A Comprehensive and Critical Compilation, Evaluation, and Selection of Physical–Chemical Property Data for Selected Polychlorinated Biphenyls

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Accurate physical–chemical properties (aqueous solubility S_W, octanol–water partition coefficient K_{OW}, vapor pressure P, Henry's law constant H, octanol–air partition coefficient K_{OA}, octanol solubility S_O) are of fundamental importance for modeling the transport and fate of organic pollutants in the environment. Energies of phase transfer are used to describe the temperature dependence of these properties. When trying to quantify the behavior of contaminant mixtures such as the polychlorinated biphenyls, consistent physical–chemical properties are required for each individual congener. A complete set of temperature dependent property data for sixteen polychlorinated biphenyls (PCB-3, 8, 15, 28, 29, 31, 52, 61, 101, 105, 118, 138, 153, 155, 180, 194) was derived, based on all experimentally obtained values reported for these congeners in the literature. Log mean values derived from the experimental data were adjusted to yield an internally consistent set of data for each congener. These adjusted data also show a greater degree of interhomologue consistency, which can be illustrated with the help of simple quantitative structure-property relationships that use molar mass and the number of chlorine substitutions in *ortho*-positions as descriptors. The extent of the required adjustment gives an indication of the uncertainty of the averaged measured values and is typically lower than might be expected from the range of the reported measured values. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1562632]

Key words: aqueous solubility, congeners, energy of phase transfer, Henry's law constant, octanol–air partition coefficient, octanol solubility, octanol–water partition coefficient, physical-chemical properties, polychlorinated biphenyls, vapor pressure.

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1. Introduction

The environmental fate of a persistent organic chemical is strongly influenced by its distribution between various phases or compartments. Environmental chemists rely traditionally on the equilibrium partitioning coefficients between the gas phase, the aqueous phase, and the liquid octanol phase to characterize phase distribution in the environment. Of particular importance in this regard are an organic chemical's aqueous solubility (S_{W}), vapor pressure (P), octanol–water partition coefficient (K_{OW}), Henry's law constant (H), octanol–air partition coefficient (K_{OA}), and solubility in octanol (S_{O}). Simple empirical relationships with these physical–chemical properties are used to describe partitioning into environmental phases and organisms. Pollutant fate models incorporate these empirical relationships and thus usually require the physical–chemical properties as input parameters. If the fate of a chemical at temperatures other than 20 or 25 °C is of interest, the temperature dependence of the physical–chemical properties becomes important. Over relatively small environmentally relevant temperature ranges, that temperature dependence can be conveniently expressed through the respective internal energies of phase transfer ΔU.

Polychlorinated biphenyls (PCBs) are among the most studied persistent organic pollutants, and much has been learned about the environmental behavior of persistent organic substances from studying PCBs. Of particular significance in this respect is the fact that the PCBs comprise a large number of congeners which differ substantially in their partitioning characteristics and environmental fate. For example, the least chlorinated congeners occur in the atmosphere as gaseous compounds, whereas decachlorobiphenyl is completely sorbed to atmospheric particles. It is possible to gain considerable insight into the fate of persistent organic pollutants in general by quantitatively understanding the differences in environmental behavior between different PCB congeners. This obviously requires quantitative knowledge of the physical–chemical properties of PCBs on a congener-specific basis.

There are numerous studies reporting physical–chemical properties of the PCBs. Even the lightest PCB congeners are rather sparingly soluble in water and have low volatility. As a result, the experimental determination of physical–chemical properties of this type of compound is a difficult task, and the reported values for a property from two independent measurements may show large discrepancy. Pontolillo and Eganhouse[1] illustrated this eloquently through a comprehensive and critical analysis of the scientific literature on the S_{W} and K_{OW} of p,p'-DDT and p,p'-DDE, two compounds with partitioning properties similar to the PCBs. Reporting errors, multilevel referencing, a common lack of precision information, as well as other problems lead to a multitude of property data with an intimidating degree of inconsistency. They concluded that it is impossible to derive the true S_{W} and K_{OW} value for these two compounds based on the available studies.

Even a cursory inspection of the available data suggests that similar problems exist for the PCBs. The issue of selecting data for the PCBs may seem even more daunting considering the large number of congeners. Nevertheless, there have been several attempts at deriving a consistent physical–chemical property data set for the PCBs. Paasivirta and collaborators derived internally consistent sets of physical–chemical property data for several classes of persistent organic compounds, including the PCBs.[2] However, they used only a very small fraction of the available empirical evidence. Shiu and Ma[3] presented an extensive review of PCB property data reported in the literature and also recommended a particular set of P, S_W, and H values, including their temperature dependence. It is not always obvious, however, how the selected values were derived. Neither were all measured data taken into account, nor are the selected property values internally consistent. Most recently, Beyer and co-workers presented an adjustment technique to derive internally consistent sets of property data for one chemical, and applied it to 12 PCB congeners.[4] They used the selected values by Shiu and Ma[3] and Mackay *et al.*[5] as a starting point, but neither evaluated whether these data were reasonable nor accounted for their relative uncertainty.

The ambition of this work was to use a rigorous and transparent procedure to derive a PCB property data set, that makes use of all available measured data. Reasons for not using a measured data point had to be stated. The outcome should be a set of properties, which is consistent in two regards:

(i) the six partitioning properties for each investigated PCB congener are consistent with each other, and
(ii) each of the six partitioning properties is consistent across homologue groups.

This was done for 16 PCB congeners by compiling and evaluating the measured data from the literature, selecting measured values through averaging or linear regression, making estimates of the uncertainty of these values, and finally applying the adjustment technique described by Beyer *et al.*[4]

2. Methods

The investigated set of compounds comprised the PCBs 3, 8, 15, 28, 29, 31, 52, 61, 101, 105, 118, 138, 153, 155, 180, and 194. A number of criteria were used in the selection of these congeners. The set needed to include a large variety of congeners, both in terms of the degree of chlorination and in terms of the substitution patterns. The set includes mono- through octachlorinated congeners, highly symmetrical congeners, such as PCB-15, and congeners with all chlorines on one of the two aromatic rings, such as PCB-29 and PCB-61. It also includes congeners with a variety of number of chlorines in the *ortho* position, including the tetra-*ortho* PCB-155. It also includes the congeners that are most commonly quantified in environmental samples, namely PCBs 28, 52, 101, 153, and 180. Finally, it was a prerequisite that a significant number of physical–chemical property measurements had been reported for a congener. It may be feasible to perform a similar analysis for a few additional PCB congeners, but for most of the 209 congeners the availability of measured data is too limited to apply the procedure with much confidence.

The following steps were involved in the process of compiling, evaluating, selecting and adjusting physical-chemical property data.

(i) Finding and Obtaining Original References: Using the Chemical Abstract Search Service Index (CASSI) and other databases,[5] we tried to obtain and identify all the published literature on measured physical–chemical properties for the selected congeners. It is quite likely that additional data sources exist that escaped our attention. Only original data sources are considered, i.e., no quoted values were included, thereby avoiding multilevel referencing.[1] Some studies reporting physical–chemical properties obtained by theoretical means such as quantitative structure–property relationships (QSPRs) were also obtained.

(ii) Compiling the Data in a Comparable Format: The measured data were compiled in spreadsheets, and converted into appropriate and identical units. The experimental temperature of the measurements was also noted. If no temperature was provided or the source indicated that the experiments were performed under ambient or room temperature conditions, we assumed a temperature of 23 °C. The vapor pressure and solubility values reported for the solid phase (P_S, S_{WS}, S_{OS}) were converted into the properties of the supercooled liquid (P_L, S_{WL}, S_{OL}) using compound specific entropy of fusion values $\Delta_{fus}S$ and melting point temperatures T_M in Eq. (1)

$$S_{WS}/S_{WL}=S_{OS}/S_{OL}=P_S/P_L =\exp(-\Delta_{fus}S\cdot(T_M/T-1)/R). \tag{1}$$

If a compound-specific $\Delta_{fus}S$ was not available, a generic default value of 56 $J\cdot K^{-1}\cdot mol^{-1}$ was used.

(iii) Eliminating Redundant and Faulty Data: At that stage data were eliminated for the following reasons:

(i) values that are identical to previously reported values by the same group and thus appear to refer to the same set of experiments.
(ii) Obviously flawed property values, identifiable as outliers that differ substantially from a cluster of other reported values for that property.
(iii) Obviously flawed property values, identifiable by being highly inconsistent with the other property values for that congener.
(iv) Indirectly measured values, specifically values derived from correlations with high performance liquid chromatography (HPLC) retention times and capacity factors, if a sufficient number of directly measured values was available. If no such direct measurements had been performed or the experimental values were found to be highly inconsistent with other properties, indirectly measured values were included.
(v) Estimated values, unless no measured values for a

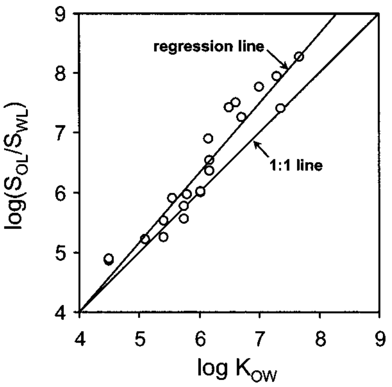

FIG. 1. Relationship between the literature-derived values for the log K_{OW} of 16 PCBs and the logarithm of the ratio of their solubilities in pure octanol and water.

particular property were available. In some cases, when no measured value had been reported, estimated values were included.

(iv) Derivation of Literature-Derived Values: For each property a literature-derived value (LDV) was calculated in one of two ways.

(i) If property values at several temperatures had been reported, the logarithm of all measured data that had not been eliminated was plotted as a function of reciprocal absolute temperature. A linear regression equation was derived, and the value of 25 °C obtained from the regression line. That value was the LDV.

(ii) If measurements had only been done within a fairly small temperature range (20–25 °C), the values were adjusted to 25 °C by using an estimated energy of phase transfer. In this case the LDV was the logarithmic mean of the noneliminated values. The logarithmic mean was considered superior to the arithmetic mean, as the latter tends to give too much weight to high values.

The LDVs for the internal energies of phase transfer ΔU were obtained as follows: If there were sufficient data of a property as a function of temperature, a ΔU was calculated as the product of the slope of the regression line and the ideal gas constant R. This approach was used for the internal energy of dissolution of the liquid substance in water ΔU_W for seven congeners. The average of these values served as the LDV for the ΔU_W of the remaining congeners. Slopes of regressions involving data from several studies served to derive the LDV for the energies of vaporization, ΔU_A, for 12 PCB congeners. For the remaining four congeners, the values reported by Falconer and Bidleman[6] were the LDVs. For four congeners, regressions involving data from more than one study served to derive internal energies of octanol–air transfer ΔU_{OA}. For the remaining congeners, the ΔU_{OA} was taken directly from one of three studies.[8,9,15] Only one study had measured the temperature dependence of the K_{OW} of PCBs.[10] The LDV for the ΔU_{OW} for all congeners was estimated based on information for a few congeners reported in that study.

The selection of LDVs for the internal energy of air–water phase transfer ΔU_{AW} presented difficulties. Only ten Hulscher *et al.*[11] and Bamford *et al.*[12] had reported directly measured temperature dependencies of the Henry's law constants of the PCBs. The former study involved only PCB congeners 28 and 52. The latter study's results for ΔU_{AW} were judged unreliable based on the unreasonably large range of reported values and the unexplained variability from congener to congener. Consistent, but theoretically derived ΔU_{AW} values for PCB homologues reported by Burkhard *et al.*[13] were scaled based on the experimental results for PCB 28 and 52 by ten Hulscher *et al.*[11] and used as LDVs.

(v) Assessing the Uncertainty of the Literature-Derived Values: For each LDV an uncertainty estimate u_X between 1 and 5 was derived based on a number of factors, including the standard deviations of the calculated averages, the standard deviations of the calculated regression parameters, a knowledge of the measurement methodology used and its inherent uncertainty, and an assessment of the general reliability of data reported by particular research groups. For example, a large u_X, indicating high uncertainty, was assigned to properties for which few or no directly measured data exist (e.g., Henry's law constant of PCB-3, K_{OW} for PCB-52) or if several reported values are highly divergent (e.g., S_W for PCB-52), whereas properties that had been measured directly several times with accepted techniques yielding comparable values would deserve a low u_X (e.g., Henry's law constant of PCB-52). Because these uncertainty parameters are used to achieve consistency among the properties for one chemical, their relative size for the properties of one congener is particularly important, whereas the relative size of u_X for one property for different chemicals is less crucial. This assessment is by necessity somewhat subjective.

(vi) Adjusting LDVs to Achieve Consistency: The LDVs were adjusted using an algorithm presented by Beyer *et al.*[4] This technique adjusts a set of physical–chemical property values in such a way that they conform to thermodynamic constraints (i.e., are internally consistent), yet deviate as little as possible from the original values. The adjusted values are referred to as final adjusted values (FAVs). Missing property values (such as the S_{OL} for 11 of the PCB congeners) are calculated at the same time. In this adjustment procedure, we make use of the uncertainty estimates u_X from step v in such a way that the least certain parameters are adjusted more strongly than the most certain ones. For a detailed account of the thermodynamic basis of the adjustment procedure and the equations on which it is based see Beyer *et al.*[4] A computer program with the algorithm is available from http://www.usf.uos.de/projects/elpos/download/adjust.en.html.

A complication arises from the mutual solubility of water and octanol, i.e., an experimentally determined K_{OW} is a quantitative expression of the partitioning between water-saturated octanol and octanol–saturated water. On the other

TABLE 1. Reported and selected physical–chemical properties for PCB-3

Registry No.	2051-62-9			
Chlorine substitution	4-monochlorobiphenyl	Melting point temperature/°C	77	
Molar mass/g·mol^{-1}	188.65	$\Delta_{\mathrm{fus}}S$/J·K^{-1}·mol^{-1}	38.03	Ref. 80

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
23	6.20E−03	1.43E−02	−1.85	Shake flask-GC	19	
4	3.51E−03	1.17E−02	−1.93	Generator column-GC	20	
20	6.39E−03	1.55E−02	−1.81			
25	7.83E−03	1.74E−02	−1.76			
32	1.13E−02	2.21E−02	−1.65			
25	6.89E−03	1.53E−02	−1.82	Generator column-HPLC	21	
25	7.11E−03	1.58E−02	−1.80	Generator column-GC	22	
25	7.06E−03	1.57E−02	−1.80	Slow stirring-GC	22	
5	4.36E−03	1.42E−02	−1.85	Equilibrium gas stripping	23	
15	5.67E−03	1.52E−02	−1.82			
25	7.26E−03	1.61E−02	−1.79			
35	1.15E−02	2.15E−02	−1.67			
45	1.61E−02	2.55E−02	−1.59			
25	4.77E−03	1.06E−02	−1.97	Generator column-GC	24	Not used, outlier
23	8.00E−05	7.82E−05	−4.11	Slow stirring-GC	25	Not used, outlier
25	7.00E−03	6.84E−03	−2.17	Slow stirring-GC	26	Not used, outlier
25		2.45E−02	−1.61	Estd., TSA	13	Not used, estimated value
25	4.57E−03	4.48E−03	−2.35	HPLC-retention index	27	Not used, estimated value
25	4.06E−03	3.96E−03	−2.40	Calcd., QSPR	28	Not used, estimated value
25	7.07E−03	1.57E−02	−1.80	Generator column-GC	29	Not used, same value as in Ref. 22
LDV at 25 °C		1.71E−02		Linear regression	19, 20, 21, 22, 23	Log $S_{\mathrm{WL}} = -631/(T/\mathrm{K}) + 0.35$, $r^2 = 0.78$ (Fig. 2)
FAV at 25 °C		2.02E−02				Log $S_{\mathrm{WL}} = -963/(T/\mathrm{K}) + 1.53$ (Fig. 2)

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	4.61	Shake flask-GC	30	
25	4.49	Generator column-HPLC	18	
25	4.37	Generator column-GC	29	
25	4.49	Generator column-GC	31	Not used, same value as in Ref. 18
25	4.69	Estd., differential substitution constants	30	Not used, estimated value
25	4.4	HPLC-k'	32	Not used, estimated value
25	4.84	Estd., TSA	31	Not used, estimated value
25	4.74	Estd., group contribution	31	Not used, estimated value
25	4.63	HPLC-retention index	27	Not used, estimated value
25	4.69	Estd., TSA	33	Not used, estimated value
25	4.49	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	4.49	Log mean	30, 18, 29	
FAV at 25 °C	4.65			

Vapor Pressure in Pa

T/°C	P_{S}	P_{L}	Log P_{L}	Method	Reference	Note
33	0.73	1.41	0.15	Knudsen effusion	35	
37	1.21	2.19	0.34			
50	3.31	4.86	0.69			
54	4.38	6.06	0.78			
59	6.75	8.67	0.94			
63	9.77	11.85	1.07			
73	19.8	20.92	1.32			
35	0.84	1.57	0.20			
41	1.47	2.49	0.40			
44	2	3.23	0.51			
50	2.95	4.33	0.64			
52	4.12	5.87	0.77			
57	5.69	7.52	0.88			
61	8.03	10.02	1.00			
62	9.66	11.88	1.07			

TABLE 1. Reported and selected physical–chemical properties for PCB-3—Continued

$T/°\mathrm{C}$	P_S	P_L	Log P_L	Method	Reference	Note
65	10.8	12.73	1.10			
67	12.4	14.21	1.15			
68	13.3	15.04	1.18			
69	14.6	16.28	1.21			
73	15.3	16.16	1.21			
4.2	0.011	0.037	−1.43	Gas saturation-GC	36	
16	0.050	0.131	−0.88			
24	0.172	0.389	−0.41			
−20	0.000 24	0.0014	−2.85	Gas saturation-GC	37	
−10	0.0013	0.0059	−2.23			
0	0.0049	0.018	−1.75			
10	0.0188	0.056	−1.26			
20	0.0677	0.165	−0.78			
30	0.223	0.454	−0.34			
−10			−1.72	GC-retention time	6	Reported as a linear equation
0			−1.19			
10			−0.70			
20			−0.25			
30			0.18			
40			0.58			
25		0.930	−0.032	GC-retention time	38	Not used, more recent values from similar methods
25		0.931	−0.031	GC-retention time	39	Not used, more recent values from similar methods
25		0.320	−0.49	GC-retention time	13	Not used, more recent values from similar methods
LDV at 25 °C			−0.33	Linear regression	35, 36, 37, 6	Log $P_L = -3737/(T/\mathrm{K}) + 12.21$, $r^2 = 0.97$ (Fig. 3)
FAV at 25 °C			−0.32			Log $P_L = -3627/(T/\mathrm{K}) + 11.84$ (Fig. 3)

Henry's Law Constant in $\mathrm{Pa \cdot m^3 \cdot mol^{-1}}$

$T/°\mathrm{C}$	H	Log H	Method	Reference	Note
25	35.95	1.56	Calcd., QSPR	28	
25	13.07	1.12	Calcd. from estimated P_L and S_L	13	Not used, obtained from P_L/S_L
LDV at 25 °C		1.56	Directly taken	28	
FAV at 25 °C		1.37			Log $H = -2664/(T/\mathrm{K}) + 10.31$

