Environmentally Relevant Properties of All 209 Polychlorinated Biphenyl Congeners for Modeling Their Fate in Different Natural and Climatic Conditions

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The temperature dependence of physical properties and degradation lifetimes in the environment of all polychlorinated biphenyl (PCB) congeners ($N = 209$) were determined. For physical properties, the coefficients A and B in equations log(property) = A(property) − B(property)/T(K) were determined by thermodynamic and QSPR methods and compared with the results of independent methods in the literature. The coefficients Apl and Bpl for liquid state vapor pressure P_L, As and Bs for solubility in water S_W, Ah and Bh for volatility k_H (or $k_H = P_L/S_W$), and Aow and Bow for lipophilicity (K_{OW}), stored in the database of the fate model program, allowed automatic temperature corrections for realistic fate and exposure modeling at variable environmental conditions. Half-lives HL(i) for degradation in compartments air ($i = 1$), water (2), soil/plants (3), and sediment (4) were determined by combination of the photolysis and biodegradation rates (from the literature) at one reference temperature (mostly 25 °C). Examples of validation procedures for both physical properties and degradation rates were given. Temperature dependences were possible to compare with sufficient independent PCB sets only for vapor pressure. Other property sets could be compared statistically at 25 °C only. Field observations gave opportunities to validate estimated properties indirectly, e.g., with fate modeling and kinetics. Such a case was presented about the role of mono-*ortho* hexa-CB congeners 156, 157, and 167 as precursors in the formation of toxic CB126, the most potent observed factor to yolk sac mortality (YSM) from 1988 to 1992 of the fry of Simojoki River salmon ($N = 40$).

1. Introduction

Polychlorinated biphenyls (PCBs) are exclusively anthropogenic persistent organic pollutants (POPs). They were detected as abundant contaminants in marine biota in 1965 by Jensen.[1] Many properties of the PCB congeners have been determined for the evaluation of their risk to man and other biota. However, any complete database of their properties needed for satisfactory environmental fate and risk estimation has not been worked out. Management of the hazard from anthropogenic chemicals in the environment to man and biota requires assessment of possible risk (Ro) to harmful effects, e.g., numerically by eq 1.

$$\mathrm{Ro} = \mathrm{PEC}/\mathrm{PNEC} \quad (1)$$

The risk is defined as the ratio of the predicted environmental concentration (PEC) and the predicted no-effect concentration (PNEC) in compartments air, water, soil/plants, sediments, and biota.[2] PNEC is evaluated by tests and QSPR (quantitative structure−property relationships) in the field of (eco)toxicology. PEC estimates of the concentrations of target chemicals (exposure levels), instead of costly analyses, can be achieved by modeling the environmental fate of the chemical. The estimate is dependent on the properties of compartments and climate of the receiving environment (model box) and on properties of the chemical modeled. One environmental chemical risk evaluation scheme is illustrated as Figure 1 in ref 3, where the role of our program for PEC exposure modeling is given to FATEMOD. It is a one-box multimedia tool designed for local and regional chemical contamination cases. It is based on Mackay's algorithm GENERIC for fugacity mass balance modeling[4] and inventions developed in the European Science Foundation (ESF) project on chemical exposure modeling[5,6] where we participated. Further, automatic temperature corrections to compound properties were included in the FATEMOD code.[3,7–9] Properties of environments are, as soon as they are estimated and validated, stored in the environmental database of the model algorithm. Properties of the chemicals needed for PEC modeling are obtained by measurements, literature searches, and QSAR (or QSPR) methods and added to the compound database.

The use of FATEMOD with previously stored model data is very fast and easy. For example, a full report from each run can be written by one click as an Excel workbook. On the contrary, to add more new environment's and/or compound's properties to the database requires a lot of research work. Especially, temperature dependency coefficients for values of vapor pressure, solubility in water, volatility k_H, and lipophilicity (n-octanol−water partition coefficient) must be determined.[3,7,8] These coefficients in the database allow automatic adjustment of the values to ambient temperatures by a model run. Degradation rates in bulk media (combinations of photolysis, hydrolysis, and biodegradation) are temperature dependent and characterized as overall half-lives at one reference temperature (mostly 25 °C) in the compound database.[3,8,9] FATEMOD makes instantly the necessary temperature corrections for compound properties for each compartment. Also pK_a is an important parameter for fast correction in the model run for the values of acidic or basic compounds in water using the algorithm presented, e.g., by Trapp and Matthies.[6] This work describes parameter evaluation for all 209 theoretically possible congeners of PCBs for modeling their fate. A great part of relevant properties are found in the literature, but temperature correction coefficients, excluding vapor pressures, and individual reaction

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rates for most PCB congeners were developed scarcely before our present work.[3,7–9] The number of congeners is challenging, but their structural simplicity (only Cl substitution on two joint phenyl skeleton groups) and extra high persistency in reactions mean that property evaluation rules can be successfully applied.

2. Materials and Methods

2.1. Constant Parameters. Structure Parameters. The substances were coded as CB1-CB209 using the numerical order principle drafted by Ballschmiter and Zell.[10] Cl position labels and an order of two congeners CB198 and CB201 were later corrected by interchanging them.[11] This change was also done in our modeling database (FATEMOD) to follow the generally used PCB nomenclature. Chemical name and registry number were checked from catalogues for all PCB congeners as was molar mass (WM; weight of the molecule) and placed in the database. Structural parameters included the square root of the number of chlorine atoms (CN), numbers of chlorines (nCl), numbers of chlorine in different positions (No, Nm, and Np) and biodegradable CH combinations: (Nchch or phenyl groups).

Molecular Descriptors (MDs). Melting point (Mp/°C, T_f/K), entropy (ΔS_f) of fusion, molar volume (V_b), solubility parameter (DB), ionization potential (IP), dipole moment (μ), excess molar refraction (E), dipolarity/polarizability (S), the hydrogen bond basicity (B), the McGovan volume (V), log gas−hexane partition coefficient (L), and total surface area for planar molecules (TSAplan) were included for property parameter calculations. The units of these parameters are listed in the Abbreviations section. The values not found in the literature were estimated using different statistical methods. The most useful method was "Stepwise Multiple Linear Regression" (SMLR). In this calculation, the MDs (and structure parameters) were added one by one in a step-by-step manner, and the regression trial was repeated until the overall correlation (R) and the significance (p) of F in ANOVA could not be improved any further by the enter/remove procedures of MDs.

Values of Most MDs. important for temperature coefficient estimates were obtained from the literature. Measured melting points were collected from three reports. Bolgar et al. reported 198 measured Mp's and compared them to the earlier literature, where 77 congeners had values in good agreement with reported ones.[12] Miller et al.[13] reported 15 Mp's and Nakajoh et al.[14] 26 Mp's of PCB congeners measured by differential scanning calorimetric (DSC) methods. Altogether, 203 measured Mp's could be included in the FATEMOD database. Mp's of six congeners (CB6, CB13, CB17, CB27, CB51, and CB59) are absent in the literature. Values for these Mp's were hard to find even by SMLR with the known Mp's as a training set and the above listed MDs as explanatory variables. The melting point values estimated by Abramowitz and Yalkowsky[15] by correlation with nCl and molecular symmetry MDs were considered to be, at present, the best candidates as interim Mp's of these six congeners.

Entropy of Fusion. (ΔS_f/J·K^{-1}·mol^{-1}) was calculated as the ratio of enthalpy of fusion (ΔH_f/J·mol^{-1}) to the melting point in Kelvin (T_f/K = Mp/°C + 273.15). Accurate measurement of these properties using the DSC method[16] is feasible from (1 to 3) mg of pure crystals. Measured enthalpies of fusion could be found for 41 PCB congeners.[13,14] While ΔS_f of some congeners are successfully measured, fusion entropies of the other congeners were estimated by stepwise multiple linear regression (SMLR) using MDs as explanatory variables. An example is the determination of T_f, ΔH_f, and ΔS_f values for all 75 polychlorinated naphthalene compounds from the DSC results of 15 pure congeners of PCNs.[17] Estimations of ΔS_f for organic molecules have been done also based on statistical increments of structure groups.[18] In this work, ΔS_f values for all 209 PCB congeners were obtained by extrapolation based on the measured entropies of fusion of the 41 PCB congeners from the literature (training set) by SMLR. ΔS_f estimates (dependent variables) were regressed by a set of MDs as independent (explanatory) variables. The MDs applied in these trials were WM, V_b, DB, CN, IP, μ, E, S, B, V, L, and TSAplan. SMLR produced the best linear result for ΔS_f values with DB, L, and E.

MDs for Solubility Estimates. V_b was calculated from increments suggested by Ruelle et al.[19] DB was calculated as the ratio of the sum of dispersion components of molar attractions F_{di}[20] and V_b[19] according to Ruelle.[21] Essential association constants of polar substituents were obtained as incremental MDs.[19,21] Solubility parameters E, S, B, V, and L for all 209 PCB congeners have been published by Abraham and Al-Hussaini.[22] Dipole moments μ for PCBs have been estimated, e.g., by Chana et al.[23] and Makino.[24] In this work, IP and μ for 131 congeners from Rayne and Ikonomou[25] were used as the training set for SMLR to estimate the missing μ and IP values. In the case of μ, the significant explanatory variables were B and L, and in the case of IP, the explanatory variables were CN, B, E, ΔH_f, and L. Also chromatographic data[26] and TSAplan[27] have been utilized as MDs in property estimations of PCBs.

2.2. Temperature Coefficients for Physical Properties. Equation for Temperature Corrections. The first log−linear temperature dependence equation on the property of chemical substances was presented more than 150 years ago. It was for vapor pressure by Clausius and Clapeyron. Their equation was also found suitable to define temperature corrections to some other environmentally important physical properties of chemicals (eq 2)

$$\log(\text{property}) = \text{Apr} - \text{Bpr}/T \tag{2}$$

Temperature Coefficients for the Vapor Pressure Values. VPLEST. Chemical substances can have two different vapor pressures: for solid state P_S and for liquid state P_L. Accordingly, they have two log−linear temperature (T/K) dependence equations, 3 and 4

$$\log P_S = \text{Aps} - \text{Bps}/T \tag{3}$$

and

$$\log P_L = \text{Apl} - \text{Bpl}/T \tag{4}$$

For molecular compounds, only the P_L (subcooled) liquid state vapor pressure is needed for modeling of PEC because a substance in the environment most certainly is distributed to the molecular level. To estimate values of P_L/Pa for FATEMOD, a QSPR program VPLEST was developed from the modified Watson method of Grain.[28] His equations for P_L from reference vapor pressure P_{L1} at reference temperature T_1 are coded 14-15, 14-24, and 14-25 in ref 28 and here as eqs 5 to 7

$$C_2 = 0.19T_1 - 18 \tag{5}$$

$$\Delta H_{v1}/T_1 \approx K_F[8.75 + R(\ln T_1 - \ln P_{L1})] \tag{6}$$

$$\ln P_L = \ln P_{L1} + (\Delta H_{v1}(T_1 - C_2)^2/0.97RT_1^2)\cdot[1/(T_1 - C_2) - 1/(T - C_2)] \tag{7}$$

ΔH_{v1} is enthalpy of vaporization (J·mol^{-1}); K_F is the structure parameter in Tables 14-4 and 14-5 in ref 28; R is the gas constant (8.3143 J·K^{-1}·mol^{-1}); and T is the ambient temperature (K) in the model run. In the VPLEST run, feed-in parameters are

