C

[1] subsurface Bering Sea whole-water, collected using a submersible pump

[2] surface microlayer Bering Sea whole-water, collected using a stainless steel mesh screen

[3] subsurface Chukchi Sea whole-water, collected using a submersible pump

[4] surface microlayer Chukchi Sea whole-water, collected using a stainless steel mesh screen

[5] surface Arctic ice

[6] sampling procedures described by Chernyak, S.M.; Rice, C.P.; McConnell, L.L. *Mar. Pollut. Bull*. **1996**, *32*, 410

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