Octanol–Air Partition Coefficient

$T/°\mathrm{C}$	Log K_{OA}	Method	Reference	Note
−10	8.37	Generator column-GC	15	Reported as a linear regression equation
0	7.88			
10	7.43			
20	7.02			
30	6.63			
−10	8.56	Generator column-GC	14	Reported as a linear regression equation, not used, inconsistent with other measurements
0	8.00			
10	7.49			
20	7.02			
0	7.86	Multicolumn GC (retention index)	9	Not used, estimated value
20	6.99			
LDV at 25 °C	6.82	Directly taken	15	Log K_{OA} vs $1/(T/\mathrm{K})$ using values from Refs. 14, 15, and 9 (Fig. 5)
FAV at 25 °C	6.78			Log $K_{OA} = 3502/(T/\mathrm{K}) - 4.97$ (Fig. 5)

Octanol Solubility in $\mathrm{mol \cdot m^{-3}}$

$T/°\mathrm{C}$	S_{OS}	S_{OL}	Log S_{OL}	Method	Reference	Note
25	608.0	1350	3.13	Shake flask-GC	40	
LDV at 25 °C		1350		Directly taken	40	
FAV at 25 °C		1151				

TABLE 2. Reported and selected physical–chemical properties for PCB-8

Registry No.	34883-43-7			
Chlorine substitution	2,4′-dichlorobiphenyl	Melting point temperature/°C	44	
Molar mass/g·mol^{-1}	223.1	$\Delta_{fus}S$/J·K^{-1} mol^{-1}	56	Default value

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	9.06E−03	1.39E−02	−1.86	Shake flask-GC	19	Adjusted to 25 °C
25	2.78E−03	4.27E−03	−2.37	Generator column-GC	24	
25	3.57E−03	5.48E−03	−2.26	Slow stirring-GC	41	Adjusted to 25 °C
23	8.29E−03	1.34E−02	−1.87	Shake flask-GC	19	Not at 25 °C
20	2.86E−03	4.96E−03	−2.30	Slow stirring-GC	41	Not at 25 °C
23	2.86E−03	2.83E−03	−2.55	Slow stirring-GC	42	Room temperature, assumed to be 23 °C
23	6.23E−04	6.17E−04	−3.21	Slow stirring-GC	25	Not used, Aroclor mixture as standard
25		5.89E−03	−2.23	Estd., TSA	13	Not used, estimated value
20		2.41E−03	−2.62	Slow stirring-GC	43	Not used, Aroclor mixture as standard
25	3.44E−03	3.41E−03	−2.47	HPLC-retention index	27	Not used, estimated value
25	2.88E−03	2.86E−03	−2.54	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		7.06E−03		Log mean	19, 24, 41	
FAV at 25 °C		6.50E−03				Log $S_{WL} = -1000/(T/K) + 1.17$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	5.04	Shake flask-GC	41	Adjusted to 25 °C
25	5.14	Generator column-GC	18	
23	5.10	Shake flask-GC	41	Not at 25 °C
25	5.10	HPLC-k'	32	Not used, estimated value
25	5.14	Generator column-GC	31	Not used, same value as in Ref. 18
25	5.22	Estd., TSA	31	Not used, estimated value
25	5.46	Estd., group contribution	31	Not used, estimated value
25	5.09	HPLC-retention index	27	Not used, estimated value
25	5.14	Generator column-GC	44	Not used, same value as in Ref. 18
25	5.07	Estd., TSA	33	Not used, estimated value
25	5.00	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	5.09	Log mean	41, 18	
FAV at 25 °C	5.12			

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
20		0.069	−1.16	Head space-GC	43	
10		0.020	−1.70	GC-retention time	45	Reported as a linear equation
20		0.058	−1.23			
30		0.158	−0.80			
40		0.400	−0.40			
10		0.034	−1.47	GC-retention time	6	Reported as a linear equation
20		0.096	−1.02			
30		0.255	−0.59			
40		0.637	−0.20			
25		0.150	−0.82	GC-retention time	39	Not used, more recent values from similar methods
25		0.142	−0.85	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−0.91	Linear regression	43, 45, 6	Log $P_L = -3818/(T/K) + 11.90$, $r^2 = 0.95$ (Fig. 3)
FAV at 25 °C			−0.83			Log $P_L = -3728/(T/K) + 11.68$ (Fig. 3)

TABLE 2. Reported and selected physical–chemical properties for PCB-8—Continued

Henry's Law Constant in Pa·m^3·mol^{-1}

T/°C	H	Log H	Method	Reference	Note
23	22.29	1.35	Equilibrium conc. ratio	46	
20	28.37	1.45	Batch equilibrium-GC	43	
25	23.30	1.37	Dynamic gas-water equilibrium	47	
4	6.01	0.78	Gas purging-GC	12	
11	9.87	0.99			
18	15.85	1.20			
25	24.89	1.40			
31	36.07	1.56			
23	96.04	1.98	Gas purging-GC	48	Not used, outlier
25	24.93	1.40	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	31.31	1.50	Estd., molecular connectivity	49	Not used, estimated value
25	30.74	1.49	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.42	Linear regression	46, 43, 47, 12	Log $H = -2428/(T/\mathrm{K}) + 9.56$, $r^2 = 0.93$ (Fig. 4)
FAV at 25 °C		1.36			Log $H = -2728/(T/\mathrm{K}) + 10.51$ (Fig. 4)

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
10	8.08	Generator column (fugacity meter)-GC	8	Reported as a linear regression equation
13	7.94			
24	7.45			
35	6.99			
43	6.67			
0	8.58	Multicolumn GC (retention index)	9	Not used, estimated value
20	7.61			
LDV at 25 °C	7.40	Directly taken	8	Log K_{OA} vs 1/(T/K) using values from Refs. 8 and 9 (Fig. 5)
FAV at 25 °C	7.34			Log $K_{OA} = 3785/(T/\mathrm{K}) - 5.35$ (Fig. 5)

Octanol Solubility in mol·m^{-3}

	S_{OL}	Method	Reference	Note
FAV at 25 °C	1301			

TABLE 3. Reported and selected physical–chemical properties for PCB-15

Registry No.	2050-68-2			
Chlorine substitution	4,4′-dichlorobiphenyl	Melting point temperature/°C	151	
Molar mass/g·mol^{-1}	223.1	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	56	Default value

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
23	3.14E−04	5.77E−03	−2.24	Shake flask-GC	19	
25	2.51E−04	4.32E−03	−2.36	Generator column-GC	24	
20	2.78E−04	5.64E−03	−2.25	Slow stirring-GC	50	
25	2.60E−04	4.48E−03	−2.35	Generator column-HPLC	21	
5	9.41E−05	3.23E−03	−2.49	Equilibrium gas stripping	23	
15	1.55E−04	3.73E−03	−2.43			
25	2.55E−04	4.40E−03	−2.36			
35	4.75E−04	6.00E−03	−2.22			
45	8.34E−04	7.86E−03	−2.10			
25		4.57E−03	−2.34	Estd., TSA	13	Not used, estimated value
25	1.63E−04	2.81E−03	−2.55	Generator column-GC	51	Not used, outlier
25	4.22E−04	7.26E−03	−3.38	HPLC-retention index	27	Not used, estimated value
25	1.08E−04	1.87E−03	−2.73	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		5.00E−03		Linear regression	19, 24, 50, 21, 23	Log $S_{WL}=-807/(T/\mathrm{K})+0.41$, $r^2=0.76$ (Fig. 3)
FAV at 25 °C		4.30E−03				Log $S_{WL}=-909/(T/\mathrm{K})+0.68$ (Fig. 3)

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	5.52	Shake flask-GC	50	Adjusted to 25 °C
25	5.36	Shake flask-GC	30	
25	5.33	Generator column-HPLC	18	
20	5.58	Shake flask-GC	50	Not at 25 °C
25	5.33	Generator column-GC	31	Not used, same value as in Ref. 18
25	5.28	Estd., differential substitution constants	30	Not used, estimated value
25	4.82	HPLC-k'	32	Not used, estimated value
25	5.25	Estd., TSA	31	Not used, estimated value
25	5.46	Estd., group contribution	31	Not used, estimated value
25	5.23	HPLC-retention index	27	Not used, estimated value
25	5.3	Estd., TSA	33	Not used, estimated value
25	5.04	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	5.35	Log mean	50, 30, 18	
FAV at 25 °C	5.36			

TABLE 3. Reported and selected physical–chemical properties for PCB-15—Continued

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
29.88	0.00515	0.076	−1.12	Knudsen effusion	52	
66.58	0.439	2.343	0.37			
76.78	1.281	5.345	0.73			
87	3.521	11.655	1.07			
10		6.03E−03	−2.22	GC-retention time	45	Reported as a linear equation
20		1.87E−02	−1.73			
30		5.41E−02	−1.27			
40		1.46E−01	−0.84			
−10	1.206E−05	7.43E−04	−3.13	Gas saturation-GC	37	
0	8.303E−05	3.44E−03	−2.46			
10	4.159E−04	1.19E−02	−1.92			
20	1.197E−03	2.43E−02	−1.61			
30	4.475E−03	6.58E−02	−1.18			
−10		1.23E−03	−2.91	GC-retention time	6	Reported as a linear equation
0		4.39E−03	−2.36			
10		1.43E−02	−1.84			
20		4.31E−02	−1.37			
30		1.20E−01	−0.92			
25			−1.11	GC-retention time	38	Not used, more recent values from similar methods
25		0.077	−1.18	GC-retention time	39	Not used, more recent values from similar methods
25		0.067	−1.29	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−1.23	Linear regression	52, 45, 37, 6	Log $P_L = -3931/(T/\mathrm{K}) + 11.89$, $r^2 = 0.99$ (Fig. 3)
FAV at 25 °C			−1.24			Log $P_L = -3829/(T/\mathrm{K}) + 11.60$ (Fig. 3)

Henry's Law Constant in $\mathrm{Pa \cdot m^3 \cdot mol^{-1}}$

T/°C	H	Log H	Method	Reference	Note
25	14.69	1.17	Gas purging-GC	53	
25	20.16	1.30	Gas purging-GC	54	
25	9.67	0.99	Wetted wall column-GC	55	
23	30.40	1.48	Equilibrium conc. ratio	46	Not used, Aroclor mixture as standard
25	11.04	1.04	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	20.16	1.30	Gas purging-GC	51	Not used, same value as in Ref. 54
25	27.40	1.44	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.15	Log mean	53, 54, 55	
FAV at 25 °C		1.13			Log $H = -2921/(T/\mathrm{K}) + 10.92$ (Fig. 4)

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
0	8.87	Multicolumn GC (retention index)	9	
20	7.88			
−10	9.31	Generator column-GC	14	Reported as a linear regression equation
0	8.78			Not used, highly inconsistent with other properties
10	8.29			
20	7.84			
LDV at 25 °C	7.65	Extrapolation	9	Log K_{OA} vs $1/(T/\mathrm{K})$ using values from Refs. 14 and 9 (Fig. 5)
FAV at 25 °C	7.85			Log $K_{OA} = 4078/(T/\mathrm{K}) - 5.83$ (Fig. 5)

Octanol Solubility in $\mathrm{mol \cdot m^{-3}}$

T/°C	S_{OS}	S_{OL}	Log S_{OL}	Method	Reference	Note
25	71.27	1227.6	3.089	Shake flask-GC	40	
4	93.33	3322.4	3.521	Shake flask-GC	56	
12	107.15	2856.7	3.456			
20	128.82	2612.9	3.417			
LDV at 25 °C		1590		Log mean	40, 56	Log S_{OL} vs $1/(T/\mathrm{K})$ using values from Refs. 40 and 56 (Fig. 6)
FAV at 25 °C		1635				

TABLE 4. Reported and selected physical–chemical properties for PCB-28

Registry No.	7012-37-5			
Chlorine substitution	2,4,4′-trichlorobiphenyl	Melting point temperature/°C	58	
Molar mass/g·mol^{-1}	257.54	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	56	Default

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	3.61E−04	7.61E−04	−3.12	Shake flask-GC	19	Adjusted to 25 °C
25	1.01E−03	2.13E−03	−2.67	Generator column-GC	24	
25	5.61E−04	1.18E−03	−2.93	Slow stirring-GC	41	Adjusted to 25 °C
25	4.50E−04	9.49E−04	−3.02	Slow stirring-GC	57	
25	4.53E−04	9.55E−04	−3.02	Generator column-GC	51	
25	2.98E−04	6.28E−04	−3.20	Generator column-GC	58	Adjusted to 25 °C
23	3.30E−04	7.32E−04	−3.14	Shake flask-GC	19	Not at 25 °C
20	4.47E−04	1.07E−03	−2.97	Slow stirring-GC	41	Not at 25 °C
22	2.60E−04	5.92E−04	−3.23	Generator column-GC	58	Not at 25 °C
23	3.83E−05	8.50E−05	−4.07	Slow stirring-GC	25	Not used, Aroclor mixture as standard
20	5.56E−04	1.33E−03	−2.88	Slow stirring-GC	43	Not used, Aroclor mixture as standard
25		1.21E−03	−2.92	Estd., TSA	13	Not used, estimated value
25	5.92E−04	1.25E−03	−2.90	HPLC-retention index	27	Not used, estimated value
25	3.44E−04	7.26E−04	−3.14	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.01E−03		Log mean	19, 24, 41, 57, 51, 58	
FAV at 25 °C		8.85E−04				Log $S_{WL}=-1147/(T/\mathrm{K})+0.79$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	5.55	Shake flask-GC	41	Adjusted to 25 °C
25	5.74	Estd., differential substitution constants	30	Not used, estimated value
20	5.62	Shake flask-GC	41	Not at 25 °C
25	5.71	HPLC-retention index	27	Not used, estimated value
25	5.67	Estd., TSA	33	Not used, estimated value
25	5.49	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	5.55	Directly taken after T adjustment	41	
FAV at 25 °C	5.66			

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
20		1.49E−02	−1.83	Head space-GC	43	
10		2.78E−03	−2.56	GC-retention time	45	Reported as a linear equation
20		9.10E−03	−2.04			
30		2.75E−02	−1.56			
40		7.75E−02	−1.11			
10		6.43E−03	−2.19	GC-retention time	6	Reported as a linear equation
20		1.99E−02	−1.70			
30		5.73E−02	−1.24			
40		1.54E−01	−0.81			
25		3.40E−02	−1.47	GC-retention index	39	Not used, more recent values from similar methods
25		2.77E−02	−1.56	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−1.63	Linear regression	43, 45, 6	Log $P_L=-4157/(T/\mathrm{K})+12.31$, $r^2=0.91$ (Fig. 3)
FAV at 25 °C			−1.57			Log $P_L=-4007/(T/\mathrm{K})+11.87$ (Fig. 3)

TABLE 4. Reported and selected physical–chemical properties for PCB-28—Continued

Henry's Law Constant in $Pa \cdot m^3 \cdot mol^{-1}$

T/°C	H	Log H	Method	Reference	Note
20	26.75	1.43	Batch equilibrium-GC	43	
25	20.27	1.31	Dynamic gas–water equilibrium	47	
10.4	8.70	0.94	Gas purging-GC	11	
20	21.20	1.33			
30.1	47.40	1.68			
34.9	50.30	1.70			
42.1	70.80	1.85			
47.9	120.60	2.08			
48.4	122.20	2.09			
4	13.13	1.12	Gas purging-GC	12	
11	19.06	1.28			
18	27.18	1.43			
25	38.14	1.58			
31	50.39	1.70			
25	22.80	1.36	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	28.95	1.46	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.52	Linear regression	43, 47, 11, 12	Log $H = -2101/(T/K) + 8.57$, $r^2 = 0.90$ (Fig. 4)
FAV at 25 °C		1.48			Log $H = -2860/(T/K) + 11.08$ (Fig. 4)

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
10	8.68	Generator column (fugacity meter)-GC	8	Reported as a linear regression equation
13	8.52			
24	7.98			
35	7.48			
43	7.13			
0	9.43	Multicolumn GC (retention index)	9	Not used, estimated value
20	8.40			
LDV at 25 °C	7.93	Directly taken	8	Log K_{OA} vs $1/(T/K)$ using values from Refs. 8 and 9 (Fig. 5)
FAV at 25 °C	7.85			Log $K_{OA} = 4102/(T/K) - 5.91$ (Fig. 5)

Octanol Solubility in $mol \cdot m^{-3}$

	S_{OL}	Method	Reference	Note
FAV at 25 °C	768			

TABLE 5. Reported and selected physical–chemical properties for PCB-29

Registry No.	15862-07-4			
Chlorine substitution	2,4,5-trichlorobiphenyl	Melting point temperature/°C	77	
Molar mass/g·mol^{-1}	257.54	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	65.2	Ref. 59

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	3.57E−04	1.40E−03	−2.85	Generator column-GC	24	
25	6.32E−04	2.48E−03	−2.61	Generator column-GC	59	
25	5.44E−04	2.13E−03	−2.67	Generator column-HPLC	21	
5	1.60E−04	1.22E−03	−2.91	Equilibrium gas stripping	23	
15	2.65E−04	1.43E−03	−2.84			
25	4.12E−04	1.62E−03	−2.79			
35	7.88E−04	2.30E−03	−2.64			
45	1.28E−03	2.82E−03	−2.55			
25		1.45E−03	−2.84	Estd., TSA	13	Not used, estimated value
25	4.47E−04	1.75E−03	−2.76	HPLC-retention index	27	Not used, estimated value
25	3.24E−04	1.27E−03	−2.90	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.86E−03		Linear regression	24, 59, 21, 23	Log $S_{WL} = -824/(T/\mathrm{K}) + 0.03$, $r^2 = 0.69$ (Fig. 2)
FAV at 25 °C		1.51E−03				Log $S_{WL} = -977/(T/\mathrm{K}) + 0.46$ (Fig. 2)

Octanol-Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	5.51	Generator column-GC	59	
25	5.81	Generator column-HPLC	18	
25	5.90	Slow stirring-GC (HPLC)	60	
25	5.77	Estd., differential substitution constants	30	Not used, estimated value
25	6.25	HPLC-k'	32	Not used, estimated value
25	5.81	Generator column-GC	31	Not used, same value as in Ref. 18
25	5.59	Estd., TSA	31	Not used, estimated value
25	6.17	Estd., group contribution	31	Not used, estimated value
25	5.52	Estd., LSER	61	Not used, estimated value
25	5.81	HPLC-retention index	27	Not used, estimated value
25	5.60	Estd., TSA	33	Not used, estimated value
25	5.49	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	5.74	Log mean	59, 18, 60	
FAV at 25 °C	5.60			

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
10		8.68E−03	−2.06	GC-retention time	6	Reported as a linear equation
20		2.64E−02	−1.58			
25		4.47E−02	−1.35			
30		7.45E−02	−1.13			
40		1.97E−01	−0.71			
25		4.44E−02	−1.35	GC-retention time	38	Not used, more recent values from similar methods
25		4.59E−02	−1.34	GC-retention time	39	Not used, more recent values from similar methods
25		3.66E−02	−1.44	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−1.35	Directly taken	6	
FAV at 25 °C			−1.34			Log $P_L = -3904/(T/\mathrm{K}) + 11.75$