P_{L1}, T_1, and temperature range taken for calculation of log P_L in one degree intervals—for environmental fate parameters, the suitable range is, e.g., from (−2 to +30) °C. Linear regression for log P_L values (converted from ln P_L's), 1/T as the explanatory variable, gives Apl as the intercept and −Bpl as the slope. The P_{L1} value for the frequently used reference temperature 25 °C can be estimated using QSPR methods like multivariate regression selecting significant explanatory variables from sets of molecular descriptors (MDs). Öberg[29] determined P_{L25} values for all PCB congeners with regression from 46 experimental values with 260 MDs from the Syracuse database.[30] We used these P_{L25} values as input parameters (P_{L1}) to VPLEST to obtain all Apl and Bpl coefficients for PCBs in the FATEMOD database. If P_{L1} is not known at any temperature, it can be calculated from known P_{S1} values at T_1 by conversion (eq 8). If either temperature coefficient pair is known, the other can be calculated by conversion eqs 9 and 10.

$$\log P_{L1} = \log P_{S1} - (\Delta S_f/R)\cdot(1 - T/T_1)/\ln 10 \quad (8)$$

$$\mathrm{Apl} = \mathrm{Aps} - \Delta S_f/(R \ln 10) \quad (9)$$

$$\mathrm{Bpl} = \mathrm{Bps} - \Delta S_f T_f/(R \ln 10) \quad (10)$$

An indirect determination of coefficients Apl and Bpl can be performed by gas chromatography.[31,32] Burkhard et al.[33] have evaluated 11 predictive methods for the estimation of the vapor pressure at 25 °C for 15 polychlorinated biphenyls. The best correlative method was based on a relationship between ΔG_V (free enthalpy of vaporization) and gas−liquid chromatographic retention indexes. Relative retention data from GC, on nonpolar columns and linear temperature program, are nearly as reliable as retention index methods for Apl and Bpl determination.[33,34] Estimates of vapor pressures for 134 PCB congeners have been done based on published retention indices and known liquid phase vapor pressures (at 25 °C) of 27 other PCB congeners by isothermal GC at 200 °C.[34] Temperature programmed GC (100 °C, 3 min, + 2 °C·min^{-1} to 245 °C) has been used for the determination of P_L for 133 PCBs by Fischer et al.[35] The temperature dependence of P_L for 32 PCB congeners has been derived from previously obtained gas chromatographic data.[32,33] Parameters for calculating saturation liquid-phase vapor pressures of 180 PCB congeners as functions of temperature and *ortho*-chlorine substitution have been presented by Falconer and Bidleman.[36] Data for 32 congeners were obtained from gas chromatographic retention data. This information was used to estimate the values for 148 other isomers whose vapor pressure at one fixed temperature had been reported.[36]

Temperature Correction Coefficients for Solubility in Water. WATSOLU. Molecules having low water solubility in the environment can have only one value of S_W in pure water.[3,6–8,37] Occurrence of both "solid state solubility" and "(subcooled) liquid state solubility" for some hydrophobic organic molecules is very improbable, while dissolution in water obviously leads to a hydrated single molecule in the usually very low environmental concentrations. Micelles etc. are of course another matter.

Measured water solubility's at 25 °C were found for 74 PCB congeners.[38–41] Recently, Huang and Hong[38] have measured aqueous solubilities for 12 non-*ortho* and mono-*ortho* PCBs at four temperatures using a modified generator-column technique. Abramowitz and Yalkowsky have estimated water solubilities for all PCBs based on estimated Mp's and TSAplan's.[15] Ruelle and Kesselring[39] have predicted water solubility of 60 PCB congeners using the general solubility equation derived from mobile order and disorder (MOD) thermodynamics. There the solubility of a hydrophobic compound depends only on molar volume and melting properties in the case of solid compounds. Some more solubility data were compiled by Patil et al.[40] who have calculated water solubility of 140 PCB congeners based on molecular connectivity. Brodsky and Ballschmiter[41] determined S_W and log K_{OW} for 154 PCBs using the retention indices obtained by RP-HPLC and structurally selected PCB congeners with known values for the regression lines.

Ruelle et al. have developed a quite successful MOD procedure for QSPR estimation of S_W values.[19,21,39] Their equations were split by us into two polynomial parts: part As including constant terms and part Bs including terms containing temperature (T/K). The WATSOLU program[3,7,8] was written from these two parts to compute coefficients As and Bs (eqs 11 to 15)

WATSOLU calculations:

Solubility in water (mol·m^{-3})

$$\log S_W = \mathrm{As} - \mathrm{Bs}/T \quad (11)$$

$$\mathrm{As} = \Delta S_f/(R \ln 10) - 0.036V_b - 0.217 \ln V_b + \sum N_{OH}(2 + \mathrm{boh})/\ln 10 + \mathrm{aAcc} + \mathrm{aDon} + 5.154 \quad (12)$$

$$\mathrm{Bs} = \Delta S_f T_f/(R \ln 10) + (\mathrm{DB} - 20.5)^2 V_b/(R \ln 10(1 + \mathrm{MAXW}/18.1)) \quad (13)$$

Association terms:

$$\mathrm{aAcc} = \sum \mathrm{vAcc}(i) \log(1 + \mathrm{KAccW}(i)/18.1) \quad (14)$$

$$\mathrm{aDon} = \sum \mathrm{vDon}(i) \log(1 + \mathrm{KDonW}(i)/18.1) \quad (15)$$

In eqs 12 to 15 vAcc(i) and vDon(i) are the numbers of active sites; KaccW(i) and KDonW(i) are stability constants for proton acceptor and donor groups in water; R (gas constant) = 8.3143; V_b = liquid state molar volume (cm^3·mol^{-1});[19] N_{OH} = number of the hydroxyl groups; boh = 1, 2, or 2.9 for prim., sec., or tert. OH, respectively; 18.1 is the molar volume of pure water; T_f = melting point (K); DB = Ruelle's solubility parameter;[21] and MAXW = the greatest value of KAccW(i) or KDonW(i) in water.

Octanol−Water Partition Coefficient K_{OW}. TDLKOW. The temperature dependence of K_{OW} is usually small.[40–43] The log K_{OW} can be estimated by reversed-phase high performance liquid chromatography (RP-HPLC)[40–45] and also its temperature dependence.[46] Hawker and Connell have calculated K_{OW} values for all PCB congeners using the TSAplan, which was highly significantly correlated with K_{OW}.[47] Some new data by Kong et al.[48,49] obtained by the so-called hydrophobic rule approach method suggest that the log K_{OW} values for nona- and decachlorinated biphenyls are very high, especially for CB209 and CB206: 10.15 and 9.22, respectively.

Ruelle expanded the applicability of the MOD method using a formula analogous with that for water solubility (see above) to determine the organic solvent/water partition, including log K_{OW25} estimation.[21] The *l*og K_{OW25} values predicted by Ruelle's algorithm were in good agreement with measured values in the literature. For temperature correction to log K_{OW}, we divided these Ruelle's formulas into temperature-independent and -dependent parts to produce coefficients Aow and Bow to a Clausius−Clapeyron type of equation (eq 16). The calculation algorithms for Aow and Bow named the TDLKOW program[3,8] are presented in eqs (16 to 22).

Octanol water partition:

$$\log K_{OW} = Aow - Bow/T \quad (16)$$

$$Aow = \Delta B + \Delta F + \Delta Acc + \Delta Don \quad (17)$$

$$\Delta B = (0.5V_b(1/124.2 - 1/18.1) + 0.5 \ln(18.1/124.2))/\ln 10 \quad (18)$$

$$\Delta F = (V_b(rw/18.1 - ro/124.2) - \Delta N_{OH}(j)(boh + rw - ro))/\ln 10 \quad (19)$$

$$\Delta Acc = \sum vAcc(i)(\log(1 + KAccO(i)/124.2)/(1 + KAccW(i)/18.1)) \quad (20)$$

$$\Delta Don = \sum vDon(i) \log((1 + KDonO(i)/124.2)/(1 + KDonW(i)/18.1)) \quad (21)$$

$$Bow = (V_b/19.1444)((DB - 20.5)2/(MAXW/18.1) - DB - 16.38)2/(1 + MAXO/124.2)) \quad (22)$$

Most molecular descriptors are defined in the previous discussion on WATSOLU. To consider the *n*-octanol partition, vAcc(*i*) and vDon(*i*) are also here numbers of active sites, but 124.2 is the reduced molar volume of water-saturated *n*-octanol; rw is the structuration factor of water = 2.0; ro is the structuration factor for water-saturated *n*-octanol = 1.275. KAccO(*i*) and KDonO(*i*) are stability constants of proton acceptor and donor groups in octanol, and MAXO is the greatest value of KAccO(*i*) or KDonO(*i*) for solute in *n*-octanol.[21]

Volatility. Henry's law constant k_H (IUPAC) is used in fate modeling to calculate air−water partition coefficient $K_{AW} = C_A/C_S$ which is dimensionless.[6] The value of k_H is temperature-dependent and approximated as $k_H = P_L/S_W$.[6] This value is practical for low solubility compounds not miscible in water.[50,51] For very hydrophilic compounds, other methods to calculate k_H values must be used to estimate volatility.[50] The measured k_H values of PCBs deviate significantly between applied laboratory methods especially for higher chlorinated congeners.[50−60] For pristine environments, the P_L/S_W ratio for k_H at each ambient temperature is a useful way to evaluate k_H for PCBs. The temperature dependence of log k_H from this ratio is determined by eq 23 by logarithmic calculus of the coefficients for log P_L (eq 4) and for log S_W (eq 11). If these thermodynamically based[19−21] variables are known, Ah and Bh can be obtained by simple conversions (eqs 24 and 25):

$$\log k_H = Ah - Bh/T \quad (23)$$

$$Ah = Apl - As \quad (24)$$

$$Bh = Bpl - Bs \quad (25)$$

Mackay and Shiu[51] have estimated the temperature dependence so that k_H is doubled as the temperature is increased from (10 to 65) °C, and Burkhardt et al.[52] have predicted an increase of one order of magnitude of k_H with a 25 °C increase in temperature. Dunnivant et al.[53,54] presented measured k_H (at 25 °C) values for 34 PCB congeners. Ten Hulscher et al. have measured values of k_H for three PCBs (CB9, CB28, CB52) at seven temperatures (from (10.4 to 48.4) °C) and values of k_H for 11 PCBs at 20 °C.[55,56] Experimentally determined values at 25 °C for 55 pure PCB congeners were reported by Brunner et al.,[57] for 12 PCBs by Fang et al.,[58] and by Murphy et al.[59] for PCBs in different Aroclor mixtures. Bamford et al.[60] have measured "Henry's law constants" for 26 PCB congeners using a gas-stripping apparatus at (4, 11, 18, 25, and 31) °C.