TABLE 5. Reported and selected physical–chemical properties for PCB-29—Continued

Henry's Law Constant in $Pa \cdot m^3 \cdot mol^{-1}$

T/°C	H	Log H	Method	Reference	Note
25	20.27	1.31	Dynamic gas-water equilibrium-GC	47	
4	12.12	1.08	Gas purging-GC	12	
11	18.04	1.26			
18	26.37	1.42			
25	37.89	1.58			
31	51.03	1.71			
25	25.33	−1.99	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	27.05	1.43	Estd., molecular connectivity	49	Not used, estimated value
25	31.82	−1.89	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.51	Linear regression	47, 12	Log $H = -1674/(T/K) + 7.13$, $r^2 = 0.78$ (Fig. 4)
FAV at 25 °C		1.48			Log $H = -2927/(T/K) + 11.30$ (Fig. 4)

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
0	9.15	Multicolumn GC (retention index)	9	
20	8.05			
−10	9.61	Generator column-GC	14	Reported as a linear regression equation
0	9.08			Not used, highly inconsistent with other properties
10	8.59			
20	8.14			
LDV at 25 °C	7.80	Extrapolation	9	Log K_{OA} vs $1/(T/K)$ using values from Refs. 9, 14 (Fig. 5)
FAV at 25 °C	7.78			Log $K_{OA} = 4175/(T/K) - 6.22$ (Fig. 5)

Octanol Solubility in $mol \cdot m^{-3}$

T/°C	S_{OS}	S_{OL}	Log S_{OL}	Method	Reference	Note
25	176.17	692	2.84	Shake flask-GC	40	
LDV at 25 °C		692		Directly taken	40	
FAV at 25 °C		1114				

TABLE 6. Reported and selected physical–chemical properties for PCB-31

Registry No.	16606-02-3			
Chlorine substitution	2,5,4′-trichlorobiphenyl	Melting point temperature/°C	64.5	
Molar mass/$g \cdot mol^{-1}$	257.54	$\Delta_{fus}S/J \cdot K^{-1} \cdot mol^{-1}$	56	Default value

Aqueous Solubility in $mol \cdot m^{-3}$

$T/°C$	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	3.49E−04	8.53E−04	−3.07	Generator column-GC	58	
23	3.71E−04	9.53E−04	−3.02	Slow stirring-GC	25	Not used, Aroclor mixture as standard
20		5.55E−04	−3.26	Slow stirring-GC	43	Not used, Aroclor mixture as standard
25		1.23E−03	−2.91	Estd., TSA	13	Not used, estimated value
25	6.61E−04	1.61E−03	−2.79	HPLC-retention index	27	Not used, estimated value
25	3.71E−04	9.05E−04	−3.04	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		8.53E−04		Directly taken	58	
FAV at 25 °C		7.54E−04				Log $S_{WL} = -1123/(T/K) + 0.64$

Octanol–Water Partition Coefficient

$T/°C$	Log K_{OW}	Method	Reference	Note
25	5.79	Generator column-GC	18	
25	5.77	Estd., differential substitution constants	30	Not used, estimated value
25	5.69	HPLC-k'	32	Not used, estimated value
25	5.79	Generator column-GC	31	Not used, same value as in Ref. 18
25	6.17	Estd., group contribution	31	Not used, estimated value
25	5.63	Estd., TSA	31	Not used, estimated value
25	5.67	Estd., TSA	33	Not used, estimated value
25	5.68	HPLC-retention index	27	Not used, estimated value
25	5.53	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	5.79	Directly taken	18	
FAV at 25 °C	5.78			

Vapor Pressure in Pa

$T/°C$	P_S	P_L	Log P_L	Method	Reference	Note
20		1.49E−02	−1.83	Head-space-GC	43	
10		2.78E−03	−2.56	GC-retention time	45	Reported as a linear equation
20		9.10E−03	−2.04			
30		2.75E−02	−1.56			
40		7.75E−02	−1.11			
10		6.58E−03	−2.18	GC-retention time	6	Reported as a linear equation
20		2.03E−02	−1.69			
30		5.81E−02	−1.24			
40		1.55E−01	−0.81			
25		4.02E−02	−1.40	GC-retention time	38	Not used, more recent values from similar method
25		3.59E−02	−1.44	GC-retention time	39	Not used, more recent values from similar method
25		3.13E−02	−1.50	GC-retention index	13	Not used, more recent values from similar method
LDV at 25 °C			−1.62	Linear regression	43, 45, 6	Log $P_L = -4149/(T/K) + 12.29$, $r^2 = 0.91$ (Fig. 3)
FAV at 25 °C			−1.59			Log $P_L = -4010/(T/K) + 11.86$ (Fig. 3)

TABLE 6. Reported and selected physical–chemical properties for PCB-31—Continued

Henry's Law Constant in Pa·m^3·mol^{-1}

T/°C	H	Log H	Method	Reference	Note
25	107.53	2.03	Gas purging-GC	48	Adjusted to 25 °C
25	23.29	1.37	Equilibrium conc. ratio	46	Adjusted to 25 °C
25	38.01	1.58	Equilibrium conc. ratio	43	Adjusted to 25 °C
25	19.25	1.28	Dynamic gas-water equilibrium-GC	47	
23	93.57	1.97	Gas purging-GC	48	Not at 25 °C
23	20.27	1.31	Equilibrium conc. ratio	46	Room temperature, assumed to be 23 °C
20	26.75	1.43	Equilibrium conc. ratio	43	Not at 25 °C
25	25.43	1.41	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	28.47	1.45	Estd., molecular connectivity	49	Not used, estimated value
25	27.78	1.44	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.57	Log mean	48, 46, 43, 47	
FAV at 25 °C		1.53			Log $H = -2887/(T/\mathrm{K}) + 11.22$

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
10	8.68	Generator column (fugacity meter)-GC	8	Reported as a linear regression equation
13	8.52			
24	7.98			
35	7.48			
43	7.13			
0	9.43	Multicolumn GC (retention index)	9	Not used, estimated value
20	8.40			
LDV at 25 °C	7.93	Directly taken	8	Log K_{OA} vs $1/(T/\mathrm{K})$ using values from Refs. 8 and 9 (Fig. 5)
FAV at 25 °C	7.94			Log $K_{OA} = 4110/(T/\mathrm{K}) - 5.84$ (Fig. 5)

Octanol Solubility in mol·m^{-3}

	S_{OL}		Method	Reference	Note
FAV at 25 °C	902	902			

TABLE 7. Reported and selected physical–chemical properties for PCB-52

Registry No.	35693-99-3			
Chlorine substitution	2,5,2′,5′-tetrachlorobiphenyl	Melting point temperature/°C	86.5	
Molar mass/g·mol^{-1}	291.99	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	46.1	Ref. 63

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	1.72E−04	5.38E−04	−3.27	Shake flask-GC	19	Adjusted to 25 °C
25	5.96E−05	1.87E−04	−3.73	Generator column-GC	58	Adjusted to 25 °C
25	3.75E−04	1.18E−03	−2.93	Generator column-GC	51	
25	5.82E−04	1.83E−03	−2.74	Generator column-HPLC	21	
23	1.58E−04	5.17E−04	−3.29	Shake flask-GC	19	Not at 25 °C
22	5.24E−05	1.76E−04	−3.75	Generator column-GC	58	Not at 25 °C
23	8.49E−04	2.79E−03	−2.55	Slow stirring-GC	42	Room temperature, assumed to be 23 °C, not used, outlier
23	7.64E−05	2.51E−04	−3.60	Slow stirring-GC	25	Not used, Aroclor mixture as standard
25		3.62E−04	−3.44	Estd., TSA	13	Not used, estimated value
20		3.87E−04	−3.41	Slow stirring-GC	43	Not used, Aroclor mixture as standard
25	1.00E−04	3.14E−04	−3.50	HPLC-retention index	27	Not used, estimated value
25	1.14E−04	3.59E−04	−3.45	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		6.82E−04		Log mean	19, 58, 51, 21	
FAV at 25 °C		4.78E−04				Log $S_{WL} = -1103/(T/K) + 0.37$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	6.26	Estd., differential substitution constants	30	
25	6.09	HPLC-k'	32	
25	5.79	HPLC-retention index	27	
25	5.84	Estd., TSA	33	
25	6.13	Estd., characteristic root index	34	
LDV at 25 °C	6.00	Log mean	30, 32, 27, 33, 34	No directly measured values
FAV at 25 °C	5.91			

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
25	2.53E−03	7.94E−03	2.10	Saturation column-GC	64	
30	4.80E−03	1.35E−02	−1.87			
20		9.04E−03	−2.04	Head space-GC	43	
10		1.20E−03	−2.92	GC-retention time	45	Reported as a linear equation
20		4.10E−03	−2.39			
30		1.29E−02	−1.89			
40		3.79E−02	−1.42			
10		2.86E−03	−2.54	GC-retention time	6	Reported as a linear equation
20		9.22E−03	−2.04			
30		2.75E−02	−1.56			
40		7.66E−02	−1.12			
25	7.33E−03	2.30E−02	−1.64	GC-retention time	65	Not used, more recent values from similar methods
25		1.19E−02	−1.92	GC-retention time	38	Not used, more recent values from similar methods
25		1.78E−02	−1.75	GC-retention index	39	Not used, more recent values from similar methods
25		1.93E−02	−1.72	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−1.97	Linear regression	64, 43, 45, 6	Log $P_L = -4190/(T/K) + 12.08$, $r^2 = 0.998$ (Fig. 3)
FAV at 25 °C			−1.92			Log $P_L = -4059/(T/K) + 11.69$ (Fig. 3)

TABLE 7. Reported and selected physical–chemical properties for PCB-52—Continued

Henry's Law Constant in Pa·m^3·mol^{-1}

T/°C	H	Log H	Method	Reference	Note
23	27.00	1.43	Equilibrium conc. ratio-GC	46	
20	12.16	1.08	Gas purging-GC	66	
20	24.12	1.38	Equilibrium conc. ratio-GC	43	
25	34.65	1.54	Gas purging-GC	54	
25	20.27	1.31	Dynamic gas–water equilibrium-GC	47	
10.4	8.60	0.93	Gas purging-GC	11	
20	16.40	1.21			
30.1	37.40	1.57			
34.9	38.80	1.59			
42.1	68.70	1.84			
47.9	109.20	2.04			
48.4	120.60	2.08			
4	11.34	1.05	Gas purging-GC	12	
11	16.13	1.21			
18	22.56	1.35			
25	31.07	1.49			
31	40.43	1.61			
23	93.57	1.97	Gas purging-GC	48	Not used, outlier
25	53.20	1.73	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	34.65	1.54	Gas purging-GC	51	Not used, same value as in Ref. 54
25	27.78	1.44	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.45	Linear regression	46, 66, 43, 54, 47, 11, 12	Log $H = -2189/(T/\mathrm{K}) + 8.79$, $r^2 = 0.88$ (Fig. 4)
FAV at 25 °C		1.40			Log $H = -2956/(T/\mathrm{K}) + 11.32$ (Fig. 4)

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
10	8.99	Generator column (fugacity meter)-GC	8	Reported as a linear regression equation
13	8.83			
24	8.27			
35	7.74			
43	7.39			
0	9.46	Multicolumn GC (retention index)	9	Not used, estimated value
20	8.49			
LDV at 25 °C	8.22	Directly taken	8	Log K_{OA} vs $1/(T/\mathrm{K})$ using values from Refs. 8 and 9 (Fig. 5)
FAV at 25 °C	8.22			Log $K_{OA} = 4251/(T/\mathrm{K}) - 6.04$ (Fig. 5)

Octanol Solubility in mol·m^{-3}

T/°C	S_{OS}	S_{OL}	Log S_{OL}	Method	Reference	Note
25	234	735	2.87	Shake flask-GC	40	
LDV at 25 °C		735		Directly taken	40	
FAV at 25 °C		799				

TABLE 8. Reported and selected physical–chemical properties for PCB-61

Registry No.	33284-53-6			
Chlorine substitution	2,3,4,5-tetrachlorobiphenyl	Melting point temperature/°C	90	
Molar mass/g·mol^{-1}	291.99	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	69.1	Ref. 59

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	6.58E−05	4.06E−04	−3.39	Generator column-GC	24	
25	7.17E−05	4.42E−04	−3.35	Generator column-GC	59	
25	4.78E−05	2.95E−04	−3.53	Generator column-GC	51	
25	4.68E−05	2.89E−04	−3.54	Generator column-GC	22	
5	1.92E−05	2.46E−04	−3.61	Equilibrium gas stripping	23	
15	3.49E−05	3.07E−04	−3.51			
25	5.34E−05	3.30E−04	−3.48			
35	9.76E−05	4.33E−04	−3.36			
45	1.92E−04	6.25E−04	−3.20			
25		4.86E−04	−3.31	Estd., TSA	13	Not used, estimated value
25	3.39E−05	2.09E−04	−3.68	Generator column-HPLC	21	Not used, outlier
25	7.76E−05	4.79E−04	−3.32	HPLC-retention index	27	Not used, estimated value
25	6.18E−05	3.81E−04	−3.42	Calcd., QSPR	28	Not used, estimated value
25	4.66E−05	2.88E−04	−3.54	Generator column-GC	29	Not used, same value as in Ref. 22
LDV at 25 °C		3.63E−04		Linear regression	24, 59, 51, 22, 23	Log $S_{WL} = -839/(T/K) - 0.626$, $r^2 = 0.72$ (Fig. 2)
FAV at 25 °C		3.46E−04				Log $S_{WL} = -1043/(T/K) + 0.037$ (Fig. 2)

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	5.72	Generator column-GC	59	
25	6.18	Generator column-GC	33	
25	6.41	Slow stirring-GC (HPLC)	60	
25	6.38	Generator column-GC	29	
25	6.39	Estd., differential substitution constants	30	Not used, estimated value
25	6.09	HPLC-k'	32	Not used, estimated value
25	6.44	HPLC-retention index	27	Not used, estimated value
25	6.04	Estd., TSA	33	Not used, estimated value
25	5.92	Estd., LSER	61	Not used, estimated value
25	5.97	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	6.17	Log mean	59, 33, 60, 29	
FAV at 25 °C	6.11			

Vapor Pressure Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
−20	5.30E−07	1.99E−05	−4.70	Generator column-GC	37	
−10	3.82E−06	9.10E−05	−4.04			
0	1.44E−05	2.25E−04	−3.65			
10	6.16E−05	6.52E−04	−3.19			
20	1.85E−04	1.36E−03	−2.87			
0		5.46E−04	−3.26	GC-retention time	6	Reported as a linear equation
10		2.01E−03	−2.70			
20		6.79E−03	−2.17			
30		2.11E−02	−1.67			
25		5.58E−03	−1.917	GC-retention index	13	Not used, estimated value
LDV at 25 °C			−2.14	Linear regression	37, 6	Log $P_L = -4330/(T/K) + 12.38$, $r^2 = 0.92$ (Fig. 3)
FAV at 25 °C			−2.16			Log $P_L = -4193/(T/K) + 11.91$ (Fig. 3)

TABLE 8. Reported and selected physical–chemical properties for PCB-61—Continued

Henry's Law Constant in $Pa \cdot m^3 \cdot mol^{-1}$

$T/°C$	H	Log H	Method	Reference	Note
25	17.5	1.24	Estd., molecular connectivity	49	
25	24.14	1.38	Calcd., QSPR	28	
25	11.4	1.06	Calcd. from estimated P_L and S_L	13	Not used, estimated value
LDV at 25 °C		1.31	Log mean	49, 28	
FAV at 25 °C		1.30			Log $H = -3150/(T/K) + 11.87$

Octanol–Air Partition Coefficient

$T/°C$	Log K_{OA}	Method	Reference	Note
0	10.19	Multicolumn GC (retention index)	9	
20	8.93			
−10	10.26		14	Reported as a linear regression equation; not used, highly inconsistent with other properties
0	9.78			
10	9.33			
20	8.92			
LDV at 25 °C	8.64	Extrapolation	9	Log K_{OA} vs $1/(T/K)$ using values from Refs. 14 and 9 (Fig. 5)
FAV at 25 °C	8.55			Log $K_{OA} = 4660/(T/K) - 7.08$ (Fig. 5)

Octanol Solubility in $mol \cdot m^{-3}$

$T/°C$	S_{OS}	S_{OL}	Log S_{OL}	Method	Reference	Note
25	140	862	2.94	Shake flask-GC	40	
LDV at 25 °C		862		Directly taken	40	
FAV at 25 °C		983				

TABLE 9. Reported and selected physical–chemical properties for PCB-101

Registry No.	37680-73-2			
Chlorine substitution	2,4,5,2’,5’-pentachlorobiphenyl	Melting point temperature/°C	77	
Molar mass/g·mol^{-1}	326.43	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	53.6	Ref. 63

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
23	8.58E−05	2.78E−04	−3.56	Shake flask-GC	19	
25	1.29E−05	3.96E−05	−4.40	Generator column-GC	24	
24	3.06E−05	9.67E−05	−4.01	Slow stirring-GC	50	
25	5.92E−05	1.82E−04	−3.74	Generator column-GC	59	
25	3.37E−05	1.04E−04	−3.98	Slow stirring-GC	57	
4	1.88E−05	1.03E−04	−3.99	Generator column-GC	67	
20	3.71E−05	1.30E−04	−3.89			
25	4.72E−05	1.45E−04	−3.84			
32	6.83E−05	1.77E−04	−3.75			
20		8.06E−05	−4.09	Slow stirring-GC	43	
25	2.07E−05	6.37E−05	−4.20	Generator column-GC	51	
23	3.16E−05	1.02E−04	−3.99	Slow stirring-GC	42	Room temperature, assumed to be 23 °C
25	1.53E−06	4.71E−06	−5.33	Generator column-GC	68	Not used, outlier
25		1.09E−04	−3.96	Estd., TSA	13	Not used, estimated value
25	2.88E−05	8.88E−05	−4.05	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		9.57E−05		Log mean	19, 24, 50, 59, 57, 67, 43, 51	
FAV at 25 °C		1.02E−04				Log $S_{WL}=-1113/(T/\mathrm{K})-0.27$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	5.92	Ratio of S_{WO} and S_{OW} measured by slow stirring	59	
25	6.50	Generator column-GC	18	
25	6.04	Shake flask-GC	50	Adjusted to 25 °C
20	6.11	Shake flask-GC	50	Not at 25 °C
25	6.85	Estd., differential substitution constants	30	Not used, estimated value
25	6.42	HPLC-k'	68	Not used, estimated value
25	7.07	HPLC-k'	32	Not used, estimated value
25	6.88	HPLC-k'	69	Not used, estimated value
25	6.50	Generator column-GC	31	Not used, same value as in Ref. 18
25	7.60	Estd., group contribution	31	Not used, estimated value
25	6.39	Estd., TSA	31	Not used, estimated value
25	6.3	HPLC-retention index	27	Not used, estimated value
25	6.50	Generator column-GC	70	Not used, same value as Ref. 18
25	6.38	Estd., TSA	33	Not used, estimated value
25	6.62	Estd., LSER	61	Not used, estimated value
25	6.64	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	6.15	Log mean	59, 18, 50	
FAV at 25 °C	6.33			

TABLE 9. Reported and selected physical–chemical properties for PCB-101—Continued

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
25	9.60E−04	2.96E−03	−2.53	Gas saturation-GC	64	
30	1.73E−03	4.70E−03	−2.33			
20		1.46E−03	−2.84	Head space-GC	43	
10		2.24E−04	−3.65	GC-retention time	45	Reported as a linear equation
20		8.35E−04	−3.08			
30		2.86E−03	−2.54			
40		9.05E−03	−2.04			
10		5.34E−04	−3.27	GC-retention time	6	Reported as a linear equation
20		1.87E−03	−2.73			
30		6.02E−03	−2.22			
40		1.80E−02	−1.74			
25	1.23E−03	3.78E−03	−2.42	GC-retention time	65	Not used, more recent values from similar methods
25		3.67E−03	−2.44	GC-retention time	38	Not used, more recent values from similar methods
25		3.82E−03	−2.42	GC-retention index	39	Not used, more recent values from similar methods
25		3.58E−03	−2.45	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−2.62	Linear regression	64, 43, 45, 6	Log $P_L = -4632/(T/\mathrm{K}) + 12.92$, $r^2 = 0.92$ (Fig. 3)
FAV at 25 °C			−2.61			Log $P_L = -4346/(T/\mathrm{K}) + 11.94$ (Fig. 3)

Henry's Law Constant in Pa·m^3·mol^{-1}

T/°C	H	Log H	Method	Reference	Note
25	28.8	1.46	Batch equilibrium-GC	43	Adjusted to 25 °C
25	25.43	1.41	Gas purging-GC	54	
4	15.75	1.20	Gas purging-GC	12	
11	22.2	1.35			
18	30.8	1.49			
25	42.1	1.62			
31	54.4	1.74			
20	18.1	1.26	Batch equilibrium-GC	43	Not at 25 °C
20	7.1	0.85	Gas purging-GC	66	Not at 25 °C
25	11.3	1.05	Gas purging-GC	66	Adjusted to 25 °C, not used, outlier
25	32.7	1.51	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	24.9	1.40	Calcd., QSPR	28	Not used, estimated value
25	25.4	1.41	Gas purging	51	Not used, same value as Ref. 54
LDV at 25 °C		1.50	Log mean	43, 54, 12	
FAV at 25 °C		1.38			Log $H = -3233/(T/\mathrm{K}) + 12.21$

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
0	10.24	Generator column-GC	15	Reported as a linear regression equation
10	9.75			
20	9.28			
30	8.85			
10	9.56	Generator column (fugacity meter)-GC	8	Reported as a linear regression equation
13	9.40			
24	8.83			
35	8.31			
0	10.25	Multicolumn GC (retention index)	9	Not used, estimated value
20	9.28			
LDV at 25 °C	8.90	Linear regression	15, 8	Log $K_{OA} = 4291/(T/\mathrm{K}) - 5.50$, $r^2 = 0.96$ (Fig. 5)
FAV at 25 °C	8.73			Log $K_{OA} = 4302/(T/\mathrm{K}) - 5.60$ (Fig. 5)

Octanol Solubility in mol·m^{-3}

	S_{OL}	Method	Reference	Note
FAV at 25 °C	534			

TABLE 10. Reported and selected physical–chemical properties for PCB-105

Registry No.	32598-14-4			
Chlorine substitution	2,3,4,3′,4′-pentachlorobiphenyl	Melting point temperature/°C	117	
Molar mass/g·mol^{-1}	326.43	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	56	Default value

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25		1.24E−04	−3.91	Estd., TSA	13	
25	3.00E−05	2.40E−04	−3.62	HPLC-retention index	27	
25	5.82E−06	4.65E−05	−4.33	Calcd., QSPR	28	
25	3.28E−06	2.62E−05	−4.58	Generator column-GC	71	Not used, highly inconsistent with other properties
LDV at 25 °C		1.11E−04		Log mean	13, 27, 28	
FAV at 25 °C		7.45E−05				Log $S_{WL} = -1285/(T/\mathrm{K}) + 0.18$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	6.61	Generator column-GC	72	
25	5.82	Generator column-GC	33	Not used, highly inconsistent with other properties
25	6.02	Slow stirring-GC	73	Not used, highly inconsistent with other properties
25	6.79	HPLC-retention index	27	Not used, estimated value
25	6.65	Estd., TSA	33	Not used, estimated value
25	6.57	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	6.61	Directly taken	72	
FAV at 25 °C	6.82			

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
0		3.03E−05	−4.52	GC-retention time	6	Reported as a linear equation
10		1.25E−04	−3.90			
20		4.67E−04	−3.33			
30		1.60E−03	−2.80			
25		9.02E−04	−3.04	GC-retention time	38	Not used, more recent values from similar methods
25		7.74E−04	−3.11	GC-retention index	39	Not used, more recent values from similar methods
25		7.07E−04	−3.15	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−3.06	Directly taken	6	
FAV at 25 °C			−2.99			Log $P_L = -4554/(T/\mathrm{K}) + 12.29$

Henry's Law Constant in Pa·m^3·mol^{-1}

T/°C	H	Log H	Method	Reference	Note
4	3.09	0.49	Gas purging-GC	12	
11	7.10	0.85			
18	15.73	1.20			
25	33.6	1.53			
31	62.5	1.80			
25	5.68	0.75	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	6.08	0.78	Estd., molecular connectivity	49	Not used, estimated value
25	10.06	1.00	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.53	Directly taken	12	
FAV at 25 °C		1.14			Log $H = -3269/(T/\mathrm{K}) + 12.10$

TABLE 10. Reported and selected physical–chemical properties for PCB-105—Continued

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
−10	12.10	Generator column-GC	15	Reported as a linear regression equation
0	11.45			
10	10.84			
20	10.28			
30	9.75			
0	11.41	Multicolumn GC (retention index)	9	Not used, estimated value
20	10.20			
LDV at 25 °C	10.0	Directly taken	15	Log K_{OA} vs $1/(T/K)$ for values from Refs. 15 and 9 (Fig. 5)
FAV at 25 °C	9.53			Log $K_{OA} = 4630/(T/K) - 6.00$ (Fig. 5)

Octanol Solubility in mol·m^{-3}

	S_{OL}	Method	Reference	Note
FAV at 25 °C	1410			

TABLE 11. Reported and selected physical–chemical properties for PCB-118

Registry No.	31508-00-6			
Chlorine substitution	2,4,5,3′,4′-pentachlorobiphenyl	Melting point temperature/°C	110	
Molar mass/g·mol^{-1}	326.43	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	56	Default value

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25		1.03E−04	−3.99	Estimated from TSA	13	
25		4.56E−05	−4.34	Slow stirring-GC	43	Adjusted to 25 °C
25	4.68E−05	3.19E−04	−3.50	HPLC-retention index	27	
25	6.10E−06	4.2E−05	−4.38	Calcd., QSPR	28	
20		4.12E−05	−4.39	Slow stirring-GC	43	Not at 25 °C
25	3.28E−06	2.24E−05	−4.65	Generator column-GC	71	Not used, highly inconsistent with other properties
LDV at 25 °C		8.88E−05		Log mean	13, 43, 27, 28	
FAV at 25 °C		6.83E−05				Log $S_{WL} = -1339/(T/K) + 0.32$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	6.49	Generator column-GC	72	
25	7.12	HPLC-k'	32	Not used, estimated value
25	6.57	HPLC-retention index	27	Not used, estimated value
25	6.74	Estd., TSA	33	Not used, estimated value
25	6.58	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	6.49	Directly taken	72	
FAV at 25 °C	6.69			

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
20		3.55E−04	−3.45	Head space-GC	43	
10		9.51E−05	−4.02	GC-retention time	45	Reported as a linear equation
20		3.75E−04	−3.43			
30		1.35E−03	−2.87			
40		4.46E−03	−2.35			
10		1.77E−04	−3.75	GC-retention time	6	Reported as a linear equation
20		6.46E−04	−3.19			
30		2.16E−03	−2.67			
40		6.70E−03	−2.17			
25		1.20E−03	−2.92	GC-retention time	38	Not used, more recent values from similar method
25		1.13E−03	−2.95	GC-retention index	39	Not used, more recent values from similar method
25		9.62E−04	−3.02	GC-retention index	13	Not used, more recent values from similar method

TABLE 11. Reported and selected physical–chemical properties for PCB-118—Continued

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
LDV at 25 °C			−3.05	Linear regression	45, 43, 6	Log $P_L = -4853/(T/\mathrm{K}) + 13.23$, $r^2 = 0.96$ (Fig. 3)
FAV at 25 °C			−3.00			Log $P_L = -4627/(T/\mathrm{K}) + 12.52$ (Fig. 3)

Henry's Law Constant in Pa·m³·mol⁻¹

T/°C	H	Log H	Method	Reference	Note
23	40.53	1.61	Equilibrium conc. ratio-GC	46	
20	8.61	0.94	Equilibrium conc. ratio-GC	43	
4	7.34	0.87	Gas purging-GC	12	
11	12.81	1.11			
18	21.79	1.34			
25	36.20	1.56			
31	54.80	1.74			
25	9.352	0.97	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	11.75	1.07	Estd., molecular connectivity	49	Not used, estimated value
25	12.73	1.10	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.51	Linear regression	46, 43, 12	Log $H = -2699/(T/\mathrm{K}) + 10.56$, $r^2 = 0.70$ (Fig. 4)
FAV at 25 °C		1.16			Log $H = -3289/(T/\mathrm{K}) + 12.19$ (Fig. 4)

Octanol–Air Partition Coefficient

T/°C		Log K_{OA}	Method	Reference	Note
−10		11.91	Generator column-GC	15	Reported as a linear regression equation
0		11.26			
10		10.65			
20		10.09			
30	9.56				
0		11.13	Multicolumn GC (retention index)	9	Not used, estimated value
20		10.04			
LDV at 25 °C		9.80	Directly taken	15	Log K_{OA} vs $1/(T/\mathrm{K})$ for values from Refs. 15 and 9 (Fig. 5)
FAV at 25 °C		9.36			Log $K_{OA} = 4646/(T/\mathrm{K}) - 6.22$ (Fig. 5)

Octanol Solubility in mol·m⁻³

	S_{OL}	Method	Reference	Note
FAV at 25 °C	918			

TABLE 12. Reported and selected physical–chemical properties for PCB-138

Registry No.	35065-28-2			
Chlorine substitution	2,3,4,2′,4′,5′-hexachlorobiphenyl	Melting point temperature/°C	79	
Molar mass/g·mol^{-1}	360.88	$\Delta_{\mathrm{fus}}S$/J·K^{-1}·mol^{-1}	56	Default value

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25		4.40E−05	−4.36	Estd., TSA	13	
25	6.60E−06	2.24E−05	−4.65	Slow stirring-GC	43	Adjusted to 25 °C
25	3.98E−06	1.35E−05	−4.87	HPLC-retention index	27	
25	4.20E−06	1.42E−05	−4.85	Calcd., QSPR	28	
20	5.21E−06	2.02E−05	−4.69	Slow stirring-GC	43	Not at 25 °C
LDV at 25 °C		2.08E−05		Log mean	13, 43, 27, 28	
FAV at 25 °C		1.87E−05				Log $S_{\mathrm{WL}} = -1437/(T/\mathrm{K}) + 0.093$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	7.44	HPLC-k'	32	
25	6.73	HPLC-retention index	27	
25	6.83	Estd., TSA	33	
LDV at 25 °C	7.00	Log mean	32, 27, 33	
FAV at 25 °C	7.22			

Vapor Pressure in Pa

T/°C	P_{S}	P_{L}	Log P_{L}	Method	Reference	Note
20		1.47E−04	−3.83	Head space-GC	43	
10		8.42E−05	−4.07	GC-retention time	45	Reported as a linear equation
20		3.41E−04	−3.47			
30		1.26E−03	−2.90			
40		4.27E−03	−2.37			
10		7.21E−05	−4.14	GC-retention time	6	Reported as a linear equation
20		2.73E−04	−3.56			
30		9.47E−04	−3.02			
40		3.03E−03	−2.52			
25		5.34E−04	−3.27	GC-retention time	38	Not used, more recent values from similar methods
25		5.03E−04	−3.30	GC-retention index	39	Not used, more recent values from similar methods
25		4.87E−04	−3.31	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−3.27	Linear regression	43, 45, 6	Log $P_{\mathrm{L}} = -5034/(T/\mathrm{K}) + 13.62$, $r^2 = 0.97$ (Fig. 3)
FAV at 25 °C			−3.25			Log $P_{\mathrm{L}} = -4770/(T/\mathrm{K}) + 12.75$ (Fig. 3)

Henry's Law Constant in Pa·m^3·mol^{-1}

T/°C	H	Log H	Method	Reference	Note
23	48.64	1.69	Equilibrium conc. ratio-GC	46	
20	7.60	0.88	Equilibrium conc. ratio-GC	43	
4	2.88	0.46	Gas purging-GC	12	
11	7.50	0.88			
18	18.68	1.27			
25	44.60	1.65			
31	91.10	1.96			
25	11.04	1.04	Calcd. from estimated P_{L} and S_{L}	13	Not used, estimated value
25	10.84	1.04	Estd., molecular connectivity	49	Not used, estimated value
25	2.13	0.33	Dynamic gas–water equilibrium	47	Not used, outlier
25	13.2	1.12	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.60	Linear regression	46, 43, 12	Log $H = -4672/(T/\mathrm{K}) + 17.27$, $r^2 = 0.86$ (Fig. 4)
FAV at 25 °C		1.48			Log $H = -3332/(T/\mathrm{K}) + 12.66$ (Fig. 4)

TABLE 12. Reported and selected physical–chemical properties for PCB-138—Continued

Octanol–Air Partition Coefficient $T/°\mathrm{C}$	Log K_{OA}	Method	Reference	Note
−10	11.85	Generator column-GC	15	Reported as a linear regression equation
0	11.21			
10	10.62			
20	10.07			
30	9.55			
10	10.30	Generator column (fugacity meter)-GC	8	Reported as a linear regression equation
13	10.14			
24	9.57			
35	9.04			
43	8.68			
10	10.72	Generator column-GC	74	Reported as a linear regression equation
20	10.19			
30	9.69			
40	9.22			
50	8.78			
0	11.34	Multicolumn GC (retention index)	9	Not used, estimated value
20	10.20			
LDV at 25 °C	9.76	Linear regression	15, 8, 74	Log $K_{OA}=4509/(T/\mathrm{K})-5.37$, $r^2=0.96$ (Fig. 5)
FAV at 25 °C	9.66			Log $K_{OA}=4510/(T/\mathrm{K})-5.47$ (Fig. 5)

Octanol Solubility in $\mathrm{mol\cdot m^{-3}}$	S_{OL}	Method	Reference	Note
FAV at 25 °C	1031			

TABLE 13. Reported and selected physical–chemical properties for PCB-153

Registry No.	35065-27-1			
Chlorine substitution	2,4,5,2′,4′,5′-hexachlorobiphenyl	Melting point temperature/°C	103	
Molar mass/g·mol^{-1}	360.88	$\Delta_{\mathrm{fus}}S$/J·K^{-1}·mol^{-1}	56	Default value

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	2.54E−05	1.48E−04	−3.83	Shake flask-GC	19	Adjusted to 25 °C
25	3.33E−06	1.94E−05	−4.71	Generator column-GC	24	
25	2.69E−06	1.56E−05	−4.81	Slow stirring-GC	50	Adjusted to 25 °C
4	1.28E−05	1.42E−04	−3.85	Generator column-GC	70	
25	2.34E−05	1.36E−04	−3.87			
40	3.54E−05	1.37E−04	−3.86			
25	4.57E−06	2.66E−05	−4.57	Generator column-GC	58	Adjusted to 25 °C
25	2.39E−06	1.39E−05	−4.86	Generator column-GC	51	
25	8.23E−06	4.79E−05	−4.32	Generator column-LSC	75	Adjusted to 25 °C
23	2.44E−05	1.50E−04	−3.82	Shake flask-GC	19	Not at 25 °C
23	2.64E−06	1.63E−05	−4.79	Slow stirring-GC	42	Not used, room temperature, assumed to be 23 °C
24	2.63E−06	1.58E−05	−4.80	Slow stirring-GC	50	Not at 25 °C
25		3.70E−05	−4.43	Estd., TSA	13	Not used, estimated
20		2.59E−05	−4.59	Slow stirring-GC	43	Not used, Aroclor mixture as standard
22	4.30E−06	2.73E−05	−4.56	Generator column-GC	58	Not at 25 °C
25	3.20E−06	1.86E−05	−4.73	HPLC-retention index	27	Not used, estimated value
25	2.45E−06	1.65E−05	−4.78	Calcd., QSPR	28	Not used, estimated value
22	7.76E−06	4.93E−05	−4.31	Generator column-LSC	75	Not at 25 °C
LDV at 25 °C		3.77E−05		Log mean	19, 24, 50, 58, 70, 51, 75	
FAV at 25 °C		3.07E−05				Log $S_{\mathrm{WL}} = -1305/(T/\mathrm{K}) - 0.14$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	6.65	Shake flask-GC	50	Adjusted to 25 °C
25	6.90	Generator column-GC	18	
25	6.58	Slow stirring-GC	73	
20	6.72	Shake flask-GC	50	Not at 25 °C
25	7.44	Estd., differential substitution constants	30	Not used, estimated value
25	6.68	HPLC-retention time	76	Not used, estimated value
25	6.90	Generator column-GC	31	Not used, same value as in Ref. 18.
25	6.90	Generator column-GC	44	Not used, same value as in Ref. 18.
25	8.31	Estd., group contribution	31	Not used, estimated value
25	6.75	Estd., TSA	31	Not used, estimated value
25	7.69	HPLC-k'	69	Not used, estimated value
25	6.80	HPLC-retention index	27	Not used, estimated value
25	6.92	Estd., TSA	33	Not used, estimated value
25	7.09	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	6.71	Log mean	50, 18, 73	
FAV at 25 °C	6.87			

TABLE 13. Reported and selected physical–chemical properties for PCB-153—Continued

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
20		2.53E−04	−3.60	Head space-GC	43	
10		5.31E−05	−4.27	GC-retention time	45	Reported as a linear equation
20		2.15E−04	−3.67			
30		7.93E−04	−3.10			
40		2.69E−03	−2.57			
10		9.69E−05	−4.01	GC-retention time	6	Reported as a linear equation
20		3.64E−04	−3.44			
30		1.26E−03	−2.90			
40		4.00E−03	−2.40			
25		6.99E−04	−3.16	GC-retention time	38	Not used, more recent values from similar methods
25		7.58E−04	−3.12	GC-retention index	39	Not used, more recent values from similar methods
25		6.63E−04	−3.18	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−3.28	Linear regression	43, 45, 6	Log $P_L = -4923/(T/\mathrm{K}) + 13.24$, $r^2 = 0.970$ (Fig. 3)
FAV at 25 °C			−3.22			Log $P_L = -4712/(T/\mathrm{K}) + 12.59$ (Fig. 3)