Degradation Half-Lives of PCBs. To model the fate of a chemical, its overall degradation half-life HL(*i*) in each compartment (*i* = air, water, soil/plants, sediment) is essential. The half-life for each compartment *i* can be calculated by eq 26. Instead of ln 2, 0.693 is used.

$$HL(i) = t_{1/2} = 0.693/(Kh + Kb + Kp) \quad (26)$$

where Kh, Kb, and Kp are (pseudo) first-order rate constants (h^{-1}) for hydrolysis (Kh; for PCBs in pristine waters is very low), biodegradation (Kb), and photodegradation (Kp). Photodegradation can occur in the atmosphere, in surface waters, and on the surface of soils and plants. Generally, the reaction with OH radicals is the most important.[61] The photolysis rate constants are dependent on temperature. For many organic compounds in the atmosphere, the increase in the reaction rate constant with OH radicals has been found to be 1.5- to 2.0-fold when the temperature was increased from (265 to 298) K.[62] In water, a 10 °C increase in temperature was observed to accelerate the photodegradation rate by a factor between 1.15 and 1.5.[9,63,64] In addition to many characteristics of the medium,[64] the biodegradation rate also depends on the temperature.[65] The EC FOCUS Group has suggested a "rule of thumb" that increasing temperature by 10 °C induces an increase in the overall degradation rate by a factor of 2.2. Walker et al. have shown that this relationship applies to the great majority of biodegradable chemicals.[65,66] Arnold and Briggs[67] have presented a factor of 2.5 to 3 for each 10 °C increase in temperature. Estimates of biodegradation half-lives of PCBs in soils and sediments vary from several years to decades.[68−71]

Degradation rates R(*i*)/h^{-1} and half-lives HL(*i*)/h of the chemical in the four compartments (*i* = 1 to 4) are needed for fate prediction.[3,8,9] On the basis of field observations and molecular structure, approximate *R*(*i*) and HL(*i*) values are estimated by eqs 27 to 30. From the reported degradation measurements in the environment, the photolysis rate in water is 10 to 20 times slower than Kp in the atmosphere. As well, the biodegradation rate in water is 10 to 20 times slower than the biodegradation rate Kb in solid surface layers of soil, plants, and sediment.[61−72] For fate modeling, we used estimates of the degradation rates in water for photolysis Kp/15 and for biodegradation Kb/15. The hydrolysis rate (Kh) in water is very slow related to photolysis and biodegradation, thus it has no observable influence on the total rate and half-life estimates (in eqs 27 to 30)

$$\text{Air} \quad (i = 1) \quad R(1) = Kp \quad HL(1) = 0.693/R(1) \quad (27)$$

$$\text{Water} \quad (i = 2) \quad R(2) = Kh + Kb/15 + Kp/15 \quad HL(2) = 0.693/R(2) \quad (28)$$

$$\text{Soil/Plants} \quad (i = 3) \quad R(3) = Kh/15 + Kb \quad HL(3) = 0.693/R(3) \quad (29)$$

$$\text{Sediment} \quad (i = 4) \quad R(4) = Kh/15 + Kb \quad HL(4) = 0.693/R(4) \quad (30)$$

As rule of thumb for temperature correction of the HL(*i*) values, a 10 °C decrease in temperature *T* from the reference value increases degradation lifetime in air by a factor of 1.2 and in other compartments by a factor of 2.[3,9] The corresponding correction equations are 31 to 34

$$HL(1)corr = HL(1)ref \cdot 1.2^{(HLT-T)/10} \quad (31)$$

$$HL(2)corr = HL(2)ref \cdot 2^{(HLT-T)/10} \quad (32)$$

$$HL(3)corr = HL(3)ref \cdot 2^{(HLT-T)/10} \quad (33)$$

$$HL(4)corr = HL(4)ref \cdot 2^{(HLT-T)/10} \quad (34)$$

To obtain reference HL(*i*) values at 25 °C for individual PCB congeners, we adopted ranges in hours for each number of chlorines (nCl) from Mackay et al.[72] Mackay's suggestion for the HL ranges of PCBs is based on experience and literature data.[60−71,73−75] The dominating degradation process of PCBs in

Table 1. Ranges of $HL_{25}(1)$ Values (Modified from Ref 72) of the PCBs in Classes of Chlorine Numbers[a]

	air(1)			soil/plants/sediment(3,4)			max	min.
nCl	min1	max1	range1	min3,4	max3,4	range3,4	Nchch	Nchch
1	100	300	200	5000	20000	15000	7	6
2	100	300	200	7000	24000	17000	6	4
3	300	1000	700	10000	36000	26000	5	2
4	1000	3000	2000	15000	48000	33000	4	0
5	1000	3000	2000	20000	80000	60000	4	0
6	3000	10000	7000	25000	95000	70000	3	0
7	3000	10000	7000	30000	110000	80000	2	0
8	10000	30000	20000	35000	125000	90000	1	0
9	10000	30000	20000	40000	150000	110000	0	0
10	50000	50000	0	60000	180000	120000	0	0

[a] The variables nCl and Nchch for all PCB congeners are listed in Table 2.

air and in pristine surface waters was found to be photolysis and in solids (soil/plants and sediments) biodegradation. UV-induced degradation (reduction to hydrogen) of *ortho*-chlorines of PCBs was generally fastest and *para*-chlorine loss the next fastest in the atmosphere, in surface water, and on solid surfaces. UV irradiation had been used to test degradation pathways and relative rates of PCB congeners in solutions.[76,77] Alkaline *n*-propanol was found to accelerate PCB degradation by UV.[78] TiO_2 was found to be an even more successful catalyst in purification of wastewaters and contaminated solids by UV treatment.[79,80] Addition of surfactants facilitated UV/TiO_2 catalysis in practical removal of PCB contamination from solids and sludges.[81] Results from these catalytic tests, when UV irradiation was analogous to sunlight,[79] could be used to evaluate the order of relative photolysis rates of PCB congeners, despite rates in the natural environment being much slower. However, if, e.g., an ozone reaction is applied together with UV,[81] the accelerated rates are too complex to allow any similar conclusion to be made.

To obtain HL reference values on individual PCB congeners, we started by calculation of the photolysis half-life in Air $HL_{25}(1)$ by using structure descriptors No and Np and by calculation of the biodegradation half-life in solids $HL_{25}(3,4)$ using descriptors Nchch (number of vicinal CH−CH arrangements) or Phen (a nonsubstituted phenyl group in the PCB molecule). Values of these MDs are listed in Table 2. The minimum and maximum values and ranges for HL(i) (modified from ref 72) in air (i = 1) and solids (i = 3,4) are presented in Table 1.

The next step to obtain reference values ($HL_{25}(i)$/h) was to calculate (using values in Table 1) relative values for each PCB molecule in each frame of range1 for air (i = 1) photolysis (eq 35) and range3,4 for solid (i = 3,4) biodegradation by eqs 36 to 37 where symbols MaxNchch is the highest and MinNchch the lowest value of Nchch in each congener group (in Table 2). Then, reaction rates in water (Kp2 and Kb2) are calculated by eqs 38 and 39, and the total degradation half-life in water HL(2) is calculated by eq 40.

$$HL_{25}(1) = \max1 - No \cdot range1 - Np \cdot range1/(2nCl) \quad (35)$$

$$\text{If } Phen = 1,\ HL_{25}(3,4) = \min3,4 \quad (36)$$

$$HL_{25}(3,4) = \min3,4 + (\max Nchch - Nchch) \cdot range3,4/\max Nchch \quad (37)$$

$$Kp2 = 0.693/HL(1)/15 \quad (38)$$

$$Kb2 = 0.693/HL(3,4)/15 \quad (39)$$

$$HL25(2) = 0.693/(Kp2 + Kb2) \quad (40)$$

3. Results and Discussion

3.1. Structure Codes, Labels, and Property Parameters. Table 1 defines the values of fastest and slowest limit and range of reference (at 298.15 K) values for half-lives of degradation $HL_{25}(i)$ in two types of media: air (i = 1) and solids (i = 3 and 4). The water compartment (i = 2) value limits and ranges for reaction were not set in Table 1 because these values were determined by eqs 35 to 40 (see Materials and Methods above).

Table 2 includes compound codes, CASRN's, chemical names, values of WM, nCl, CN, No, Nm, Np, biodegradable CH combinations (Nchch or Phenyl groups), and Mp's. 203 PCB congeners had measured values of Mp's in the literature.[12–16] Melting points of six congeners were not reported. Therefore, their QSPR estimates[15] were taken as interim Mp values (for CB6, CB13, CB17, CB27, CB51, and CB59). Possible effects of 10 °C errors in these Mp values were tested for their influence on the temperature coefficients from WATSOLU (see details in Section 3.2 and in Table 6). Table 2 presents also entropies of fusion (ΔS_f/J·K^{-1}·mol^{-1}) estimated by SMLR and their SEs of prediction. Further details on ΔS_f estimation are presented in Section 3.2, Table 7, and Figure 1.

Table 3 presents molecular descriptors (MDs), constant parameters for determination or validation of temperature correction coefficients of the physical properties of PCBs. They include molar volume V_b and solubility parameter DB calculated from increments of Ruelle et al.,[19] van Krevelen,[20] and Ruelle.[21] The solubility parameters E, S, B, V, and L in Table 3 were from Abraham and Al-Hussaini.[22] MDs IP and μ were mostly from Rayne and Ikonomou[25]—some values were obtained by SMLR, with structure parameters nCl, No, Nm, Np, and CN (Table 2) as predictors. Association constants (KaccW) for chlorines were determined by a WATSOLU run for log S_{W25} and by a TDLKOW run for log K_{ow25} values searching the best fit with the experimental literature values of S_{W25}.[38–41] The KaccW value was reported by Ruelle[21] to be 30, which is in fair agreement with tested values of CB4-CB209 for S_W. KaccW values for *n*-octanol−water partition from the TDLKOW test were 30 for dichloro-PCBs but smaller for CB16-CB209. One more MD listed in Table 3 was the total surface area for planar molecules (TSAplan), a popular predictor for Mp's, vapor pressures, solubilities S_{W25}, H_{25} values, and log K_{OW}'s for PCBs.[15,25,46,88]

Table 4 presents temperature coefficients Apl and Bpl for liquid state vapor pressure P_L/Pa, As and Bs for solubility S_W/mol·m^{-3} in water; Aow and Bow for *n*-octanol−water partition ratio K_{OW}, and Ah and Bh for Henry's law constant k_H/Pa·m^3·mol^{-1}. Calculation of P_L coefficients by a VPLEST run was based on liquid state vapor pressure at 25 °C, P_{L25}/Pa, by Öberg[29] as the input value (included in Table 4).

Table 5 presents values of Kp in air and Kb in solids (soil, plants, sediments).The third degradation rate (Kh, for hydrolysis) is taken as zero. The table also presents estimates of half lives $HL_{25}(1)$ in air, $HL_{25}(2)$ in surface water, and $HL_{25}(3,4)$ for solids calculated by eqs 35 to 40. In the FATEMOD database, the corresponding values $HL_{25}(1)$, $HL_{25}(2)$, $HL_{25}(3)$, and $HL_{25}(4)$ are presented in the table by two significant numbers (rounded).