Henry's Law Constant in $\mathrm{Pa \cdot m^3 \cdot mol^{-1}}$

T/°C	H	Log H	Method	Reference	Note
23	27.00	1.43	Equilibrium conc. ratio-GC	46	
20	6.08	0.78	Gas purging-GC	66	
25	12.46	1.10	Gas purging-GC	53	
20	10.03	1.00	Batch equilibrium-GC	43	
25	13.37	1.13	Gas purging-GC	51	
4	6.50	0.81	Gas purging-GC	12	
11	13.52	1.13			
18	27.20	1.43			
25	52.80	1.72			
31	91.20	1.96			
25	17.93	1.25	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	13.37	1.13	Gas purging-GC	54	Not used, same value as Ref. 51
25	2.33	0.37	Dynamic gas-water equilibrium-GC	47	Not used, outlier
25	16.7	1.22	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.40	Linear regression	46, 66, 53, 43, 51, 12	Log $H = -2584/(T/\mathrm{K}) + 10.07$, $r^2 = 0.39$ (Fig. 4)
FAV at 25 °C		1.30			Log $H = -3407/(T/\mathrm{K}) + 12.72$ (Fig. 4)

Octanol–Air Partition Coefficient

T/°C	Log K_{OA}	Method	Reference	Note
0	11.17	Generator column-GC	15	Reported as a linear regression equation
10	10.56			
20	10.00			
30	9.47			
10	10.16	Generator column (fugacity meter)-GC	8	Reported as a linear regression equation
13	9.99			
24	9.42			
35	8.89			
0	11.03	Multicolumn GC (retention index)	9	Not used, estimated value
20	9.99			
LDV at 25 °C	9.52	Linear regression	15, 8	Log $K_{OA} = 4966/(T/\mathrm{K}) - 7.14$, $r^2 = 0.923$ (Fig. 5)
FAV at 25 °C	9.44			Log $K_{OA} = 4903/(T/\mathrm{K}) - 7.00$ (Fig. 5)

Octanol Solubility in $\mathrm{mol \cdot m^{-3}}$

	S_{OL}	Method	Reference	Note
FAV at 25 °C	675			

TABLE 14. Reported and selected physical–chemical properties for PCB-155

Registry No.	33979-03-2			
Chlorine substitution	2,2′,4,4′,6,6′-hexachlorobiphenyl	Melting point temperature/°C	113	
Molar mass/g·mol^{-1}	360.88	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	45.3	Ref. 59

Aqueous Solubility in mol·m^{-3}

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	6.18E−06	3.09E−05	−4.51	Generator column-GC	51	
22	7.87E−06	4.22E−05	−4.37	Generator column-GC	58	
25	9.12E−06	4.55E−05	−4.34	Generator column-GC	22	
25	7.87E−06	3.93E−05	−4.41	Slow stirring-GC	26	
25	9.12E−06	4.55E−05	−4.34	Generator column-GC	77	
5	2.77E−06	2.30E−05	−4.64	Equilibrium gas stripping	23	
15	4.71E−06	3.00E−05	−4.52			
25	7.76E−06	3.87E−05	−4.41			
35	1.19E−05	4.73E−05	−4.32			
45	1.77E−05	5.68E−05	−4.25			
25	2.49E−06	1.25E−05	−4.90	Generator column-GC	24	Not used, outlier
25	1.13E−06	5.64E−06	−5.25	Generator column-GC	59	Not used, outlier
25		2.81E−05	−4.55	Estd., TSA	13	Not used, estimated value
25	7.59E−06	3.79E−05	−4.42	HPLC-retention index	27	Not used, estimated value
25	6.30E−06	3.14E−05	−4.50	Calcd., QSPR	28	Not used, estimated value
25	9.12E−06	4.59E−05	−4.34	Generator column-GC	29	Not used, same value as Ref. 22
LDV at 25 °C		3.93E−05		Linear regression	51, 58, 22, 26, 77, 23	Log $S_{WL} = -861/(T/K) - 1.52$, $r^2 = 0.80$ (Fig. 2)
FAV at 25 °C		3.82E−05				Log $S_{WL} = -1268/(T/K) - 0.16$ (Fig. 2)

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	7.55	Generator column-GC	59	
25	7.29	Slow stirring-GC (HPLC)	60	
25	7.24	Generator column-GC	29	
25	6.39	HPLC-k'	78	Not used, estimated value
25	7.12	Estd., differential substitution constants	30	Not used, estimated value
25	6.39	HPLC-t'_R	76	Not used, estimated value
25	8.31	Estd., HPLC-MS	76	Not used, estimated value
25	6.54	HPLC-retention index	27	Not used, estimated value
25	6.41	Estd., TSA	33	Not used, estimated value
25	7.20	Estd., LSER	61	Not used, estimated value
25	7.24	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	7.36	Log mean	59, 60, 29	
FAV at 25 °C	7.19			

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
−10	1.63E−06	2.09E−05	−4.68	Gas saturation-GC	37	
0	1.19E−05	1.13E−04	−3.95			
10	8.04E−05	5.83E−04	−3.23			
20	3.25E−04	1.83E−03	−2.74			
30	7.79E−04	3.46E−03	−2.46			
10		6.65E−04	−3.18	GC-retention time	6	Reported as a linear equation
20		2.20E−03	−2.66			
30		6.69E−03	−2.17			
40		1.90E−02	−1.72			
25		1.60E−03	−2.80	GC-retention time	65	Not used, more recent values from similar methods
25		4.43E−03	−2.35	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−2.48	Linear regression	37, 6	Log $P_L = -4697/(T/K) + 13.27$, $r^2 = 0.98$ (Fig. 3)
FAV at 25 °C			−2.46			Log $P_L = -4562/(T/K) + 12.85$ (Fig. 3)

TABLE 14. Reported and selected physical–chemical properties for PCB-155—Continued

Henry's Law Constant in $Pa \cdot m^3 \cdot mol^{-1}$

$T/°C$	H	Log H	Method	Reference	Note
25	76.50	1.88	Gas purging-GC	51	
25	157.05	2.20	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	11.65	1.07	Gas purging-GC	53	Not used, more recent values using same approach
25	76.50	1.88	Gas purging-GC	54	Not used, same value as in Ref. 51
25	85.25	1.93	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		1.88	Log mean	51	
FAV at 25 °C		1.96			Log $H = -3294/(T/K) + 13.01$

Octanol–Air Partition Coefficient

$T/°C$	Log K_{OA}	Method	Reference	Note
0	10.19	Multicolumn GC (retention index)	9	Estimated value
20	9.13			
−10	10.48	Generator column-GC	14	Not used, highly inconsistent with other properties
0	10.02			
10	9.59			
20	9.18			
LDV at 25 °C	8.89	Extrapolation	9	Log K_{OA} vs $1/(T/K)$ for values from Refs. 14 and 9 (Fig. 5)
FAV at 25 °C	9.14			Log $K_{OA} = 4357/(T/K) - 5.47$ (Fig. 5)

Octanol Solubility in $mol \cdot m^{-3}$

	S_{OL}	Method	Reference	Note
FAV at 25 °C	1948			

TABLE 15. Reported and selected physical–chemical properties for PCB-180

Registry No.	35065-29-3			
Chlorine substitution	2,3,4,5,2′,4′,5′-heptachlorobiphenyl	Melting point temperature/°C	112	
Molar mass/$g \cdot mol^{-1}$	395.32	$\Delta_{fus}S/J \cdot K^{-1} \cdot mol^{-1}$	56	Default value

Aqueous Solubility in $mol \cdot m^{-3}$

T/°C	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25		1.66E−05	−4.78	Estd., TSA	13	
25		1.08E−05	−4.97	Slow stirring-GC	43	Adjusted to 25 °C
25	7.94E−07	5.67E−06	−5.25	HPLC-retention index	27	
25	5.70E−07	4.07E−06	−5.39	Calcd., QSPR	28	
20		9.74E−06	−5.01	Slow stirring-GC	43	Not at 25 °C
LDV at 25 °C		8.01E−06		Log mean	13, 43, 27, 28	No directly measured values at 25 °C
FAV at 25 °C		1.32E−05				Log $S_{WL} = -1356/(T/K) - 0.33$

Octanol–Water Partition Coefficient

T/°C	Log K_{OW}	Method	Reference	Note
25	7.21	HPLC-retention index	27	
25	7.36	Estd., TSA	33	
LDV at 25 °C	7.29	Log mean	27, 33	No directly measured values
FAV at 25 °C	7.16			

Vapor Pressure in Pa

T/°C	P_S	P_L	Log P_L	Method	Reference	Note
0		3.73E−06	−5.43	GC-retention time	6	Reported as a regression equation
10		1.67E−05	−4.78			
20		6.77E−05	−4.17			
30		2.50E−04	−3.60			
25		1.29E−04	−3.89	GC-retention time	38	Not used, more recent values from similar methods
25		1.32E−04	−3.88	GC-retention index	39	Not used, more recent values from similar methods
25		5.06E−04	−3.30	GC-retention index	13	Not used, more recent values from similar methods
20		3.14E−05	−4.50	Head space-GC	43	Not used, Aroclor mixture as standard
LDV at 25 °C			−3.88	Directly taken	6	
FAV at 25 °C			−3.97			Log $P_L = -4809/(T/K) + 12.16$

Henry's Law Constant in $Pa \cdot m^3 \cdot mol^{-1}$

T/°C	H	Log H	Method	Reference	Note
25	53.0	0.72	Equilibrium conc. ratio-GC	43	
25	1.01	0.01	Dynamic gas–water equilibrium-GC	47	Adjusted to 25 °C
4	0.43	−0.37	Gas purging-GC	12	
11	2.03	0.31			
18	8.96	0.95			
25	37.00	1.57			
31	118.50	2.07			
25	30.40	1.48	Calcd. from estimated P_L and S_L	13	Not used, estimated value
20	3.24	0.51	Equilibrium conc. ratio-GC	43	Not at 25 °C
25	10.88	1.04	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		0.77	Log mean	43, 47, 12	
FAV at 25 °C		0.93			Log $H = -3453/(T/K) + 12.49$

TABLE 15. Reported and selected physical–chemical properties for PCB-180—Continued

Octanol–Air Partition Coefficient $T/°\mathrm{C}$	Log K_{OA}	Method	Reference	Note
0	11.90	Generator column-GC	15	Reported as a linear regression equation
10	11.32			
20	10.77			
30	10.26			
10	10.57	Generator column (fugacity meter)-GC	8	Reported as a linear regression equation
13	10.42			
24	9.92			
35	9.44			
0	11.94	Multi-column GC (retention index)	9	Not used, estimated value
20	10.72			
LDV at 25 °C	10.12	Linear regression	15, 8	Log $K_{\mathrm{OA}} = 4975/(T/\mathrm{K}) - 6.55$, $r^2 = 0.79$ (Fig. 5)
FAV at 25 °C	10.16			Log $K_{\mathrm{OA}} = 4845/(T/\mathrm{K}) - 6.09$ (Fig. 5)

Octanol Solubility in mol·m^{-3}	S_{OL}	Method	Reference	Note
FAV at 25 °C	633			

TABLE 16. Reported and selected physical–chemical properties for PCB-194

Registry No.	35694-08-7			
Chlorine substitution	2,3,4,5,2′,3′,4′,5′-octachlorobiphenyl	Melting point temperature/°C	157	
Molar mass/$g\cdot mol^{-1}$	429.77	$\Delta_{fus}S/J\cdot K^{-1}\cdot mol^{-1}$	56	Default value

Aqueous Solubility in $mol\cdot m^{-3}$

$T/°C$	S_{WS}	S_{WL}	Log S_{WL}	Method	Reference	Note
25	5.44E−08	1.07E−06	−5.97	Shake flask-GC	19	Adjusted to 25 °C
25	6.33E−07	1.25E−05	−4.90	Generator column-GC	24	
25	2.60E−06	5.12E−05	−4.29	Generator column-GC	58	Adjusted to 25 °C
23	4.90E−08	1.03E−06	−5.99	Shake flask-GC	19	Not at 25 °C
22	2.21E−06	4.82E−05	−4.32	Generator column-GC	58	Not at 25 °C
25		8.13E−06	−5.09	Estd., TSA	13	Not used, estimated value
25	2.00E−07	3.94E−06	−5.40	HPLC-retention index	27	Not used, estimated value
25	4.90E−08	9.66E−07	−6.01	Calcd., QSPR	28	Not used, estimated value
LDV at 25 °C		8.82E−06		Log mean	19, 24, 58	
FAV at 25 °C		5.59E−06				Log $S_{WL}=-1533/(T/K)-0.11$

Octanol–Water Partition Coefficient

$T/°C$	Log K_{OW}	Method	Reference	Note
25	7.67	Generator column-GC	33	
25	8.68	Estd., differential substitution constants	30	Not used, estimated value
25	7.62	HPLC-retention index	27	Not used, estimated value
25	7.80	Estd., TSA	33	Not used, estimated value
25	8.07	Estd., characteristic root index	34	Not used, estimated value
LDV at 25 °C	7.67	Directly taken	33	
FAV at 25 °C	7.76			

Vapor Pressure in Pa

$T/°C$	P_S	P_L	Log P_L	Method	Reference	Note
0		4.50E−07	−6.35	GC-retention time	6	Reported as a linear equation
10		2.25E−06	−5.65			
20		1.01E−05	−5.00			
30		4.08E−05	−4.39			
25		1.93E−05	−4.72	GC-retention index	39	Not used, more recent values from similar methods
25		3.86E−04	−3.41	GC-retention index	13	Not used, more recent values from similar methods
LDV at 25 °C			−4.69	Directly taken	6	
FAV at 25 °C			−4.61			Log $P_L=-5099/(T/K)+12.49$

Henry's Law Constant in $Pa\cdot m^3\cdot mol^{-1}$

$T/°C$	H	Log H	Method	Reference	Note
25	6.79	0.83	Calcd., QSPR	28	
25	47.52	1.68	Calcd. from estimated P_L and S_L	13	Not used, estimated value
25	1.01	0.0057	Dynamic gas–water equilibrium	47	Not used, highly inconsistent with other properties
LDV at 25 °C		0.83	Directly taken	28	
FAV at 25 °C		0.64			Log $H=-3566/(T/K)+12.60$

Octanol–Air Partition Coefficient

$T/°C$	Log K_{OA}	Method	Reference	Note
0	12.83	Multicolumn GC (retention index)	9	
20	11.59			
LDV at 25 °C	11.31	Extrapolation	9	
FAV at 25 °C	11.13			Log $K_{OA}=4906/(T/K)-5.33$

Octanol Solubility in $mol\cdot m^{-3}$

	S_{OL}	Method	Reference	Note
FAV at 25 °C	1331			

TABLE 17. Literature-derived values and assigned uncertainty estimates for the physical–chemical properties at 25 °C

	S_{WL}/mol·m^{-3}		K_{OW}		P_{L}/Pa		H/Pa·m^3·mol^{-1}		K_{OA}		S_{OL}/mol·m^{-3}	
Compound	LDV	u_{W}	LDV	u_{OW}	LDV	u_{A}	LDV	u_{AW}	LDV	u_{OA}	LDV	u_{O}
PCB-3	1.71E−02	1	3.09E+04	1	4.80E−01	1	36.0	5	6.58E+06	1	1350.2	1
PCB-8	7.36E−03	2	1.23E+05	1	1.23E−01	3	26.2	2	2.53E+07	2		
PCB-15	5.00E−03	2	2.53E+05	1	5.04E−02	1	14.2	2	4.50E+07	2	1721.3	1
PCB-28	1.01E−03	2	3.58E+05	3	2.36E−02	2	33.1	1	8.58E+07	2		
PCB-29	1.86E−03	2	5.50E+05	2	4.47E−02	2	32.6	3	6.28E+07	5	691.7	5
PCB-31	8.53E−04	3	6.17E+05	3	2.38E−02	2	36.8	4	8.58E+07	2		
PCB-52	6.82E−04	4	1.05E+06	4	1.06E−02	2	28.2	1	1.65E+08	2	735.3	3
PCB-61	3.63E−04	2	1.49E+06	4	7.21E−03	2	20.6	5	4.38E+08	5	862.2	3
PCB-101	1.05E−04	3	1.42E+06	4	2.41E−03	2	31.4	4	7.90E+08	1		
PCB-105	1.11E−04	5	4.07E+06	2	8.74E−04	2	33.6	5	1.02E+10	4		
PCB-118	8.88E−05	5	3.09E+06	2	8.93E−04	2	32.0	5	6.61E+09	4		
PCB-138	2.08E−05	5	9.98E+06	5	5.39E−04	2	39.5	4	5.72E+09	2		
PCB-153	3.77E−05	3	5.11E+06	5	5.29E−04	2	25.0	3	3.28E+09	2		
PCB-155	3.93E−05	1	2.29E+07	4	3.31E−03	2	76.5	4	7.71E+08	5		
PCB-180	8.01E−06	5	1.93E+07	5	1.32E−04	2	5.84	4	1.37E+10	1		
PCB-194	8.82E−06	5	4.68E+07	3	2.05E−05	2	6.79	5	2.02E+11	5		

TABLE 18. Internally consistent physical–chemical properties at 25 °C after adjustment.[a] The required percentage of adjustment to achieve consistency is also given.[b]

	S_{WL}/mol·m^{-3}		K_{OW}		P_{L}/Pa		H/Pa·m^3·mol^{-1}		K_{OA}		S_{OL}/mol·m^{-3}	
Compound	FAV	Adj.	FAV	Adj.	FAV	Adj.	FAV	Adj.	FAV	Adj.	FAV	Adj.
PCB-3	2.02E−02	18%	4.42E+04	43%	4.77E−01	−1%	23.6	−34%	5.98E+06	−9%	1.2E+03	−15%
PCB-8	6.49E−03	−12%	1.31E+05	7%	1.48E−01	21%	22.8	−13%	2.18E+07	−14%	1.3E+03	
PCB-15	4.29E−03	−14%	2.27E+05	−10%	5.73E−02	14%	13.4	−6%	7.07E+07	57%	1.6E+03	−5%
PCB-28	8.85E−04	−13%	4.61E+05	29%	2.70E−02	15%	30.5	−8%	7.05E+07	−18%	7.7E+02	
PCB-29	1.51E−03	−19%	4.01E+05	−27%	4.56E−02	2%	30.2	−8%	6.06E+07	−4%	1.1E+03	61%
PCB-31	7.54E−04	−12%	6.08E+05	−1%	2.58E−02	9%	34.2	−7%	8.67E+07	1%	9.0E+02	
PCB-52	4.78E−04	−30%	8.10E+05	−18%	1.20E−02	13%	25.1	−11%	1.65E+08	0%	8.0E+02	9%
PCB-61	3.46E−04	−5%	1.28E+06	−14%	6.93E−03	−4%	20.0	−3%	3.52E+08	−20%	9.8E+02	14%
PCB-101	1.02E−04	−3%	2.16E+06	52%	2.46E−03	2%	24.1	−23%	5.38E+08	−11%	5.3E+02	
PCB-105	7.45E−05	−33%	6.54E+06	61%	1.03E−03	17%	13.8	−59%	3.40E+09	−67%	1.4E+03	
PCB-118	6.83E−05	−23%	4.87E+06	58%	9.91E−04	11%	14.5	−55%	2.30E+09	−65%	9.2E+02	
PCB-138	1.87E−05	−10%	1.64E+07	64%	5.63E−04	4%	30.1	−24%	4.54E+09	−21%	1.0E+03	
PCB-153	3.07E−05	−19%	7.44E+06	46%	6.06E−04	15%	19.8	−21%	2.76E+09	−16%	6.7E+02	
PCB-155	3.82E−05	−3%	1.53E+07	−33%	3.49E−03	6%	91.4	19%	1.38E+09	79%	1.9E+03	
PCB-180	1.32E−05	65%	1.45E+07	−25%	1.08E−04	−18%	8.13	39%	1.46E+10	7%	6.3E+02	
PCB-194	5.59E−06	−37%	5.78E+07	24%	2.46E−05	20%	4.40	−35%	1.34E+11	−34%	1.3E+03	

[a] Method for adjustment: iterative (see text).