3.2. Discussion. The constant parameters from the catalogues of Beilstein and Chemical Abstracts (CASRN), structure specific names, nCl, CN, No, Nm, Np, Nchch, and Phen (Table 2) are self-evident. The molecular descriptors (MDs, Table 3) V_b, DB, IP, μ, E, S, B, V, and L were taken

Table 2. No, Nm, Np, Nc Codes, CASNRs, and Chemical Names and Values of WMs, nCl, CN, (SQRT of nCl), Nchch, Phen, Mp, ΔS_{fpred}, and SEpred for all PCB Congeners[b]

			WM	chlorines		Cl positions			biodeggroup		Mp	SMLR prediction	
code	CASRN	chemical name	g·mol^{-1}	nCl	CN	No	Nm	Np	Nchch	Phen	°C	ΔS_{fpred}	SEpred
CB1	2051-60-7	2-chlorobiphenyl	188.639	1	1.000	1	0	0	7	1	34	46.10	2.55
CB2	2051-61-8	3-chlorobiphenyl	188.639	1	1.000	0	1	0	6	1	17	50.23	2.40
CB3	2051-62-9	4-chlorobiphenyl	188.639	1	1.000	0	0	1	6	1	78	51.82	2.48
CB4	13029-08-8	2,2′-dichlorobiphenyl	223.090	2	1.414	2	0	0	6	0	61	46.22	2.28
CB5	16605-91-7	2,3-dichlorobiphenyl	223.090	2	1.414	1	1	0	6	1	28	55.36	1.53
CB6	25569-80-6	2,3′-dichlorobiphenyl	223.090	2	1.414	1	1	0	5	0	36[a]	50.35	2.08
CB7	33284-50-3	2,4-dichlorobiphenyl	223.090	2	1.414	1	0	1	5	1	25	53.70	1.61
CB8	34883-43-7	2,4′-dichlorobiphenyl	223.090	2	1.414	1	0	1	5	0	46	51.94	2.15
CB9	34883-39-1	2,5-dichlorobiphenyl	223.090	2	1.414	1	1	0	5	1	23	52.29	1.67
CB10	33146-45-1	2.6-dichlorobiphenyl	223.090	2	1.414	2	0	0	6	1	36	46.01	2.36
CB11	2050-67-1	3,3′-dichlorobiphenyl	223.090	2	1.414	0	2	0	4	0	30	54.48	2.08
CB12	2974-92-7	3,4-dichlorobiphenyl	223.090	2	1.414	0	1	1	5	0	50	60.73	1.64
CB13	2974-90-5	3,4′-dichlorobiphenyl	223.090	2	1.414	0	1	1	4	1	51[a]	56.07	2.24
CB14	34883-41-5	3,5-dichlorobiphenyl	223.090	2	1.414	0	2	0	4	0	36	57.68	1.48
CB15	2050-68-2	4,4′-dichlorobiphenyl	223.090	2	1.414	0	0	2	4	0	152	57.67	2.42
CB16	38444-78-9	2,2′,3-tri...	257.533	3	1.732	2	1	0	5	0	29	55.24	1.26
CB17	37680-66-3	2,2′,4-tri...	257.533	3	1.732	2	0	1	5	0	35[a]	53.58	1.36
CB18	37680-65-2	2,2′,5-tri...	257.533	3	1.732	2	1	0	4	0	46	52.18	1.46
CB19	38444-73-4	2,2′,6-tri...	257.533	3	1.732	3	0	0	6	0	92	50.53	1.64
CB20	38444-84-7	2,3,3′-tri...	257.533	3	1.732	1	2	0	4	0	45	59.37	1.22
CB21	55702-46-0	2,3,4-tri...	257.533	3	1.732	1	1	1	5	1	103	62.53	1.52
CB22	38444-85-8	2,3,4′-tri...	257.533	3	1.732	1	1	1	4	0	73	60.98	1.37
CB23	55720-44-0	2,3,5-tri...	257.533	3	1.732	1	2	0	4	1	41	57.34	1.75
CB24	58702-45-9	2,3,6-tri...	257.533	3	1.732	2	1	0	5	1	57	56.11	1.81
CB25	55712-37-3	2,3′,4-tri...	257.533	3	1.732	1	1	1	3	0	37	57.71	1.19
CB26	38444-81-4	2,3′,5-tri...	257.533	3	1.732	1	2	0	3	0	43	56.29	1.17
CB27	38444-76-7	2,3′,6-tri...	257.533	3	1.732	2	1	0	4	0	46[a]	53.88	1.32
CB28	7012-37-5	2,4,4′-tri...	257.533	3	1.732	1	0	2	3	0	59	59.31	1.28
CB29	15862-07-4	2,4,5-tri...	257.533	3	1.732	1	1	1	4	1	79	59.13	1.60
CB30	35693-92-6	2,4,6-tri...	257.533	3	1.732	2	0	1	4	1	65	54.98	1.91
CB31	16606-02-3	2,4′,5-tri...	257.533	3	1.732	1	1	1	3	0	65	57.89	1.19
CB32	38444-77-4	2,4′,6-tri...	257.533	3	1.732	2	0	1	4	0	56	56.26	1.26
CB33	38444-86-9	2′,3,4-tri...	257.533	3	1.732	1	1	1	4	0	62	60.61	1.34
CB34	37680-68-5	2′,3,5-tri...	257.533	3	1.732	1	2	0	3	0	58	55.33	1.21
CB35	37680-69-6	3,3′,4-tri...	257.533	3	1.732	0	2	1	3	0	67	64.74	1.68
CB36	38444-87-0	3,3′,5-tri...	257.533	3	1.732	0	3	0	2	0	79	61.00	1.30
CB37	38444-90-5	3,4,4′-tri...	257.533	3	1.732	0	1	2	3	0	90	66.33	1.93
CB38	53555-66-1	3,4,5-tri...	257.533	3	1.732	0	2	1	4	1	72	66.38	1.66
CB39	38444-88-1	3,4′,5-tri...	257.533	3	1.732	0	2	1	2	0	88	61.05	1.28
CB40	38444-93-8	2,2′,3,3′-tetra...	291.980	4	2.000	2	2	0	4	0	124	63.81	1.46
CB41	52663-59-9	2,2′,3,4-tetra...	291.980	4	2.000	2	1	1	3	0	50	56.54	1.22
CB42	36559-22-5	2,2′,3,4′-tetra...	291.980	4	2.000	2	1	1	4	0	70	62.14	1.46
CB43	70362-46-8	2,2′,3,5′-tetra...	291.980	4	2.000	2	2	0	3	0	46	51.35	1.31
CB44	41464-39-5	2,2′,3,5′-tetra...	291.980	4	2.000	2	2	0	2	0	50	60.72	1.52
CB45	70362-45-7	2,2′,3,6-tetra...	291.980	4	2.000	3	1	0	4	0	81	50.12	1.44
CB46	41464-47-5	2,2′,3,6′-tetra...	291.980	4	2.000	3	1	0	4	0	127	59.07	1.56
CB47	2437-79-8	2,2′,4,4′-tetra...	291.980	4	2.000	2	0	2	2	0	46	60.46	1.50
CB48	70362-47-9	2,2′,4,5-tetra...	291.980	4	2.000	2	1	1	3	0	87	53.14	1.21
CB49	41464-40-8	2,2′,4,5′-tetra...	291.980	4	2.000	2	1	1	2	0	69	59.05	1.60
CB50	62796-65-8	2,2′,4,6-tetra...	291.980	4	2.000	3	0	1	3	0	48	48.71	1.59
CB51	68194-04-7	2,2′,4,6′-tetra...	291.980	4	2.000	3	0	1	3	0	45[a]	57.41	1.67
CB52	35693-99-3	2,2′,5,5′-tetra...	291.980	4	2.000	2	2	0	2	0	87	57.63	1.75
CB53	41464-41-9	2,2′,5,6′-tetra...	291.980	4	2.000	3	1	0	3	0	105	56.00	1.84
CB54	15968-05-5	2,2′,6,6′-tetra...	291.980	4	2.000	4	0	0	4	0	198	54.35	1.96
CB55	74338-24-2	2,3,3′,4-tetra...	291.980	4	2.000	1	2	1	4	0	87	60.67	1.45
CB56	41464-43-1	2,3,3′,4′-tetra...	291.980	4	2.000	1	2	1	3	0	99	69.15	1.78
CB57	70424-67-8	2,3,3′,5-tetra...	291.980	4	2.000	1	3	0	2	0	88	55.48	1.09
CB58	41464-49-7	2,3,3′,5′-tetra...	291.980	4	2.000	1	3	0	2	0	129	63.87	1.51
CB59	74472-33-6	2,3,3′,6-tetra...	291.980	4	2.000	2	2	0	3	0	42[a]	53.47	1.17
CB60	33025-41-1	2,3,4,4′-tetra...	291.980	4	2.000	1	1	2	3	0	147	62.27	1.68
CB61	33284-53-6	2,3,4,5-tetra...	291.980	4	2.000	1	2	1	4	1	93	63.77	1.23
CB62	54230-23-7	2,3,4,6-tetra...	291.980	4	2.000	2	1	1	4	1	79	57.29	1.13
CB63	74472-34-7	2,3,4′,5-tetra...	291.980	4	2.000	1	2	1	2	0	90	57.08	1.15
CB64	52663-58-8	2,3,4′,6-tetra...	291.980	4	2.000	2	1	1	3	0	88	55.84	1.19
CB65	33284-54-7	2,3,5,6-tetra...	291.980	4	2.000	2	1	1	4	1	79	58.39	1.07
CB66	32598-10-0	2,3′,4,4′-tetra...	291.980	4	2.000	1	1	2	2	0	128	67.49	1.64
CB67	73557-53-8	2,3′,4,5-tetra...	291.980	4	2.000	1	2	1	2	0	64	57.27	1.16
CB68	73575-52-7	2,3′,4,5′-tetra...	291.980	4	2.000	1	2	1	1	0	93	62.21	1.51
CB69	60233-24-1	2,3′,4,6-tetra...	291.980	4	2.000	2	1	1	2	0	54	51.21	1.33
CB70	32598-11-1	2,3′,4′,5-tetra...	291.980	4	2.000	1	2	1	2	0	105	68.39	1.72
CB71	41464-46-4	2,3′,4′,6-tetra...	291.980	4	2.000	2	1	1	3	0	37	64.44	1.47
CB72	41464-42-0	2,3′,5,5′-tetra...	291.980	4	2.000	1	3	1	1	0	108	60.79	1.59
CB73	74338-23-1	2,3′,5′,6-tetra...	291.980	4	2.000	2	2	0	2	0	72	59.16	1.62