[b] If no percentage of adjustment is given, no LDV existed and the value was calculated from the other properties.

TABLE 19. Literature-derived values and assigned uncertainty estimates for the internal energies of phase transfer in kJ·mol^{-1}

Compound	ΔU_W		u_W	ΔU_{OW}		u_{OW}	ΔU_A		u_A	ΔU_{AW}		u_{AW}	ΔU_{OA}		u_{OA}	ΔU_O		u_O
PCB-3	12.1	W1	3	−20	OW1	5	69.1	A1	1	44.9	AW1	4	−66.4	OA1	2			
PCB-8	14.8	W2	5	−21	OW1	5	70.6	A2	2	47.4	AW1	4	−73.1	OA2	2			
PCB-15	15.5	W3	5	−21	OW1	5	72.8	A3	2	47.4	AW1	4	−75.9	OA3	5	−10.2	O1	5
PCB-28	14.8	W2	5	−22	OW1	5	77.1	A2	2	50.0	AW2	2	−80.2	OA2	2			
PCB-29	15.8	W4	3	−22	OW1	5	74.2	A4	2	49.9	AW1	4	−84.3	OA3	5			
PCB-31	14.8	W2	5	−22	OW1	5	77.0	A2	2	48.6	AW1	4	−80.2	OA2	2			
PCB-52	14.8	W2	5	−23	OW1	5	77.7	A5	2	52.0	AW2	2	−83.1	OA2	2			
PCB-61	16.1	W5	3	−24	OW1	5	80.4	A6	2	52.3	AW1	4	−96.6	OA3	5			
PCB-101	13.1	W6	3	−24	OW1	5	86.2	A5	2	54.4	AW1	4	−83.5	OA4	1			
PCB-105	14.8	W2	5	−24	OW1	5	88.6	A4	2	54.4	AW1	4	−89.6	OA1	1			
PCB-118	14.8	W2	5	−24	OW1	5	90.4	A2	2	54.4	AW1	4	−89.9	OA1	1			
PCB-138	14.8	W2	5	−25	OW1	5	93.9	A2	2	56.2	AW1	4	−86.3	OA5	1			
PCB-153	14.8	W2	5	−25	OW1	5	91.8	A2	2	56.2	AW1	4	−95.1	OA4	1			
PCB-155	16.5	W7	3	−25	OW1	5	87.5	A6	1	56.3	AW1	4	−81.3	OA3	5			
PCB-180	14.8	W2	5	−26	OW1	5	94.1	A4	2	57.9	AW1	4	−95.3	OA4	4			
PCB-194	14.8	W2	5	−27	OW1	5	101.0	A4	2	59.5	AW1	4	−95.1	OA3	5			

W1:	regression of log S_{WL} vs $1/T$ using data from Refs. 19, 20, 21, 22, and 23.
W2:	average of experimentally derived ΔU_W for PCBs 3, 15, 29, 61, 101, and 155.
W3:	regression of log S_{WL} vs $1/T$ using data from Refs. 19, 21, 23, 24, and 50.
W4:	regression of log S_{WL} vs $1/T$ using data from Refs. 21, 23, 24, and 59.
W5:	regression of log S_{WL} vs $1/T$ using data from Refs. 22, 23, 24, 51, and 59.
W6:	Ref. 67.
W7:	regression of log S_{WL} vs $1/T$ using data from Refs. 22, 23, 26, 51, 58, and 77.
OW1:	an empirical value derived from Ref. 10.
A1:	regression of log P_L vs $1/T$ using data from Refs. 6, 35, 36, and 37.
A2:	regression of log P_L vs $1/T$ using data of Refs. 6, 43, and 45.
A3:	regression of log P_L vs $1/T$ using data from Refs. 6, 37, 45, and 52.
A4:	Ref. 6.
A5:	regression of log P_L vs $1/T$ using data from Refs. 6, 43, 45, and 64.
A6:	regression of log P_L vs $1/T$ using data from Refs. 6 and 37.
AW1:	from Ref. 13, calibrated with a factor of 0.846, a ratio of ΔU_{AW} from Ref. 79 to those from Ref. 11 for PCB-28 and PCB-52.
AW2:	Ref. 11.
OA1:	Ref. 11.
OA2:	Ref. 8.
OA3:	derived from data given in Ref. 9.
OA4:	regression of log K_{OA} vs $1/T$ using data from Refs. 15 and 8.
OA5:	regression of log K_{OA} vs $1/T$ using data from Refs. 15, 8, and 74.

TABLE 20. Internal energies of phase transfer after adjustment.[a] The required percentage of adjustment to achieve consistency is also given.[b]

	ΔU_W/kJ·mol^{-1}		ΔU_{OW}/kJ·mol^{-1}		ΔU_A/kJ·mol^{-1}		ΔU_{AW}/kJ·mol^{-1}		ΔU_{OA}/kJ·mol^{-1}		ΔU_O/kJ·mol^{-1}	
Compound	FAV	Adj.	FAV	Adj.	FAV	Adj.	FAV	Adj.	FAV	Adj.	FAV	Adj.
PCB-3	18.4	53%	−18.5	−7%	67.0	−3%	48.5	8%	−67.0	1%	−0.1	
PCB-8	19.1	29%	−22.7	8%	68.9	−2%	49.8	5%	−72.5	−1%	−3.6	
PCB-15	17.4	13%	−24.6	17%	70.8	−3%	53.4	13%	−78.1	3%	−7.3	−29%
PCB-28	22.0	48%	−26.3	19%	74.2	−4%	52.3	5%	−78.5	−2%	−4.3	
PCB-29	18.7	19%	−26.4	20%	72.3	−3%	53.6	7%	−79.9	−5%	−7.7	
PCB-31	21.5	45%	−25.9	18%	74.3	−3%	52.8	9%	−78.7	−2%	−4.4	
PCB-52	21.1	42%	−27.3	19%	75.2	−3%	54.1	4%	−81.4	−2%	−6.2	
PCB-61	20.0	24%	−31.4	31%	77.8	−3%	57.8	11%	−89.2	−8%	−11.4	
PCB-101	21.2	61%	−23.8	−1%	80.8	−6%	59.7	10%	−83.5	0%	−2.7	
PCB-105	24.6	66%	−28.6	19%	84.7	−4%	60.1	11%	−88.7	−1%	−4.0	
PCB-118	25.6	73%	−28.5	19%	86.1	−5%	60.5	11%	−89.0	−1%	−2.8	
PCB-138	27.5	86%	−25.0	0%	88.8	−5%	61.3	9%	−86.3	0%	2.5	
PCB-153	25.0	69%	−31.1	25%	87.7	−4%	62.8	12%	−93.9	−1%	−6.2	
PCB-155	24.3	47%	−22.8	−9%	84.9	−3%	60.6	8%	−83.4	3%	1.5	
PCB-180	26.0	75%	−29.1	12%	89.6	−5%	63.6	10%	−92.8	−3%	−3.2	
PCB-194	29.4	98%	−28.1	4%	95.2	−6%	65.8	11%	−93.9	−1%	1.2	

[a] Method for adjustment: iterative (see text).

[b] If no percentage of adjustment is given, no LDV existed and the value was calculated from the other properties.

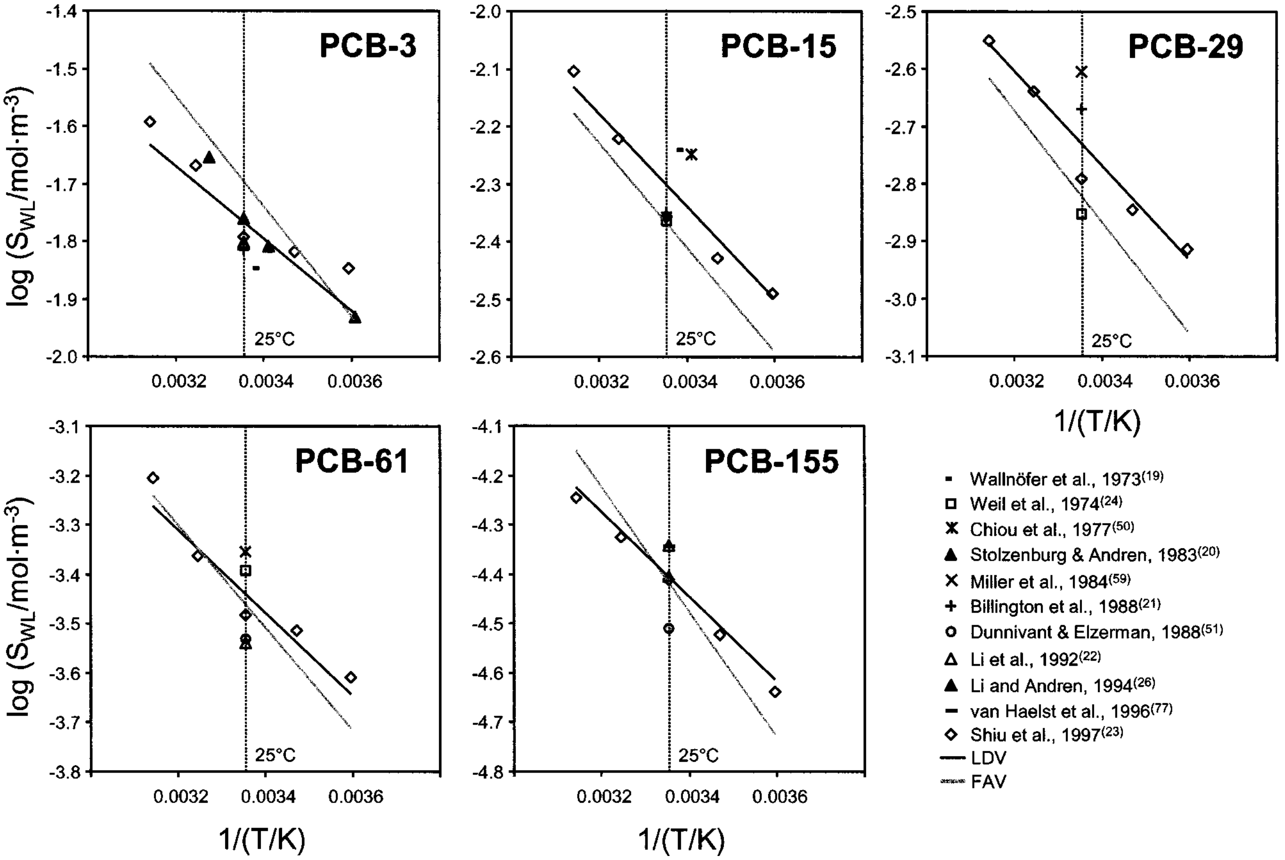

FIG. 2. Relationships between the logarithm of the liquid solubility of 5 PCBs in water and reciprocal absolute temperature.

hand, S_W and K_{AW} are usually determined with pure water, and S_{OS} and K_{OA} with pure octanol. If the presence of the other solvent notably affects the solubility of the solutes in water or octanol, the adjustment procedure needs to take this into account by deriving a corrective regression that relates the experimentally determined K_{OW} values with the ratio of the solubilities in pure octanol S_O and pure water S_W. Whereas Beyer *et al.*[4] presented such a regression, we derived one here that is specific for the PCBs and based on the LDVs derived in step 4.

In addition to the five LDVs for directly measured solubilities in octanol, we derived S_{OL} for all 16 congeners using

$$S_{OL}=K_{OA}\cdot P_L/(R\cdot T) \tag{2}$$

and the LDVs for K_{OA} and P_L. We then combined these with the LDVs for solubility in water S_{WL} to calculate the ratio of the solubilities in pure octanol and pure water. The logarithm of that ratio was then plotted (Fig. 1) and regressed against the LDVs for the $\log K_{OW}$

$$\log(S_{OL}/S_{WL})=(1.16\pm0.08)\cdot\log K_{OW}-(0.64\pm0.50),$$

$$n=21, r^2=0.914. \tag{3}$$

The relationship is very similar to that found by Beyer *et al.*[4] and indicates that the mutual solubility effect increases with hydrophobicity, to result in deviation between K_{OW} and S_{OL}/S_{WL} by 1/2 an order of magnitude for the most hydrophobic PCB congeners.

Several steps in this procedure relied to some extent on our subjective judgement rather than a prescribed set of numerical rules or a statistical test. From the experience gained during this study, we have come to the conclusion that a completely standardized approach to data selection is likely neither feasible nor desirable. During data selection procedures, situations will inevitably occur that are much better resolved through the subjective expert judgement of the compiler than by an inflexible set of rules and numerical procedures. Unfortunately, this implies that different people would derive different sets of FAVs using the same procedure and the same experimental data, i.e., the method is not entirely reproducible in the scientific sense. The variability between FAV data sets derived by different experts will however be within the measurement uncertainty of the original data.

In any case, our knowledge of physical–chemical properties is cumulative. LDV selection, uncertainty assignment, and consistency adjustment to FAVs (steps iv, v, and vi) thus need to be seen as an iterative process that would need to be continuously updated as new measurements are made and become available. One could even argue that the procedure could highlight urgent data gaps, where new and more reli-

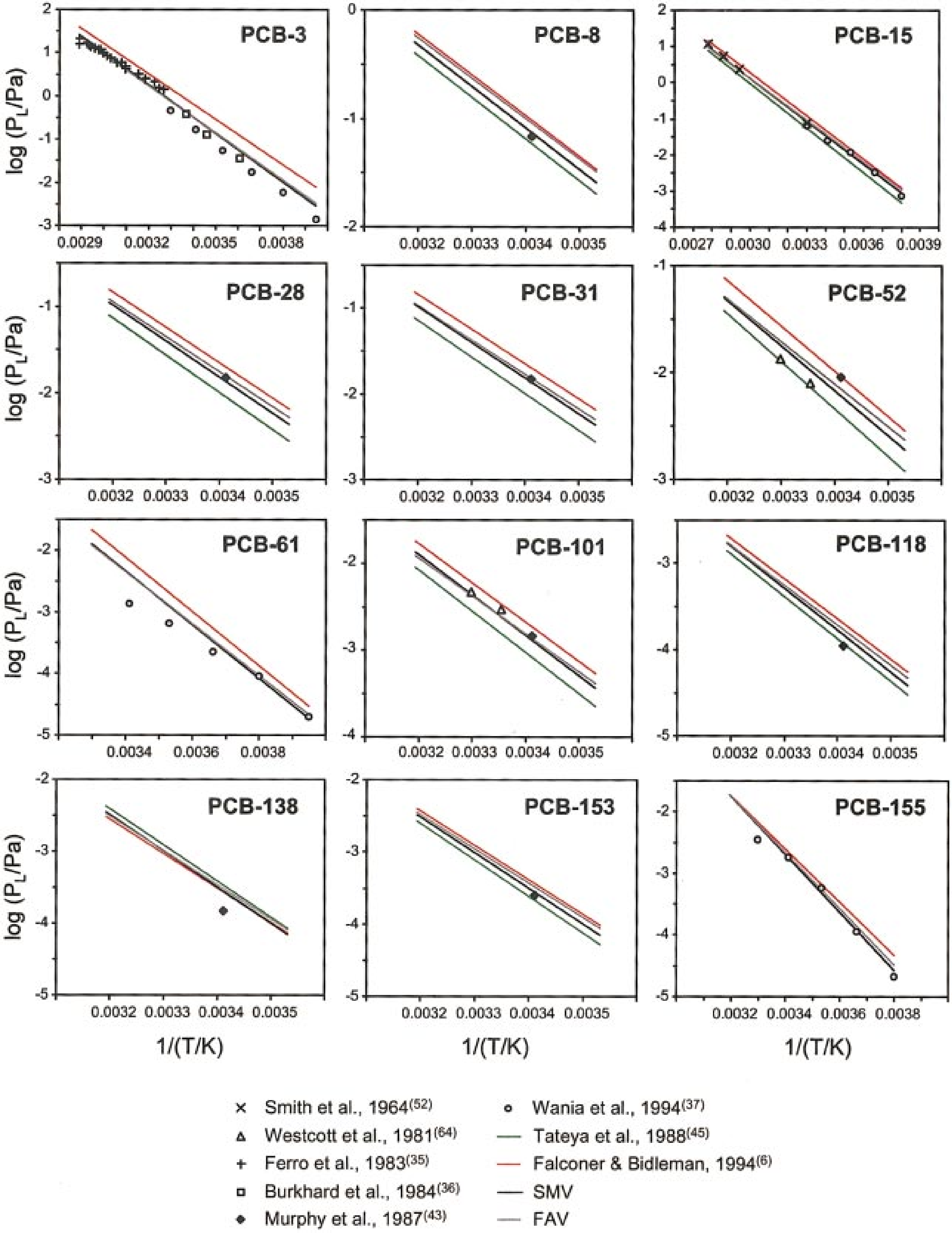

FIG. 3. Relationships between the logarithm of the liquid vapor pressure of 12 PCBs and reciprocal absolute temperature.