Table 2. Continued

			WM	chlorines		Cl positions			biodeggroup		Mp	SMLR prediction	
code	CASRN	chemical name	g·mol^{-1}	nCl	CN	No	Nm	Np	Nchch	Phen	°C	ΔS_{fpred}	SEpred
CB74	32690-93-0	2,4,4′,5-tetra...	291.980	4	2.000	1	1	2	2	0	129	58.85	1.31
CB75	32598-12-2	2,4,4′,6-tetra...	291.980	4	2.000	2	0	2	2	0	63	52.80	1.24
CB76	70362-48-0	2′,3,4,5-tetra...	291.980	4	2.000	1	2	1	3	0	135	61.17	1.55
CB77	32598-13-3	3,3′,4,4′-tetra...	291.980	4	2.000	0	2	2	2	0	181	74.52	2.40
CB78	70362-49-1	3,3′,4,5-tetra...	291.980	4	2.000	0	3	1	2	0	120	65.28	2.00
CB79	41464-48-6	3,3′,4,5′-tetra...	291.980	4	2.000	0	3	1	1	0	123	69.22	1.79
CB80	33284-52-5	3,3′,5,5′-tetra...	291.980	4	2.000	0	4	0	0	0	173	64.99	1.57
CB81	70362-50-4	3,4,4′,5-tetra...	291.980	4	2.000	0	2	2	2	0	163	66.11	2.12
CB82	52663-62-4	2,2′,3,3′,4-penta...	326.427	5	2.236	2	2	1	3	0	121	65.08	1.31
CB83	60145-20-2	2,2′,3,3′,5-penta...	326.427	5	2.236	2	3	0	2	0	84	59.89	1.17
CB84	52663-60-2	2,2′,3,3′,6-penta...	326.427	5	2.236	3	2	0	3	0	110	58.67	1.16
CB85	65510-45-4	2,2′,3,4,4′-penta...	326.427	5	2.236	2	1	2	2	0	49	63.42	1.18
CB86	55312-69-1	2,2′,3,4,5-penta...	326.427	5	2.236	3	1	1	3	0	86	55.47	1.40
CB87	38380-02-8	2,2′,3,4,5′-penta...	326.427	5	2.236	2	2	1	2	0	114	62.01	1.13
CB88	55215-17-3	2,2′,3,4,6-penta...	326.427	5	2.236	3	1	1	3	0	67	47.37	1.74
CB89	73575-57-2	2,2′,3,4,6′-penta...	326.427	5	2.236	3	1	1	3	0	86	60.36	1.07
CB90	68194-07-0	2,2′,3,4′,5-penta...	326.427	5	2.236	2	2	1	1	0	53	58.23	1.24
CB91	68194-05-8	2,2′,3,4′,6-penta...	326.427	5	2.236	3	1	1	2	0	63	57.00	1.26
CB92	52663-61-3	2,2′,3,5,5′-penta...	326.427	5	2.236	2	3	0	1	0	61	56.82	1.40
CB93	73575-56-1	2,2′,3,5,6-penta...	326.427	5	2.236	3	2	0	3	0	98	47.07	1.77
CB94	73575-55-0	2,2′,3,5,6′-penta...	326.427	5	2.236	3	2	0	1	0	83	55.18	1.48
CB95	38379-99-6	2,2′,3,5′,6-penta...	326.427	5	2.236	3	2	0	2	0	100	55.60	1.43
CB96	73575-54-9	2,2′,3,6,6′-penta...	326.427	5	2.236	4	1	0	3	0	120	53.95	1.54
CB97	41464-51-1	2,2′,3′,4,5-penta...	326.427	5	2.236	2	2	1	2	0	83	61.68	1.13
CB98	60233-25-2	2,2′,3′,4,6-penta...	326.427	5	2.236	3	1	1	2	0	95	55.62	1.40
CB99	38380-01-1	2,2′,4,4′,5-penta...	326.427	5	2.236	2	1	2	1	0	60	60.07	1.12
CB100	39485-83-1	2,2′,4,4′,6-penta...	326.427	5	2.236	3	0	2	1	0	79	53.96	1.57
CB101	37680-73-2	2,2′,4,5,5′-penta...	326.427	5	2.236	2	2	1	1	0	79	58.65	1.21
CB102	68194-06-9	2,2′,4,5,6′-penta...	326.427	5	2.236	3	1	1	1	0	72	56.96	1.26
CB103	60145-21-3	2,2′,4,5′,6-penta...	326.427	5	2.236	3	1	1	2	0	70	52.54	1.79
CB104	56558-16-8	2,2′,4,6,6′-penta...	326.427	5	2.236	4	0	1	2	0	88	51.09	1.90
CB105	32598-14-4	2,3,3′,4,4′-penta...	326.427	5	2.236	1	2	2	2	0	118	71.99	2.18
CB106	70424-69-0	2,3,3′,4,5-penta...	326.427	5	2.236	1	2	2	2	0	86	59.45	1.62
CB107	70424-68-9	2,3,3′,4′,5-penta...	326.427	5	2.236	1	3	1	1	0	97	65.26	1.34
CB108	70362-41-3	2,3,3′,4,5′-penta...	326.427	5	2.236	1	3	1	1	0	122	67.49	1.56
CB109	74472-35-8	2,3,3′,4,6-penta...	326.427	5	2.236	2	2	1	2	0	71	56.08	1.43
CB110	38380-03-9	2,3,3′,4′,6-penta...	326.427	5	2.236	2	2	1	2	0	55	64.03	1.22
CB111	39635-32-0	2,3,3′,5,5′-penta...	326.427	5	2.236	1	4	0	0	0	108	59.98	1.26
CB112	74472-36-9	2,3,3′,5,6-penta...	326.427	5	2.236	2	3	0	2	0	93	51.20	1.43
CB113	68194-10-5	2,3,3′,5′,6-penta...	326.427	5	2.236	2	3	0	1	0	57	58.75	1.23
CB114	74472-37-0	2,3,4,4′,5-penta...	326.427	5	2.236	1	2	2	2	0	99	61.19	1.84
CB115	74472-38-1	2,3,4,4′,6-penta...	326.427	5	2.236	2	1	2	2	0	65	53.11	1.38
CB116	18259-05-7	2,3,4,5,6-penta...	326.427	5	2.236	2	2	1	4	1	125	49.92	2.71
CB117	68194-11-6	2,3,4′,5,6-penta...	326.427	5	2.236	2	2	1	2	0	171	55.89	1.42
CB118	31508-00-6	2,3′,4,4′,5-penta...	326.427	5	2.236	1	2	2	1	0	113	67.05	1.50
CB119	56558-17-9	2,3′,4,4′,6-penta...	326.427	5	2.236	2	1	2	1	0	77	60.99	1.10
CB120	68194-12-7	2,3′,4,5,5′-penta...	326.427	5	2.236	1	3	1	0	0	133	61.75	1.19
CB121	56558-18-0	2,3′,4,5′,6-penta...	326.427	5	2.236	2	2	1	0	0	95	55.75	1.48
CB122	76842-07-4	2′,3,3′,4,5-penta...	326.427	5	2.236	1	3	1	2	0	118	68.93	1.73
CB123	65510-44-3	2′,3,4,4′,5-penta...	326.427	5	2.236	1	2	2	1	0	135	67.27	1.53
CB124	70424-70-3	2′,3,4,5,5′-penta...	326.427	5	2.236	1	3	1	1	0	117	65.87	1.39
CB125	74472-39-2	2′,3,4,5,6′-penta...	326.427	5	2.236	2	2	1	2	0	127	64.22	1.24
CB126	57465-28-8	3,3′,4,4′,5-penta...	326.427	5	2.236	0	3	2	2	0	161	72.76	2.22
CB127	39635-33-1	3,3′,4,5,5′-penta...	326.427	5	2.236	0	4	1	0	0	153	69.02	1.73
CB128	38380-07-3	2,2′,3,3′,4,4′-hexa...	360.874	6	2.449	2	2	2	2	0	152	66.85	1.68
CB129	55215-18-4	2,2′,3,3′,4,5-hexa...	360.874	6	2.449	2	3	1	2	0	104	64.01	1.37
CB130	52663-66-8	2,2′,3,3′,4,5′-hexa...	360.874	6	2.449	2	3	1	1	0	116	61.66	1.22
CB131	61798-70-7	2,2′,3,3′,4,6-hexa...	360.874	6	2.449	3	2	1	2	0	137	55.93	1.30
CB132	38380-05-1	2,2′,3,3′,4,6‘-hexa...	360.874	6	2.449	3	2	1	2	0	118	60.44	1.13
CB133	35694-04-3	2,2′,3,3′,5,5′-hexa...	360.874	6	2.449	2	4	0	0	0	129	56.47	1.39
CB134	52704-70-8	2,2′,3,3′,5,6-hexa...	360.874	6	2.449	3	3	0	1	0	133	55.61	1.36
CB135	52744-13-5	2,2′,3,3′,5,6′-hexa...	360.874	6	2.449	3	3	0	1	0	103	55.25	1.39
CB136	38411-22-2	2,2′,3,3′,6,6’-hexa...	360.874	6	2.449	4	2	0	2	0	115	54.02	1.42
CB137	35694-06-5	2,2′,3,4,4′,5-hexa...	360.874	6	2.449	2	2	2	1	0	82	62.35	1.24
CB138	35065-28-2	2,2′,3,4,4′,5′-hexa...	360.874	6	2.449	2	2	2	1	0	80	63.45	1.32
CB139	56030-56-9	2,2′,3,4,4′,6-hexa...	360.874	6	2.449	3	1	2	1	0	77	57.04	1.18
CB140	59291-64-4	2,2′,3,4,4′,6′-hexa...	360.874	6	2.449	3	1	2	1	0	71	55.07	1.45
CB141	52712-04-6	2,2′,3,4,5,5′-hexa...	360.874	6	2.449	2	3	1	1	0	89	60.93	1.20
CB142	41411-61-4	2,2′,3,4,5,6-hexa...	360.874	6	2.449	3	2	1	3	0	137	46.64	2.48
CB143	68194-15-0	2,2′,3,4,5,6′-hexa...	360.874	6	2.449	3	2	1	2	0	90	59.30	1.12
CB144	68194-14-9	2,2′,3,4,5′,6-hexa...	360.874	6	2.449	3	2	1	1	0	74	52.85	1.63
CB145	74472-40-5	2,2′,3,4,6,6′-hexa...	360.874	6	2.449	4	1	1	2	0	137	51.20	1.75
CB146	51908-16-8	2,2′,3,4′,5,5′-hexa...	360.874	6	2.449	2	3	1	0	0	90	58.30	1.24
CB147	68194-13-8	2,2′,3,4′,5,6-hexa...	360.874	6	2.449	3	2	1	1	0	138	53.91	1.50