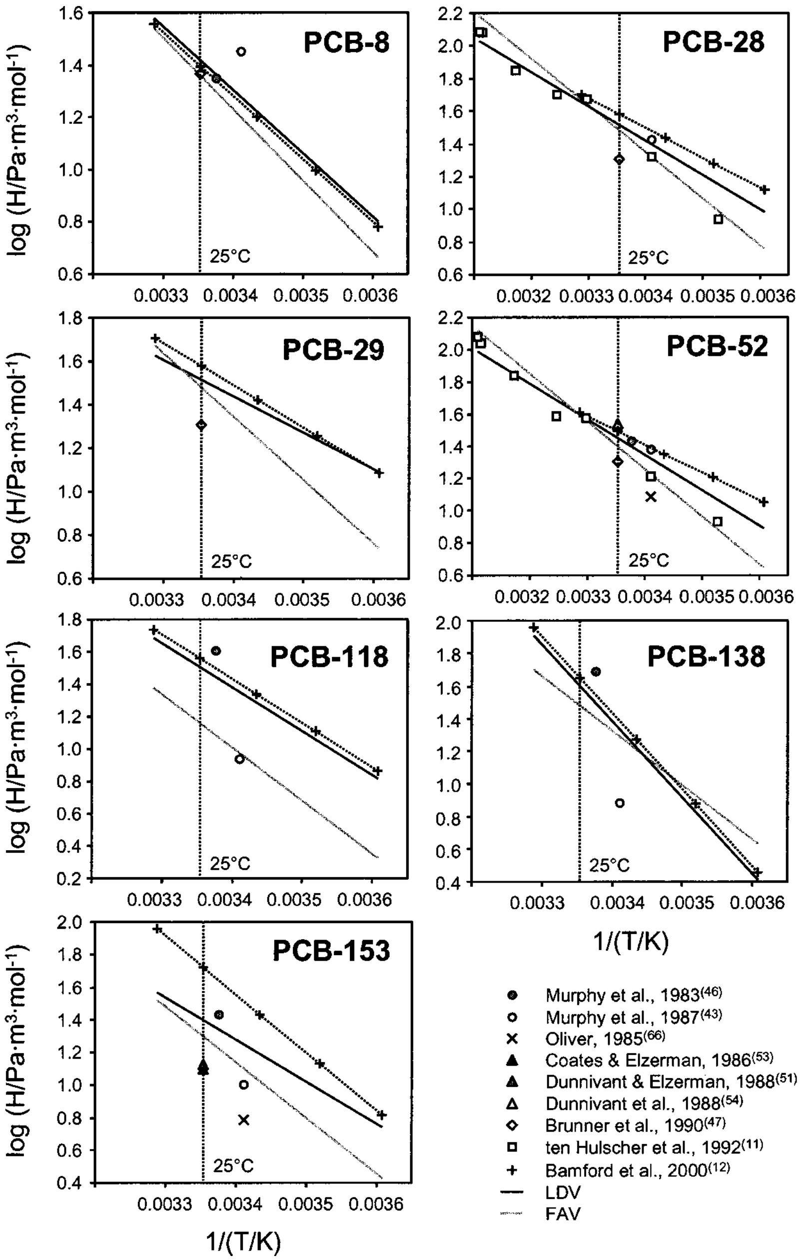

FIG. 4. Relationships between the logarithm of the Henry's law constant of 7 PCBs and reciprocal absolute temperature.

able measurements would be most valuable in constraining the physical–chemical property data set for a particular compound.

3. Results

Tables 1–16 present the water solubility S_W, octanol–water partition coefficient $\log K_{OW}$, vapor pressure P, Henry's law constant H, octanol–air partition coefficient K_{OA}, and octanol solubility S_O, in that sequence for each of the 16 PCB congeners. At the top of each subtable are the data that were included in the derivation of the LDVs, including the experimental temperature, the method used, and the reference. For comparison and completeness, the data that were not included in the derivation of the LDVs are listed in the bottom part of the subtables, together with the reason for exclusion. In these tables, the following acronyms were used: total surface area (TSA), liquid scintillation counter (LSC), linear solvation energy relationship (LSER) and gas chromatography (GC).

For P_L and K_{OA}, some investigators simply report the experimental data as a linear equation.[6,8] In such cases, discrete values were calculated for four or five temperatures, which were either the experimental temperatures indicated in the reference or temperatures in the environmentally relevant range. A similar approach was taken with the Henry's law constants reported by Bamford *et al.*,[12] which are the results of a regression analysis and not the actual measured values. Although this approach appears appropriate when the actual experimental temperatures are known,[8,12] it should be noted that it will underestimate the true uncertainty of the measured data and the correlation coefficients for regressions in-

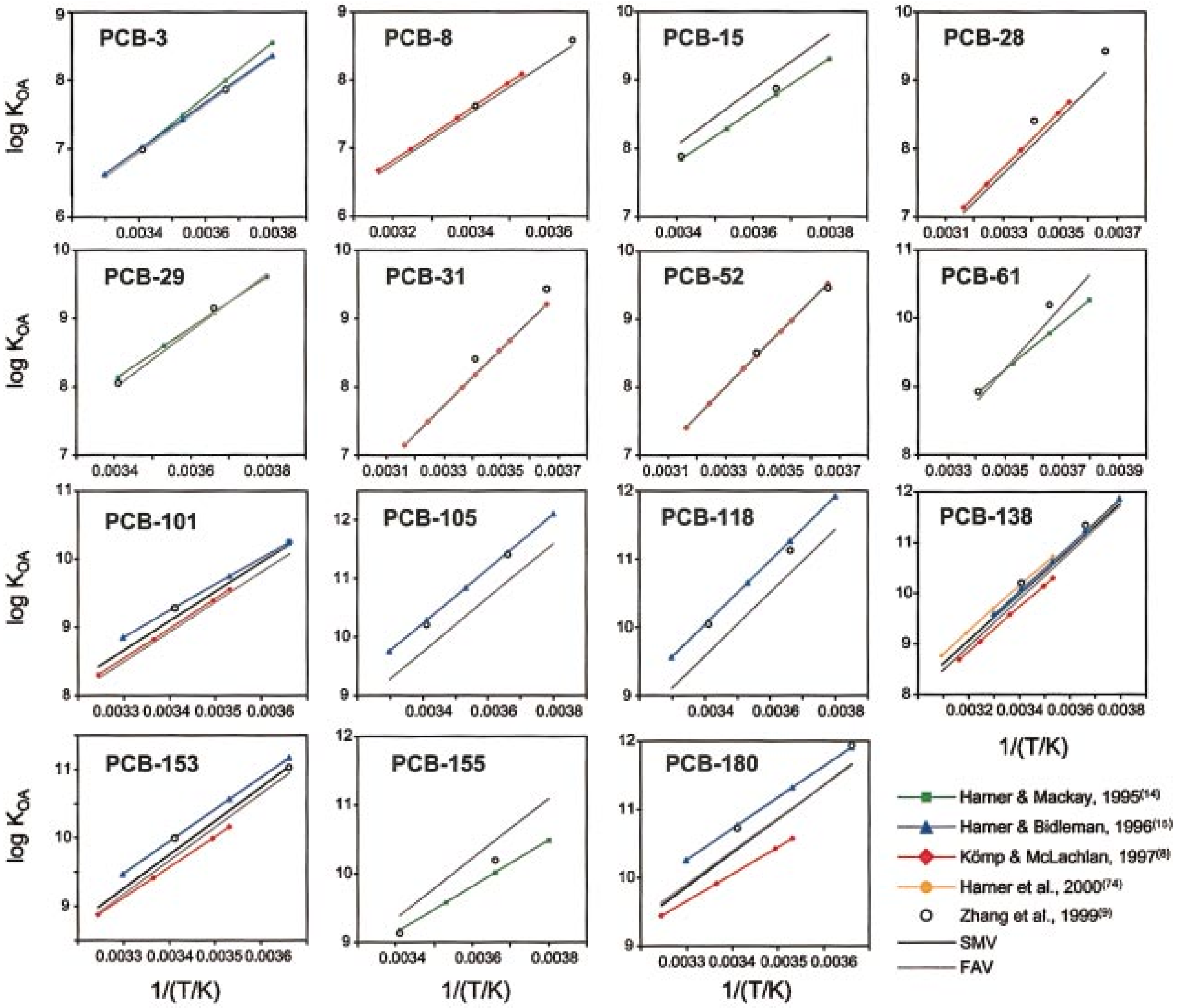

FIG. 5. Relationships between the logarithm of the octanol-air partition coefficient of 15 PCBs and reciprocal absolute temperature.

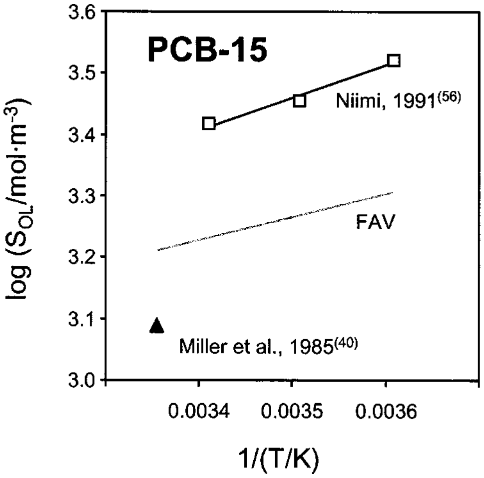

FIG. 6. Relationships between the logarithm of the liquid solubility in octanol of PCB-15 and reciprocal absolute temperature.

cluding such data points will be artificially high. The approach is even more arbitrary for data sets where the temperature dependence was derived indirectly[6] and not from a series of measurements at discrete temperatures in the relevant temperature range. Although deficient, this approach is all that appears possible and is clearly preferable to averaging ΔU_A from different studies or the slopes of different linear regression equations, because the slopes are not independent of the respective intercepts.

The LDVs and the FAVs at 25 °C for each property are also included in Tables 1–16. A summary of the LDVs at 25 °C is presented in Table 17 along with the uncertainty estimates u_X assigned to each property. The corresponding FAVs and percentage adjustment are listed in Table 18. The internal energies of phase transfer ΔU, their origin, and uncertainty estimate are presented in Table 19, whereas the FAVs for the ΔU and the required percentage of adjustment are presented in Table 20.

If a sufficient number of measurements at different temperatures had been made, plots of the logarithm of the property versus the reciprocal absolute temperature were constructed. These plots include the linear curves representing the LDVs and FAVs. Figure 2 shows such plots for the water solubility of five PCB congeners and Fig. 3 for the vapor pressure of 12 congeners. Plots for the Henry's law constant of seven PCBs, and the K_{OA} for 15 congeners are shown in Figs. 4 and 5, respectively. Only for PCB-15 were there experimental measurements of the solubility in octanol at several temperatures (Fig. 6).

By using the following equations together with the FAVs in Tables 19 and 20, values of the properties at a particular temperature can be obtained:

$$\log P_L(T) = \log P_L(25\,°C) - (\Delta U_A + R\cdot 298.15\ K)/(\ln(10)\cdot R)\cdot(1/T - 1/298.15\ K), \tag{4}$$

$$\log H(T) = \log H(25\,°C) - (\Delta U_{AW} + R\cdot 298.15\ K)/(\ln(10)\cdot R)\cdot(1/T - 1/298.15\ K), \tag{5}$$

$$\log S_{WL}(T) = \log S_{WL}(25\,°C) - \Delta U_W/(\ln(10)\cdot R)\cdot(1/T - 1/298.15\ K), \tag{6}$$

$$\log S_{OL}(T) = \log S_{OL}(25\,°C) - \Delta U_O/(\ln(10)\cdot R)\cdot(1/T - 1/298.15\ K), \tag{7}$$

$$\log K_{AW}(T) = \log K_{AW}(25\,°C) - \Delta U_{AW}/(\ln(10)\cdot R)\cdot(1/T - 1/298.15\ K), \tag{8}$$

$$\log K_{OW}(T) = \log K_{OW}(25\,°C) - \Delta U_{OW}/(\ln(10)\cdot R)\cdot(1/T - 1/298.15\ K), \tag{9}$$

$$\log K_{OA}(T) = \log K_{OA}(25\,°C) - \Delta U_{OA}/(\ln(10)\cdot R)\cdot(1/T - 1/298.15\ K). \tag{10}$$

Alternatively, the FAV equations given in the last row of each subtable in Tables 1–16 can be used.

4. Discussion

4.1. Need for Adjustment

The literature-derived values were reasonably consistent. The maximum applied adjustment to the LDVs of the values at 25 °C was 80%. In general however, much smaller adjustments on the order of 20% were sufficient to bring the five or six LDVs for one congener into agreement. The variability in the entries for a property in Tables 1–16 gives an approximate indication of the uncertainty of the measured values, which is likely considerably higher than the measurement precision reported for individual data points or techniques by some studies (e.g., Ref. 8). The required adjustments are normally well within this measurement uncertainty for these properties and indicate that the procedures applied in the selection of the LDVs already eliminated some of the experimental error. The smallest adjustments were necessary for the tri-and tetrachlorinated congeners, the largest for the penta- and hexachlorinated congeners. One might have expected the need for larger adjustments for properties of the heaviest congeners, which are the most difficult to measure, but the LDVs of PCBs 180 and 194 were surprisingly consistent. Whereas upward and downward adjustments were necessary for K_{OW} and K_{OA}, the S_{WL} and H generally needed to be decreased to achieve consistency.

The adjustment applied to the ΔU values never exceeded 100% and was on average less than 20%. Only the temperature dependence of the water solubilities had to be adjusted by more than 50% for half of the congeners. This however, amounts to less than 15 $kJ\cdot mol^{-1}$ and is thus still within the likely uncertainty range of these parameters, which have not been measured very frequently. The adjustments were usually in one direction. ΔU_W was always increased, whereas ΔU_A and ΔU_{OA} had to be decreased slightly, typically by less than 4 $kJ\cdot mol^{-1}$, to be in accordance with each other. The FAVs for ΔU_{AW} were higher than the LDVs by about 5 $kJ\cdot mol^{-1}$, and thus are very close to the set of theoretically derived values presented by Burkhard *et al.*[13] Although assigned a very high uncertainty, u_{OW}, the values for ΔU_{OW} only had to be adjusted downward by about 3 $kJ\cdot mol^{-1}$.

4.2. Potential Sources of Error in the Adjustment Procedure

There is the possibility that a perfectly good value for a property is adjusted on the basis of measured values for another property that may be flawed. The likelihood of this occurring is minimized through the use of the uncertainty estimates, which prevents the most certain values from being adjusted too much. Whether an inappropriate adjustment occurred can be checked by visually judging to what extent the FAV lines in Figs. 2–6 are reasonable representations of the reported measured values, and whether the FAV values at the bottom of Tables 1–16 fall within the range of reported values. Although deviations between FAVs and measured values are obvious in cases when only a limited number of measurements for a particular property had been reported, the FAVs are usually well within the range of reported values and are, thus, in agreement with the empirical evidence.

Although the procedure in step vi generally leads to a reduction in the error of the individual property values, it should be noted that there is also the possibility that error is introduced during the property adjustment. This can occur as a result of the solid/liquid conversion [Eq. (1)] and the $\log S_{OL}/S_{WL}$ versus $\log K_{OW}$ correction [Eq. (3)].

At environmentally relevant temperatures, most PCB congeners are solids, and only the vapor pressure and the solubility in water and octanol of the solid substances is experimentally accessible. The conversion to liquid properties depends on the knowledge of the entropy or enthalpy of fusion, which has not been determined for a large number of

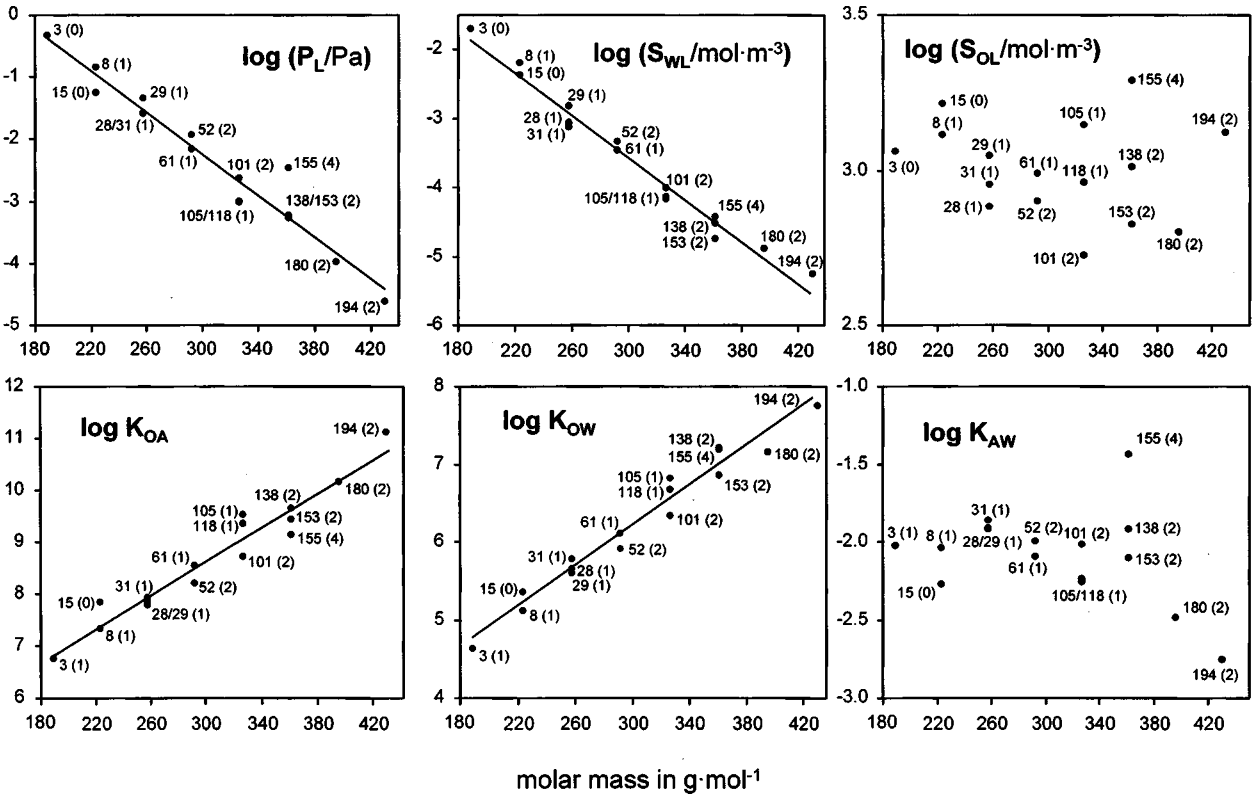

FIG. 7. Relationship between the logarithm of the final adjusted values of six physical–chemical properties at 25 °C and the molar mass for 16 PCB congeners. The number of chlorines in ortho position is given in brackets.

PCB congeners, including many of those included in this study. Uncertain entropies of fusion or the use of a default value for substances with a high melting point can lead to very significant errors in the calculated liquid property. (Since solid solubilities and vapor pressure are adjusted by the same extent/factor, this generally does not affect the consistency adjustment between groups of three properties such as $P/S_W/K_{AW}$ or $P/S_O/K_{OA}$, but it is a potential source of error when all six physical–chemical properties are adjusted to conform to thermodynamic constraints.)