Table 2. Continued

			WM	chlorines		Cl positions			biodeggroup		Mp	SMLR prediction	
code	CASRN	chemical name	g·mol^{-1}	nCl	CN	No	Nm	Np	Nchch	Phen	°C	ΔS_{fpred}	SEpred
CB148	74472-41-6	2,2′,3,4′,5,6′-hexa...	360.874	6	2.449	3	2	1	0	0	81	52.21	1.71
CB149	38380-04-0	2,2′,3,4′,5′,6-hexa...	360.874	6	2.449	3	2	1	1	0	79	57.04	1.21
CB150	68194-08-1	2,2′,3,4′,6,6′-hexa...	360.874	6	2.449	4	1	1	1	0	77	50.98	1.78
CB151	52663-63-5	2,2′,3,5,5′,6-hexa...	360.874	6	2.449	3	3	0	1	0	100	52.53	1.71
CB152	68194-09-2	2,2′,3,5,6,6′-hexa...	360.874	6	2.449	4	2	0	2	0	127	50.90	1.82
CB153	35065-27-1	2,2′,4,4′,5,5′-hexa...	360.874	6	2.449	2	2	2	0	0	104	60.05	1.17
CB154	60145-22-4	2,2′,4,4′,5,6′-hexa...	360.874	6	2.449	3	1	2	0	0	70	53.99	1.46
CB155	33979-03-2	2,2′,4,4′,6,6′-hexa...	360.874	6	2.449	4	0	2	0	0	113	47.94	2.19
CB156	38380-08-4	2,3,3′,4,4′,5-hexa...	360.874	6	2.449	1	3	2	1	0	131	69.36	1.99
CB157	69782-90-7	2,3,3′,4,4′,5′-hexa...	360.874	6	2.449	1	3	2	1	0	162	70.70	2.18
CB158	74472-42-7	2,3,3′,4,4′,6-hexa...	360.874	6	2.449	2	2	2	1	0	112	61.28	1.19
CB159	39635-35-3	2,3,3′,4,5,5′-hexa...	360.874	6	2.449	1	4	1	0	0	150	65.64	1.54
CB160	41411-62-5	2,3,3′,4,5,6-hexa	360.874	6	2.449	2	3	1	2	0	100	50.80	2.45
CB161	74474-43-8	2,3,3′,4,5′,6-hexa	360.874	6	2.449	2	3	1	0	0	106	56.00	1.39
CB162	39635-34-2	2,3,3′,4′,5,5′-hexa	360.874	6	2.449	1	4	1	0	0	144	67.06	1.70
CB163	74472-44-9	2,3,3′,4′,5,6-hexa	360.874	6	2.449	2	3	1	1	0	123	60.98	1.20
CB164	74472-45-0	2,3,3′,4′,5′,6-hexa	360.874	6	2.449	2	3	1	1	0	94	64.29	1.40
CB165	74472-46-1	2,3,3′,5,5′,6-hexa	360.874	6	2.449	2	4	0	0	0	152	57.01	1.35
CB166	41411-63-6	2,3,4,4′,5,6-hexa	360.874	6	2.449	2	2	2	2	0	167	55.81	2.75
CB167	52663-72-6	2,3′,4,4′,5,5′-hexa	360.874	6	2.449	1	3	2	0	0	127	67.30	1.73
CB168	59291-65-5	2,3′,4,4′,5′,6-hexa	360.874	6	2.449	2	2	2	0	0	111	61.25	1.19
CB169	32774-16-6	3,3′,4,4′,5,5′-hexa	360.874	6	2.449	0	4	2	0	0	210	76.88	3.12
CB170	35065-30-6	2,2′,3,3′,4,4′,5-hpta	395.321	7	2.646	2	3	2	1	0	139	66.02	1.92
CB171	52663-71-5	2,2′,3,3′,4,4′,6-hpta	395.321	7	2.646	3	2	2	1	0	119	57.94	1.43
CB172	52663-74-8	2,2′,3,3′,4,5,5′-hpta	395.321	7	2.646	2	4	1	0	0	137	60.83	1.55
CB173	68194-16-1	2,2′,3,3′,4,5,6-hpta	395.321	7	2.646	3	3	1	2	0	205	55.40	1.72
CB174	38411-25-5	2,2′,3,3′,4,5,6′-hpta	395.321	7	2.646	3	3	1	2	0	131	59.64	1.46
CB175	40186-70-7	2,2′,3,3′,4,5′,6-hpta	395.321	7	2.646	3	3	1	0	0	123	52.74	1.80
CB176	52663-65-7	2,2′,3,3′,4,6,6′-hpta	395.321	7	2.646	4	2	1	1	0	103	49.19	2.22
CB177	52663-70-4	2,2′3,3′,4′,5,6-hpta	395.321	7	2.646	3	3	1	1	0	154	59.94	1.41
CB178	52663-67-9	2,2′,3,3′,5,5′,6-hpta	395.321	7	2.646	3	4	0	0	0	112	53.20	1.75
CB179	35065-29-3	2,2′,3,3′,5,6,6′-hpta	395.321	7	2.646	4	3	0	1	0	131	48.89	2.30
CB180	35065-29-3	2,2′,3,4,4′,5,5′-hpta	395.321	7	2.646	2	3	2	0	0	114	65.65	1.88
CB181	74472-47-2	2,2′,3,4,4′,5,6-hpta	395.321	7	2.646	3	2	2	1	0	126	53.71	1.72
CB182	60145-23-5	2,2′,3,4,4′,5,6′-hpta	395.321	7	2.646	3	2	2	0	0	110	56.60	1.47
CB183	52663-69-1	2,2′,3,4,4′,5′,6-hpta	395.321	7	2.646	3	2	2	0	0	95	54.58	1.59
CB184	74472-48-3	2,2′,3,4,4′,6,6′-hpta	395.321	7	2.646	4	1	2	0	0	117	48.47	2.17
CB185	52712-05-7	2,2′,3,4,5,5′,6-hpta	395.321	7	2.646	4	2	1	1	0	150	52.31	1.77
CB186	74472-49-4	2,2′,3,4,5,6,6′-hpta	395.321	7	2.646	4	2	1	2	0	198	50.66	1.82
CB187	52663-68-0	2,2′,3,4′,5,5′,6-hpta	395.321	7	2.646	3	3	1	0	0	105	54.22	1.66
CB188	74487-85-7	2,2′,3,4′,5,6,6′-hpta	395.321	7	2.646	4	2	1	0	0	135	48.17	2.25
CB189	39635-31-9	2,3,3′,4,4′,5,5′-hpta	395.321	7	2.646	1	4	2	0	0	163	69.87	2.38
CB190	41411-64-7	2,3,3′,4,4′,5,6-hpta	395.321	7	2.646	2	3	2	1	0	124	60.74	1.99
CB191	74472-50-7	2,3,3′,4,4′,5′,6-hpta	395.321	7	2.646	2	3	2	0	0	115	58.76	1.85
CB192	74472-51-8	2,3,3′,4,5,5′,6-hpta	395.321	7	2.646	2	4	1	0	0	174	55.50	1.74
CB193	69782-91-8	2,3,3′,4′,5,5′,6-hpta	395.321	7	2.646	2	4	1	0	0	141	61.48	1.57
CB194	35694-08-7	2,2′,3,3′,4,4′,5,5′-oc	429.768	8	2.828	2	4	2	0	0	160	65.31	2.25
CB195	52663-78-2	2,2′,3,3′,4,4′,5,6-oc	429.768	8	2.828	3	3	2	1	0	172	57.86	2.22
CB196	42740-50-1	2,2′,3,3′,4,4′,5,6′-oc	429.768	8	2.828	3	3	2	0	0	129	57.41	1.87
CB197	33091-17-7	2,2′,3,3′,4,4′,6,6′-oc	429.768	8	2.828	4	2	2	0	0	139	49.33	2.32
CB198	68194-17-2	2,2′,3,3′,4,5,5′,6-oc	429.768	8	2.828	3	4	1	0	0	197	55.53	1.95
CB199	52663-73-7	2,2′,3,3′,4,5,6,6′-oc	429.768	8	2.828	4	3	1	1	0	176	54.23	2.15
CB200	40186-71-8	2,2′,3,3′,4,5′,6,6′-oc	429.768	8	2.828	4	3	1	0	0	143	54.30	1.92
CB201	52663-75-9	2,2′,3,3′,4,5,5′,6′-oc	429.768	8	2.828	3	4	1	0	0	158	51.01	2.18
CB202	2136-99-4	2,2′,3,3′,5,5′,6,6′-oc	429.768	8	2.828	4	4	0	0	0	161	48.71	2.46
CB203	52663-76-0	2,2′,3,4,4′,5,5′,6-oc	429.768	8	2.828	3	3	2	0	0	113	52.14	2.23
CB204	74472-52-9	2,2′,3,4,4′,5,6,6′oc	429.768	8	2.828	4	2	2	0	0	179	40.69	3.43
CB205	74472-53-0	2,3,3′,4,4′,5,5′,6-oc	429.768	8	2.828	2	4	2	0	0	199	61.71	2.47
CB206	40186-72-9	22′33′44′55′6-nona	464.215	9	3.000	3	4	2	0	0	204	57.67	2.64
CB207	52663-79-3	22′33′44′566′-nona	464.215	9	3.000	4	3	2	0	0	215	49.59	2.65
CB208	52663-77-1	22′33′4′55′66′-nona	464.215	9	3.000	4	4	1	0	0	181	49.27	2.69
CB209	2051-24-3	decachlorobiphenyl	498.662	10	3.162	4	4	2	0	0	320	50.30	3.34

[a] Interim estimate.[15] Non-marked (measured) values of Mp's.[11–14] [b] For units, see Abbreviations/Symbols.

or calculated from literature data (see Materials and Methods). Some missing values were determined and validated by SMLR, where the explanatory variables were taken and removed from least-squares regression until the overall correlation reached its maximal and the standard deviation its minimal value.

Melting Points. Literature values of measured Mp's[12–14] were in fair agreement with each other. Mp values of CB6, CB13, CB17, CB27, CB51, and CB59 were selected from Abramowitz and Yalkowsky[15] as interim Mp's in the FATEMOD database. Test runs of those values with WATSOLU values (Table 6) indicated that a possible deviation of ± 10 °C caused only small errors in the model results. Bs values deviated 3 %, when ΔS_{fpred} was kept constant. The deviation in the S_{W25} value was 20 % (Table 6). These influences were tolerable for fate modeling where uncertain-

Table 3. Molecular Descriptors (MDs; Constant Parameters for PCBs[a])

	molar volume	solubil. parameter	solute descriptors[d]					RRT descriptors[e]		assoc. constants WATSOLU	assoc. constants TDLKOW	total surface area
code	V_b[b]	DB[c]	*E*	*S*	*B*	*V*	*L*	IP	μ	KaccW	KaccW	TSAplan[f]
CB1	174.9	18.01	1.48	1.07	0.20	1.4466	6.336	9.1431	1.6592	61	70	195.45
CB2	174.9	18.01	1.51	1.05	0.18	1.4466	6.667	9.0092	2.1102	61	70	201.95
CB3	174.9	18.01	1.50	1.05	0.18	1.4466	6.718	8.9968	2.1219	61	70	209.12
CB4	189.8	18.12	1.60	1.22	0.20	1.5690	6.815	9.3409	2.3729	38	30	200.80
CB5	189.8	17.54	1.63	1.20	0.18	1.5690	7.168	9.0996	2.8756	38	30	210.34
CB6	189.8	18.12	1.63	1.20	0.18	1.5690	7.146	9.1939	3.1952	38	30	212.97
CB7	189.8	17.54	1.62	1.20	0.18	1.5690	7.042	9.1939	2.3797	38	30	213.14
CB8	189.8	18.12	1.62	1.20	0.18	1.5690	7.197	8.9736	3.0419	38	30	213.14
CB9	189.8	17.54	1.63	1.20	0.18	1.5690	7.001	9.1939	0.6462	38	30	212.97
CB10	189.8	17.54	1.66	1.22	0.20	1.5690	6.765	9.4256	1.1074	38	30	206.46
CB11	189.8	18.12	1.66	1.18	0.16	1.5690	7.477	9.1555	3.0637	38	30	219.47
CB12	189.8	17.54	1.65	1.18	0.16	1.5690	7.531	9.0476	3.6633	38	30	217.73
CB13	189.8	18.12	1.65	1.18	0.16	1.5690	7.528	9.0274	1.8599	38	30	219.64
CB14	189.8	17.54	1.65	1.18	0.16	1.5690	7.365	9.0476	2.6916	38	30	219.47
CB15	189.8	18.12	1.64	1.18	0.16	1.5690	7.580	8.9261	0.0038	38	30	219.81
CB16	204.7	17.68	1.75	1.35	0.17	1.6914	7.647	9.3630	3.4657	33	20	215.69
CB17	204.7	17.68	1.74	1.35	0.17	1.6914	7.521	9.4016	3.0134	33	20	218.50
CB18	204.7	17.68	1.75	1.35	0.17	1.6914	7.480	9.2820	1.7985	33	20	218.32
CB19	204.7	17.68	1.72	1.35	0.17	1.6914	7.284	9.2674	1.5435	33	20	211.82
CB20	204.7	17.68	1.78	1.33	0.15	1.6914	7.978	9.1708	3.8108	33	20	227.86
CB21	204.7	17.20	1.77	1.33	0.15	1.6914	7.907	9.1584	3.4026	33	20	226.11
CB22	204.7	17.68	1.77	1.33	0.15	1.6914	8.030	9.1584	3.0539	33	20	238.08
CB23	204.7	17.20	1.78	1.33	0.15	1.6914	7.660	9.1708	2.0166	33	20	227.86
CB24	204.7	17.20	1.75	1.35	0.17	1.6914	7.487	9.3113	1.2872	33	20	221.35
CB25	204.7	17.68	1.77	1.33	0.15	1.6914	7.852	9.1584	2.9499	33	20	230.66
CB26	204.7	17.68	1.78	1.33	0.15	1.6914	7.810	9.1708	1.5747	33	20	230.49
CB27	204.7	17.68	1.76	1.35	0.17	1.6914	7.608	9.4274	2.8332	33	20	223.99
CB28	204.7	17.68	1.76	1.33	0.15	1.6914	7.904	8.9951	1.4836	33	20	230.83
CB29	204.7	17.20	1.77	1.33	0.15	1.6914	7.722	9.1584	2.4080	33	20	228.74
CB30	204.7	17.20	1.74	1.35	0.17	1.6914	7.390	9.2922	0.8875	33	20	224.16
CB31	204.7	17.68	1.77	1.33	0.15	1.6914	7.862	9.0594	1.4831	33	20	230.66
CB32	204.7	17.68	1.74	1.35	0.17	1.6914	7.667	9.3560	3.1938	33	20	224.16
CB33	204.7	17.68	1.77	1.33	0.15	1.6914	8.010	9.1584	4.2878	33	20	228.75
CB34	204.7	17.68	1.78	1.33	0.15	1.6914	7.758	9.1708	3.1831	33	20	230.49
CB35	204.7	17.68	1.80	1.31	0.13	1.6914	8.341	9.0991	3.6950	33	20	235.25
CB36	204.7	17.68	1.79	1.31	0.13	1.6914	8.102	9.0121	1.9693	33	20	236.99
CB37	204.7	17.68	1.79	1.31	0.13	1.6914	8.392	9.0041	1.8103	33	20	235.42
CB38	204.7	17.20	1.80	1.31	0.13	1.6914	8.223	9.0245	3.7954	33	20	233.33
CB39	204.7	17.68	1.80	1.31	0.15	1.6914	8.140	9.1412	0.2906	33	20	237.16
CB40	219.6	17.30	1.90	1.48	0.15	1.8138	8.480	9.3554	4.1320	30	15	230.52
CB41	219.6	18.08	1.89	1.48	0.15	1.8138	8.386	9.4779	4.1515	30	15	231.47
CB42	219.6	17.30	1.89	1.48	0.15	1.8138	8.354	9.4323	3.2404	30	15	233.38
CB43	219.6	18.08	1.90	1.48	0.15	1.8138	8.139	9.3554	2.9027	30	15	233.21
CB44	219.6	17.30	1.90	1.48	0.15	1.8138	8.312	9.3417	2.6289	30	15	233.21
CB45	219.6	17.30	1.87	1.48	0.15	1.8138	7.966	9.3222	2.0716	30	15	226.71
CB46	219.6	17.30	1.87	1.48	0.15	1.8138	8.116	9.3791	3.2021	30	15	223.71
CB47	219.6	17.30	1.88	1.48	0.15	1.8138	8.227	9.4352	1.9572	30	15	236.19
CB48	219.6	17.30	1.89	1.48	0.15	1.8138	8.201	9.3791	3.1452	30	15	234.10
CB49	219.6	17.30	1.89	1.48	0.15	1.8138	8.186	9.3569	1.5616	30	15	236.01
CB50	219.6	17.30	1.86	1.48	0.15	1.8138	7.854	9.3058	2.0288	30	15	229.51
CB51	219.6	17.30	1.86	1.48	0.15	1.8138	7.990	9.3058	2.9092	30	15	229.51
CB52	219.6	17.30	1.90	1.48	0.15	1.8138	8.144	9.3211	0.3289	30	15	235.84
CB53	219.6	17.30	1.87	1.48	0.15	1.8138	7.949	9.3182	1.6969	30	15	229.34
CB54	219.6	17.30	1.84	1.48	0.15	1.8138	7.753	9.2810	0.0225	30	15	217.18
CB55	219.6	18.08	1.92	1.46	0.13	1.8138	8.717	9.2092	3.6538	30	15	243.63
CB56	219.6	17.30	1.92	1.46	0.13	1.8138	8.842	9.1360	4.2079	30	15	243.63
CB57	219.6	18.08	1.93	1.46	0.13	1.8138	8.470	9.2216	2.3122	30	15	245.38
CB58	219.6	17.30	1.93	1.46	0.13	1.8138	8.590	9.2216	3.0996	30	15	245.38
CB59	219.6	18.08	1.91	1.48	0.15	1.8138	8.290	9.3748	2.6288	30	15	238.87
CB60	219.6	18.08	1.91	1.46	0.13	1.8138	8.769	9.0616	2.3708	30	15	243.80
CB61	219.6	17.62	1.92	1.46	0.13	1.8138	8.687	9.1264	3.1497	30	15	241.72
CB62	219.6	17.62	1.89	1.48	0.15	1.8138	8.228	9.3430	1.9591	30	15	237.13
CB63	219.6	18.08	1.92	1.46	0.13	1.8138	8.522	9.2092	1.1037	30	15	245.55
CB64	219.6	18.08	1.89	1.48	0.15	1.8138	8.348	9.3695	2.3990	30	15	239.04
CB65	219.6	17.62	1.89	1.48	0.15	1.8138	8.288	9.3430	1.0650	30	15	236.24
CB66	219.6	17.30	1.91	1.46	0.13	1.8138	8.716	9.1642	2.7777	30	15	246.44
CB67	219.6	18.08	1.92	1.46	0.13	1.8138	8.532	9.2092	2.0413	30	15	246.28
CB68	219.6	17.30	1.92	1.46	0.13	1.8138	8.464	9.2092	1.5604	30	15	248.18
CB69	219.6	18.08	1.89	1.48	0.15	1.8138	8.096	9.3430	1.6480	30	15	241.68
CB70	219.6	17.30	1.89	1.46	0.13	1.8138	8.694	9.1206	2.8497	30	15	246.26
CB71	219.6	17.30	1.89	1.48	0.15	1.8138	8.479	9.3356	4.2563	30	15	239.76
CB72	219.6	17.30	1.93	1.46	0.13	1.8138	8.422	9.2216	1.7095	30	15	248.01
CB73	219.6	17.30	1.90	1.48	0.15	1.8138	8.227	9.4944	3.3923	30	15	241.50

Table 3. Continued

	molar volume	solubil. parameter	solute descriptors[d]					RRT descriptors[e]		assoc. constants WATSOLU	assoc. constants TDLKOW	total surface area
code	V_b[b]	DB[c]	*E*	*S*	*B*	*V*	*L*	IP	μ	KaccW	KaccW	TSAplan[f]
CB74	219.6	18.08	1.91	1.46	0.13	1.8138	8.583	9.0513	0.1659	30	15	246.43
CB75	219.6	18.08	1.88	1.48	0.15	1.8138	8.147	9.3765	1.2029	30	15	241.85
CB76	219.6	18.08	1.91	1.46	0.13	1.8138	8.709	9.1968	4.4101	30	15	244.35
CB77	219.6	17.30	1.94	1.44	0.11	1.8138	9.205	9.0758	2.6939	30	15	251.02
CB78	219.6	18.08	1.94	1.44	0.11	1.8138	9.039	9.1841	2.9249	30	15	250.85
CB79	219.6	17.30	1.95	1.44	0.11	1.8138	8.952	9.2028	1.6318	30	15	252.77
CB80	219.6	17.30	1.96	1.44	0.11	1.8138	8.757	9.3957	0.0018	30	15	254.51
CB81	219.6	18.08	1.94	1.44	0.11	1.8138	9.084	9.0853	1.6329	30	15	251.02
CB82	234.5	17.70	2.04	1.61	0.13	1.9362	9.218	9.4805	4.1672	29	12	246.36
CB83	234.5	17.70	2.05	1.61	0.13	1.9362	8.971	9.4062	3.1319	29	12	248.10
CB84	234.5	17.70	2.02	1.61	0.13	1.9362	8.798	9.3728	3.1241	29	12	241.60
CB85	234.5	17.70	2.03	1.61	0.13	1.9362	9.092	9.5374	3.0059	29	12	249.16
CB86	234.5	18.42	2.04	1.61	0.13	1.9362	9.006	9.3813	3.9256	29	12	247.07
CB87	234.5	17.70	2.04	1.61	0.13	1.9362	9.051	9.3852	2.8258	29	12	248.99
CB88	234.5	18.42	2.01	1.61	0.13	1.9362	8.459	9.3566	2.7631	29	12	242.48
CB89	234.5	17.70	2.01	1.61	0.13	1.9362	8.855	9.3566	4.1122	29	12	242.48
CB90	234.5	17.70	2.04	1.61	0.13	1.9362	8.845	9.3945	1.8574	29	12	250.90
CB91	234.5	17.70	2.01	1.61	0.13	1.9362	8.672	9.3878	2.4133	29	12	244.40
CB92	234.5	17.70	2.05	1.61	0.13	1.9362	8.804	9.3826	1.4540	29	12	250.73
CB93	234.5	18.42	2.02	1.61	0.13	1.9362	8.478	9.3690	2.1435	29	12	241.60
CB94	234.5	17.70	2.02	1.61	0.13	1.9362	8.608	9.3690	2.9372	29	12	244.23
CB95	234.5	17.70	2.02	1.61	0.13	1.9362	8.631	9.3647	1.3284	29	12	244.23
CB96	234.5	17.70	1.99	1.61	0.13	1.9362	8.435	9.3318	1.7001	29	12	232.06
CB97	234.5	17.70	2.04	1.61	0.13	1.9362	9.033	9.3938	2.6848	29	12	248.99
CB98	234.5	17.70	2.01	1.61	0.13	1.9362	8.597	9.3566	3.0994	29	12	244.40
CB99	234.5	17.70	2.03	1.61	0.13	1.9362	8.910	9.3645	1.4861	29	12	251.79
CB100	234.5	17.70	2.00	1.61	0.13	1.9362	8.471	9.3814	1.4675	29	12	247.20
CB101	234.5	17.70	2.04	1.61	0.13	1.9362	8.868	9.3662	1.6694	29	12	251.62
CB102	234.5	17.70	2.01	1.61	0.13	1.9362	8.670	9.3566	3.3516	29	12	254.12
CB103	234.5	17.70	2.01	1.61	0.13	1.9362	8.429	9.3566	0.3248	29	12	247.03
CB104	234.5	17.70	1.98	1.61	0.13	1.9362	8.244	9.3194	1.9633	29	12	234.87
CB105	234.5	17.70	2.04	1.59	0.11	1.9362	9.594	9.1248	3.2839	29	12	259.41
CB106	234.5	18.42	2.07	1.59	0.11	1.9362	9.329	9.2170	2.9969	29	12	259.24
CB107	234.5	17.70	2.07	1.59	0.11	1.9362	9.334	9.2600	2.3794	29	12	261.15
CB108	234.5	17.70	2.04	1.59	0.11	1.9362	9.349	9.2736	2.2792	29	12	261.15
CB109	234.5	18.42	2.04	1.61	0.13	1.9362	9.039	9.4259	1.6465	29	12	254.65
CB110	234.5	17.70	2.04	1.61	0.13	1.9362	9.161	9.3968	3.5745	29	12	254.65
CB111	234.5	17.70	2.08	1.59	0.11	1.9362	9.082	9.4383	1.1584	29	12	262.90
CB112	234.5	18.42	2.05	1.61	0.13	1.9362	8.809	9.4062	1.6167	29	12	253.76
CB113	234.5	17.70	2.05	1.61	0.13	1.9362	8.909	9.4062	2.5592	29	12	256.39
CB114	234.5	18.42	2.06	1.59	0.11	1.9362	9.388	9.3327	1.2902	29	12	259.41
CB115	234.5	18.42	2.03	1.61	0.13	1.9362	8.842	9.4011	1.1179	29	12	254.82
CB116	234.5	19.10	2.04	1.61	0.13	1.9362	8.998	9.3773	2.2892	29	12	250.10
CB117	234.5	18.42	2.04	1.61	0.13	1.9362	9.029	9.3621	0.9921	29	12	253.93
CB118	234.5	17.70	2.06	1.59	0.11	1.9362	9.396	9.1133	1.4495	29	12	262.04
CB119	234.5	17.70	2.03	1.61	0.13	1.9362	8.960	9.4217	2.4832	29	12	257.45
CB120	234.5	17.70	2.07	1.59	0.11	1.9362	9.143	9.2600	0.1750	29	12	263.78
CB121	234.5	17.70	2.04	1.61	0.13	1.9362	8.710	9.3938	1.4346	29	12	259.20
CB122	234.5	17.70	2.07	1.59	0.11	1.9362	9.534	9.2600	3.9154	29	12	259.24
CB123	234.5	17.70	2.06	1.59	0.11	1.9362	9.408	9.2476	2.6630	29	12	262.04
CB124	234.5	17.70	2.07	1.59	0.11	1.9362	9.367	9.2600	3.2203	29	12	261.87
CB125	234.5	17.70	2.04	1.61	0.13	1.9362	9.171	9.3938	5.1239	29	12	255.37
CB126	234.5	17.70	2.11	1.57	0.09	1.9362	9.884	9.1512	1.5976	29	12	266.63
CB127	234.5	17.70	2.10	1.74	0.09	1.9362	9.645	9.2818	1.3134	29	12	268.37
CB128	249.4	18.04	2.18	1.74	0.11	2.0586	9.957	9.5646	1.0650	29	8	262.13
CB129	249.4	18.04	2.19	1.74	0.11	2.0586	9.838	9.4446	3.6820	29	8	261.96
CB130	249.4	18.04	2.19	1.74	0.11	2.0586	9.710	9.4372	2.6897	29	8	263.88
CB131	249.4	18.04	2.16	1.74	0.11	2.0586	9.292	9.4446	2.9158	29	8	257.37
CB132	249.4	18.04	2.16	1.74	0.11	2.0586	9.537	9.4208	3.4750	29	8	257.37
CB133	249.4	18.04	2.20	1.74	0.11	2.0586	9.463	9.4570	1.5151	29	8	265.62
CB134	249.4	18.04	2.17	1.74	0.11	2.0586	9.310	9.4198	2.6443	29	8	256.49
CB135	249.4	18.04	2.17	1.74	0.11	2.0586	9.290	9.3928	2.3434	29	8	259.12
CB136	249.4	18.04	2.14	1.74	0.11	2.0586	9.117	9.3826	1.7971	29	8	246.95
CB137	249.4	18.04	2.18	1.74	0.11	2.0586	9.712	9.4426	2.2649	29	8	264.76
CB138	249.4	18.04	2.18	1.74	0.11	2.0586	9.772	9.4126	2.2490	29	8	264.76
CB139	249.4	18.04	2.12	1.74	0.11	2.0586	9.317	9.3950	1.2125	29	8	260.18
CB140	249.4	18.04	2.18	1.74	0.11	2.0586	9.316	9.4322	2.7166	29	8	260.18
CB141	249.4	18.04	2.19	1.74	0.11	2.0586	9.670	9.4121	2.4700	29	8	264.59
CB142	249.4	19.13	2.16	1.74	0.11	2.0586	9.257	9.3805	3.4218	29	8	255.46
CB143	249.4	18.04	2.16	1.74	0.11	2.0586	9.475	9.4074	4.1224	29	8	258.09
CB144	249.4	18.04	2.16	1.74	0.11	2.0586	9.124	9.4072	1.4837	29	8	260.00
CB145	249.4	18.04	2.13	1.74	0.11	2.0586	8.928	9.3701	2.9126	29	8	247.84
CB146	249.4	18.04	2.19	1.74	0.11	2.0586	9.527	9.4364	1.1375	29	8	266.51