The other issue is the correction for the mutual solubility of octanol and water. The scatter apparent in Fig. 1 and the large standard errors of the linear regression coefficients in the corrective Eq. (3) suggest that this effect is poorly quantified. There is even a possibility that it is an artifact caused by the fact that property measurements are much more diffi-

TABLE 21. Quantitative structure–property relationships between the final adjusted values (FAVs) of five physical–chemical properties at 25 °C and the molar mass M_m and the number of chlorine substitutions in *ortho* position $n_{ortho\text{-Cl}}$. In each case the number of data points was 16

Parameter	Regression equation			r^2	r^2_{adj}
$\log(P_L/\mathrm{Pa})$	$-(0.016\pm0.001)$	$\cdot M_m$	$+(2.8\pm0.3)$	0.947	0.943
	$-(0.0206\pm0.0005)$	$\cdot M_m+(0.38\pm0.03)\cdot n_{ortho\text{-Cl}}$	$+(3.4\pm0.1)$	0.995	0.994
$\log K_{OA}$	(0.016 ± 0.001)	$\cdot M_m$	$+(3.7\pm0.3)$	0.943	0.939
	(0.0199 ± 0.0009)	$\cdot M_m-(0.34\pm0.06)\cdot n_{ortho\text{-Cl}}$	$+(3.1\pm0.2)$	0.984	0.981
$\log(S_{WL}/\mathrm{mol\cdot m^{-3}})$	$-(0.0152\pm0.0006)$	$\cdot M_m$	$+(1.0\pm0.2)$	0.976	
$\log K_{OW}$	(0.0127 ± 0.0006)	$\cdot M_m$	$+(2.4\pm0.2)$	0.965	
$\log(H/\mathrm{Pa\cdot m^3\cdot mol^{-1}})$	$-(0.0015\pm0.0010)$	$\cdot M_m$	$+(1.8\pm0.3)$	0.13	0.06
	$-(0.0051\pm0.0008)$	$\cdot M_m+(0.35\pm0.06)\cdot n_{ortho\text{-Cl}}$	$+(2.4\pm0.2)$	0.77	0.74
$\Delta U_A/\mathrm{kJ\cdot mol^{-1}}$	(0.122 ± 0.007)	$\cdot M_m$	$+(42.6\pm2.2)$	0.955	0.952
	(0.139 ± 0.008)	$\cdot M_m-(1.6\pm0.6)\cdot n_{ortho\text{-Cl}}$	$+(39.8\pm2.1)$	0.972	0.967
$\Delta U_{OA}/\mathrm{kJ\cdot mol^{-1}}$	$-(0.10\pm0.01)$	$\cdot M_m$	$-(52.7\pm4.4)$	0.788	0.773
	$-(0.13\pm0.02)$	$\cdot M_m+(2.9\pm1.2)\cdot n_{ortho\text{-Cl}}$	$-(47.8\pm4.3)$	0.851	0.829
$\Delta U_W/\mathrm{kJ\cdot mol^{-1}}$	(0.047 ± 0.006)	$\cdot M_m$	$+(8.2\pm1.8)$	0.822	
$\Delta U_{AW}/\mathrm{kJ\cdot mol^{-1}}$	(0.075 ± 0.005)	$\cdot M_m$	$+(34.4\pm1.6)$	0.939	0.935
	(0.085 ± 0.007)	$\cdot M_m-(1.0\pm0.5)\cdot n_{ortho\text{-Cl}}$	$+(32.7\pm1.6)$	0.955	0.949

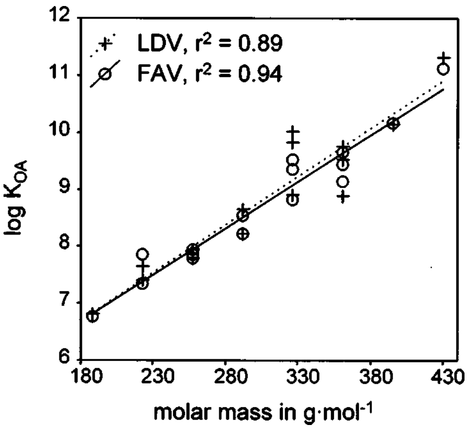

FIG. 8. Relationship between the logarithm of the octanol–air partition coefficient and the molar mass for 16 PCB congeners before and after adjustment.

cult and subject to much greater error with decreasing volatility and water solubility.

In some cases these two issues may result in inappropriate or unnecessary adjustments, i.e., properties are being adjusted to correct for an apparent inconsistency even though that inconsistency is a result of uncertain solid/liquid conversions or uncertainty concerning the effect of mutual solubility. A FAV that is different from the bulk of the reported measurements and, thus, contrary to the weight of empirical evidence may indicate a situation where these two issues conspired to introduce error in the adjusted values. This may, for example, be the case for the aqueous solubility value of PCB-3 (Fig. 2). This is, however, rare and in most cases the FAV is well within the range of measured values (see, e.g., Fig. 3).

4.3. Judging Data Quality from a Comparison with FAVs

Data from particular studies that consistently and systematically deviate from the FAVs may suggest bias or error in these data. For example, the Henry's law constants reported by Bamford *et al.*[12] are consistently higher than the FAVs (Fig. 4). For the smaller PCB congeners the difference is small, but the discrepancy tends to increase with the degree of chlorination, consistent with increasing experimental difficulty in measuring H for sparingly soluble substances. Similarly, the temperature dependence of the K_{OA} values reported by Harner and Mackay[14] tends to be low when compared to the FAVs for ΔU_{OA}. These were the very first direct measurements of K_{OA} values for PCBs and, thus, may have been subject to higher uncertainty than the values reported later.

Applying similar reasoning, the analysis may also suggest the absence of significant bias in studies which report data that are close to the FAVs. The K_{OA} values by Kömp and McLachlan,[8] for example, tend to be very close to the FAVs (Fig. 5), suggesting that they tend to be consistent with the bulk of the available property data for the PCBs. Data from such studies should be given preference, when property val-

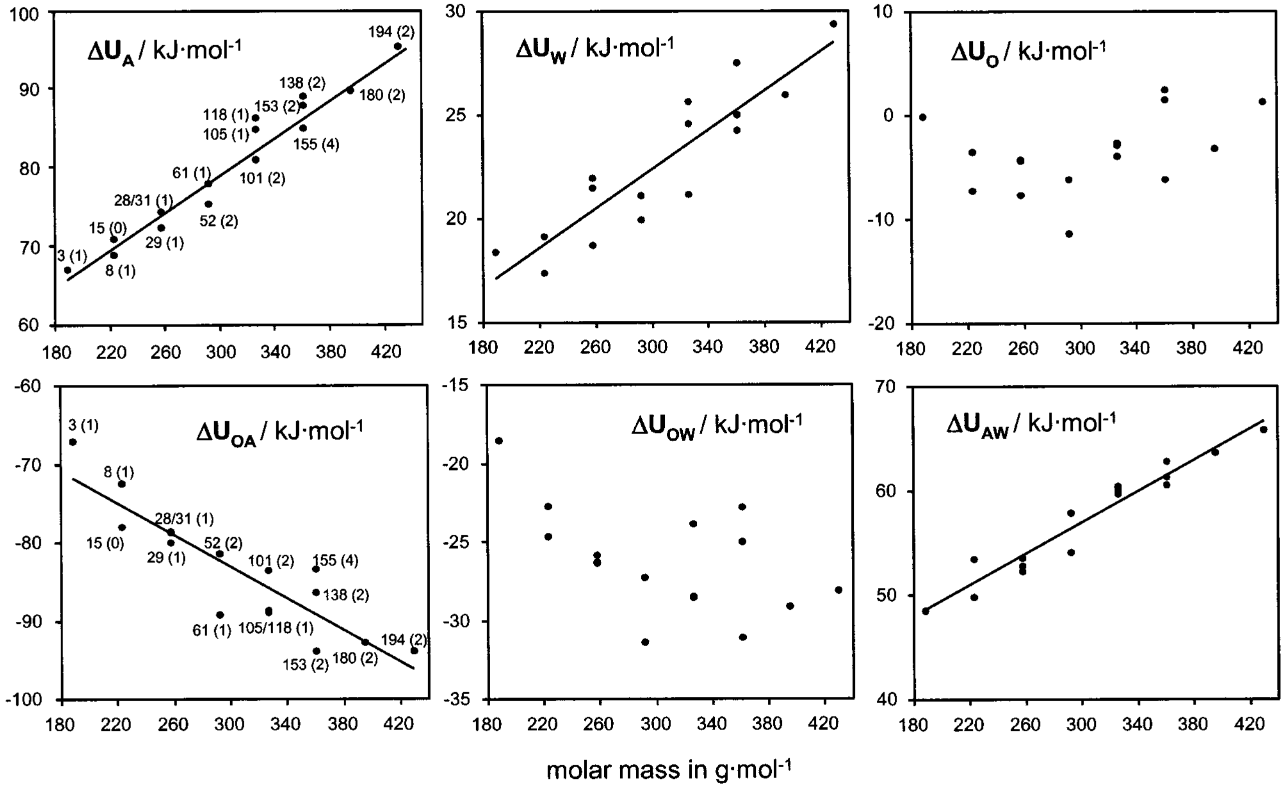

FIG. 9. Relationship between six internal energies of phase transfer and the molar mass for 16 PCB congeners.

ues for PCB congeners other than those included in this study are to be selected.

4.4. Structure–Property Relationships

When trying to develop QSPRs for the physical–chemical properties of PCBs, two options have been pursued in the past. The first option is to use unadjusted data from a variety of sources as, e.g., compiled in various databases or handbooks.[5] Such data sets are subject to significant experimental scatter and lead to QSPR relationships that may ''explain'' mostly experimental uncertainty rather than variances in properties that are truly caused by differences in molecular structure. Such relationships may still show high r^2, but may require more structural parameters than necessary. The more common option is to work with a set of data from one experimental study, which essentially amounts to an interpolation. Due to the high consistency of such data sets, the degree of explanation expressed by r^2 is usually high. However, the predictions from such QSPRs will be subject to the same bias that the experimental data may possess, and consistency with data from other studies or with other physical–chemical property is usually not assured. For example, Zhang *et al.*[9] interpolated the K_{OA} values for PCBs reported by Harner and co-workers[14,15] using gas chromatographic retention times on a variety of stationary phases. Although the predictive relationships show very high r^2 values, the predicted values are not in agreement with the experimental K_{OA} values reported by Kömp and McLachlan.[8]

The set of FAVs for 16 PCB congeners that was derived in this study should be a good starting point for the development of QSPRs, because it takes into account all empirical evidence, yet is also highly consistent. In fact, we believe that a simple QSPR analysis can aid in the assessment of the extent of consistency and experimental error in a data set. Specifically, due to the strong structural similarity between the various PCB congeners, we would expect that:

(i) Properties of PCB congeners change in a consistent manner with molecular size. For example, we would expect water solubility and vapor pressure to decrease steadily with increasing degree of chlorination. Similar smooth relationships are expected for the energies of phase transfer.

(ii) Differences in the physical–chemical properties between congeners of one homologue group may occur, but must have a rational explanation based on the structure of the congeners. It is, for example, well established that the planarity of the PCB congener, as determined by the number of chlorines in the *ortho* position to the C–C bridge connecting the two aromatic rings, has a strong impact on the volatility of PCBs,[6] and rational arguments can be made how this structural characteristic relates to the interaction between PCB molecules and thus vapor pressure.

To evaluate the extent to which the final data set adheres to these expectations, we plotted the logarithm of the properties against the molar mass of the PCB congeners in Fig. 7. Linear relationships were observed for P_{L}, S_{WL}, $\log K_{\mathrm{OA}}$, and $\log K_{\mathrm{OW}}$ (Table 21). The P_{L} and K_{OA} of the investigated congeners range over 4 orders of magnitude, S_{WL} over 3.5, and K_{OW} over 3 orders magnitude. Because the effect of size on water solubility appears to be somewhat smaller than the effect on volatility, there is a slightly decreasing trend of H with increasing molar mass, although the overall range is small (1.5 orders of magnitude) and the scatter large. The solubility in octanol has a range of only 1/2 an order of magnitude, i.e., is very similar for the various congeners.

The extent of scatter in the plots for $\log P_{\mathrm{L}}$, $\log S_{\mathrm{WL}}$, $\log K_{\mathrm{OW}}$, and $\log K_{\mathrm{OA}}$ decreases when FAVs are used instead of LDVs. An example is given in Fig. 8: Whereas molar mass can only explain 89% of the variability in the LDVs for K_{OA}, that fraction rises to 94% upon adjustment. This suggests that the adjustment procedure is successful in eliminating some of the experimental error. In all four cases, the actual regression equations, i.e., the values for intercept and slope, change only marginally when FAVs are used instead of LDVs, indicating that the adjustments do not impact on the extent to which molar mass influences a property.

The remaining scatter is smallest for $\log S_{\mathrm{WL}}$ ($r^2=0.976$) and $\log K_{\mathrm{OW}}$ ($r^2=0.965$), and slightly larger for $\log P_{\mathrm{L}}$ ($r^2=0.947$) and $\log K_{\mathrm{OA}}$ ($r^2=0.943$). However, in the case of P_{L} and K_{OA}, that scatter is not random, but strongly related to the number of *ortho*-chlorines. Vapor pressure increases and K_{OA} decreases with the number of *ortho*-chlorines, i.e., the more planar congeners have a lower volatility. Together, M_m and $n_{ortho\text{-Cl}}$ explain 99.5% of the variability in the P_{L}-FAV and 98.4% of the variability in K_{OA}-FAV. There is a slight hint that S_{WL} increases, and K_{OW} decreases with increasing $n_{ortho\text{-Cl}}$, but it is not statistically significant (i.e., r^2_{adj} does not increase upon adding $n_{ortho\text{-Cl}}$ to the regression equation). The S_{WL} for sparingly water soluble compounds such as the PCBs is strongly related to molecular size, because of the high energetic cost of forming a cavity in water. Planarity will only have a minor effect on the size of that cavity, and M_m alone thus explains most of the observed variability in S_{WL}. P_{L} and K_{OA}, on the other hand, are controlled by the extent to which the PCB molecules can interact with like molecules or octanol, and this interaction is more dependent on planarity. Therefore, M_m and $n_{ortho\text{-Cl}}$ are required to explain the observed variability in P_{L} and K_{OA}. The very small variability in the FAVs not explained by M_m and $n_{ortho\text{-Cl}}$ (less than 3.5% for K_{OW}, 2.4% for S_{WL}, 1.6% for K_{OA}, and 0.5% for P_{L}) may indicate the size of remaining experimental error in the FAVs.

The QSPRs for $\log P_{\mathrm{L}}$ and $\log K_{\mathrm{OA}}$ show remarkable similarity. The absolute value of the slopes of the regressions with M_m (0.016 ± 0.01) are identical, as are the standard errors of the intercepts. Also, the regressions with both M_m and $n_{ortho\text{-Cl}}$ are very similar. This is consistent with FAVs for the octanol solubility, which are similar for all congeners. The activity coefficient in octanol varies only between 3.2 and 10 for the 16 congeners. The uncertainty of these numbers is likely in the same order as this range, suggesting that for PCBs P_L and K_{OA} convey the same information and are interchangeable.

Whereas the $\log K_{AW}$ versus M_m plot at first looks very scattered and molar mass explains a mere 13% of the variability, the combination of M_m and $n_{ortho\text{-Cl}}$ explains a surprising 77% of the variability in the K_{AW}-FAV. Incidentally, the same two parameters explained less than 50% of the variability in the K_{AW}-LDV, suggesting that the adjustment procedure was particularly effective in reducing experimental error in the HLC data set. Chemicals with a large number of *ortho*-chlorines, most notably PCB-155, have an unusually high Henry's law constant, because nonplanarity increases vapor pressure, but has only a minor effect on aqueous solubility.

ΔU_W, ΔU_A, ΔU_{OA}, and ΔU_{AW} are also correlated with M_m (Fig. 9). Considering that measured energies of phase transfer tend to be quite uncertain and the fact that they were not regressed on a log transformed basis, the QSPRs are very good, especially for ΔU_A and ΔU_{AW} which have a r^2 of 0.94 and higher (Table 21). In the case of ΔU_A, ΔU_{OA}, and ΔU_{AW}, accounting for $n_{ortho\text{-Cl}}$ significantly improves the regressions. A higher number of *ortho*-chlorines decreases ΔU_A and ΔU_{AW}, but decreases ΔU_{OA}.

Although there is only a poor correlation of ΔU_{OW} and ΔU_O with M_m, the FAVs of the two properties for the 16 PCBs fall into a reasonable range. Due to the lack of measured values almost all the ΔU_O were obtained by the difference from the other ΔU. Kömp and McLachlan[8] postulated through calculation that the ΔU_O for the PCBs should have a value close to zero, which is consistent with the data obtained in this work.

In the absence of experimental data, the regression equations in Table 21 may serve to estimate reasonable and internally consistent physical–chemical properties and their temperature dependence for PCB congeners other than those 16 that were included in this study.

5. Conclusions

The rigorous and transparent procedure of evaluating, selecting, and adjusting physical–chemical property that was applied in this study was shown to be able to identify and eliminate a large part of the experimental error in the available measured data and to yield a consistent and complete data set with significantly reduced uncertainty. By using information for all partitioning properties simultaneously rather than one at a time, it is easier to constrain the range in which the true value for a property will lie. For example, whereas it may be impossible to decide on the true value for the S_W and K_{OW} of DDT and DDE based on even the most comprehensive review of the literature,[1] that task would almost certainly be easier if experimental data on K_{OA}, K_{AW}, P_L, and S_O are being considered as well. When performing such adjustments for a series of structurally related substances such as the PCB congeners in this study, it is further possible to estimate the extent of the remaining error in the adjusted data from unexplainable and inconsistent deviations from simple QSPRs.

The final adjusted data set should be useful when seeking to interpret the differential fate of PCB congeners in the environment, e.g., divergent partitioning of planar and nonplanar PCBs into atmospheric particles,[7] or global fractionation patterns of PCB mixtures.[16] They will also be indispensable in chemical fate modeling, especially when the intention is to evaluate the fate of individual congeners or understand changes in congeneric composition. Finally, the data set may form the basis for the development or evaluation of predictive methods such as QSPRs or correlation techniques with chromatographic data. In fact, we believe it is virtually imperative to conduct a thorough and comprehensive data evaluation such as presented here prior to embarking on QSPRs. QSPRs based on highly selective data sets, especially those based on data from a single experimental study, may suggest a high predictive power, but will generate predictions that are neither in agreement with all empirical evidence nor consistent with QSPR predictions for other properties of the same set of compounds.

In many cases, such as an uncertainty analysis for a model calculation,[17] a quantitative estimate of the uncertainty of a physical–chemical property is required. Most data compilations do not include such information, and even many experimental studies fail to report a quantitative expression of the confidence in the reported values. Standard deviations of the mean of all reported measurements of a property value probably overestimate the real uncertainty of that value, because they do not weigh the quality of the data being averaged. Sometimes the number of reported measurements is simply too small to calculate meaningful statistical measures of uncertainty. The exercise presented here provides information that may serve as a basis for estimating the uncertainty of a physical–chemical property value. In particular, the extent of adjustment required to achieve consistency, listed in Tables 18 and 20, should be useful in this regard, because it is both dependent on the extent of inconsistency from other properties for that chemical and on the uncertainties u_x assigned to a particular property value.

6. Acknowledgments

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