Table 3. Continued

	molar volume	solubil. parameter	solute descriptors[d]					RRT descriptors[e]		assoc. constants WATSOLU	assoc. constants TDLKOW	total surface area
code	V_b[b]	DB[c]	*E*	*S*	*B*	*V*	*L*	IP	μ	KaccW	KaccW	TSAplan[f]
CB147	249.4	18.04	2.16	1.74	0.11	2.0586	9.182	9.4074	1.3714	29	8	259.29
CB148	249.4	18.04	2.16	1.74	0.11	2.0586	9.089	9.4074	1.2872	29	8	261.92
CB149	249.4	18.04	2.16	1.74	0.11	2.0586	9.352	9.3859	2.5235	29	8	260.00
CB150	249.4	18.04	2.13	1.74	0.11	2.0586	8.916	9.4074	1.4744	29	8	249.76
CB151	249.4	18.04	2.17	1.74	0.11	2.0586	9.142	9.3539	0.4765	29	8	259.12
CB152	249.4	18.04	2.14	1.74	0.11	2.0586	8.947	9.3826	2.1358	29	8	246.95
CB153	249.4	18.04	2.18	1.74	0.11	2.0586	9.587	9.3892	0.2222	29	8	267.39
CB154	249.4	18.04	2.15	1.74	0.11	2.0586	9.151	9.3950	1.3871	29	8	262.81
CB155	249.4	18.04	2.12	1.74	0.11	2.0586	8.715	9.3577	0.0236	29	8	252.56
CB156	249.4	18.04	2.21	1.72	0.09	2.0586	10.200	9.1801	1.9422	29	8	275.01
CB157	249.4	18.04	2.21	1.72	0.09	2.0586	10.273	9.2045	2.5965	29	8	275.01
CB158	249.4	18.04	2.18	1.74	0.11	2.0586	9.654	9.4342	1.8872	29	8	270.64
CB159	249.4	18.04	2.20	1.72	0.09	2.0586	9.962	9.3155	0.3759	29	8	276.76
CB160	249.4	19.13	2.19	1.74	0.11	2.0586	9.590	9.4355	1.9111	29	8	267.62
CB161	249.4	18.04	2.19	1.74	0.11	2.0586	9.402	9.4942	1.2130	29	8	272.17
CB162	249.4	18.04	2.20	1.72	0.09	2.0586	10.039	9.2869	2.1579	29	8	276.76
CB163	249.4	18.04	2.19	1.74	0.11	2.0586	9.673	9.4119	2.2989	29	8	296.54
CB164	249.4	18.04	2.19	1.74	0.11	2.0586	9.853	9.4596	3.7658	29	8	270.25
CB165	249.4	18.04	2.20	1.74	0.11	2.0586	9.492	9.4570	1.3758	29	8	271.28
CB166	249.4	19.13	2.18	1.74	0.11	2.0586	9.827	9.4322	0.2043	29	8	267.79
CB167	249.4	18.04	2.21	1.72	0.09	2.0586	10.088	9.1886	1.3742	29	8	277.64
CB168	249.4	18.04	2.18	1.74	0.11	2.0586	9.652	9.4553	2.7602	29	8	273.06
CB169	249.4	18.04	2.21	1.70	0.09	2.0586	10.609	9.2257	0.0023	29	8	282.23
CB170	264.3	18.35	2.33	1.87	0.09	2.1810	10.577	9.4891	2.6594	30	7	277.74
CB171	264.3	18.35	2.30	1.87	0.09	2.1810	10.031	9.4932	2.4835	30	7	273.15
CB172	264.3	18.35	2.34	1.87	0.09	2.1810	10.330	9.4664	1.8798	30	7	279.48
CB173	264.3	18.73	2.31	1.87	0.09	2.1810	10.092	9.4582	3.0701	30	7	270.35
CB174	264.3	18.35	2.31	1.87	0.09	2.1810	10.159	9.4502	3.2821	30	7	272.98
CB175	264.3	18.35	2.31	1.87	0.09	2.1810	9.783	9.3960	1.4879	30	7	274.89
CB176	264.3	18.35	2.31	1.87	0.09	2.1810	9.590	9.4582	2.2652	30	7	262.73
CB177	264.3	18.35	2.28	1.87	0.09	2.1810	10.069	9.4209	2.5907	30	7	272.26
CB178	264.3	18.35	2.31	1.87	0.09	2.1810	9.808	9.3966	1.1800	30	7	274.01
CB179	264.3	18.35	2.32	1.87	0.09	2.1810	9.609	9.3492	1.5915	30	7	261.84
CB180	264.3	18.35	2.29	1.87	0.09	2.1810	10.415	9.4422	1.1012	30	7	280.37
CB181	264.3	18.73	2.30	1.87	0.09	2.1810	9.965	9.4429	1.5352	30	7	273.15
CB182	264.3	18.35	2.30	1.87	0.09	2.1810	9.958	9.4603	2.2555	30	7	275.78
CB183	264.3	18.35	2.30	1.87	0.09	2.1810	9.848	9.4379	1.2085	30	7	275.78
CB184	264.3	18.35	2.27	1.87	0.09	2.1810	9.409	9.4085	1.2687	30	7	265.53
CB185	264.3	18.73	2.31	1.87	0.09	2.1810	9.924	9.4294	1.6440	30	7	272.98
CB186	264.3	18.73	2.28	1.87	0.09	2.1810	9.728	9.4209	3.3322	30	7	260.81
CB187	264.3	18.35	2.31	1.87	0.09	2.1810	9.864	9.4026	1.1976	30	7	274.89
CB188	264.3	18.35	2.28	1.87	0.09	2.1810	9.428	9.4209	0.1864	30	7	264.64
CB189	264.3	18.35	2.36	1.85	0.07	2.1810	10.893	9.2523	0.8902	30	7	290.81
CB190	264.3	18.73	2.33	1.87	0.09	2.1810	10.454	9.4858	1.5244	30	7	283.40
CB191	264.3	18.73	2.33	1.87	0.09	2.1810	10.346	9.4830	2.2313	30	7	286.03
CB192	264.3	18.73	2.34	1.87	0.09	2.1810	10.204	9.4871	0.0437	30	7	285.14
CB193	264.3	18.35	2.34	1.87	0.09	2.1810	10.365	9.4471	2.5393	30	7	285.14
CB194	279.2	18.62	2.48	2.00	0.06	2.3034	11.186	9.4946	1.3732	31	5	293.34
CB195	279.2	18.98	2.45	2.00	0.06	2.3034	10.830	9.4227	2.2706	31	5	286.12
CB196	279.2	18.62	2.45	2.00	0.06	2.3034	10.650	9.4951	1.1951	31	5	288.15
CB197	279.2	18.62	2.42	2.00	0.06	2.3034	10.104	9.4810	1.4030	31	5	278.50
CB198	279.2	18.62	2.46	2.00	0.06	2.3034	10.583	9.4351	1.1400	31	5	287.87
CB199	279.2	28.98	2.43	2.00	0.06	2.3034	10.386	9.4330	2.0603	31	5	275.70
CB200	279.2	18.62	2.43	2.00	0.06	2.3034	10.410	9.4237	2.4968	31	5	277.62
CB201	279.2	18.98	2.46	2.00	0.06	2.3034	10.668	9.3979	1.1420	31	5	287.87
CB202	279.2	18.62	2.44	2.00	0.06	2.3034	10.141	9.4103	0.0147	31	5	276.73
CB203	279.2	18.98	2.48	2.00	0.06	2.3034	10.625	9.4599	0.0761	31	5	288.75
CB204	279.2	18.98	2.52	2.00	0.06	2.3034	10.143	9.5096	1.3758	31	5	278.50
CB205	279.2	18.98	2.48	2.00	0.06	2.3034	11.146	9.5260	1.3804	31	5	299.00
CB206	294.1	19.21	2.60	2.13	0.04	2.4258	11.450	9.5036	0.9629	29	5	301.73
CB207	294.1	19.21	2.57	2.13	0.04	2.4258	10.904	9.4362	1.1790	29	5	291.48
CB208	294.1	19.21	2.58	2.13	0.04	2.4258	10.922	9.4176	1.1773	29	5	290.59
CB209	309.0	19.74	2.72	2.26	0.02	2.5482	11.703	9.4862	0.0157	31	5	304.45

[a] Data missing in a few cases in the literature were completed by SMLR. Dimensions (Units) are listed in the Abbreviations section. [b] Ref 19. [c] Refs 20 and 21. [d] Ref 22. [e] Ref 25. [f] Ref 15.

ties in environmental factors are great. Therefore, use of these six interim Mp values appeared to be sufficient in model-based estimations for environmental fate, until their Mps are successfully measured. These six estimated MPs are listed together with 203 measured ones taken in the FATEMOD database in Table 2.

Entropy of Fusion (ΔS_f). This is essential for conversion of the P_S to P_L values (eqs 8 to 10) and in application of

Table 4. Temperature Correction Coefficients for Physical Properties of PCBs[a]

	vapor pressure: VPLEST			solubility in water: WATSOLU			log K_{ow}: TDLKOW			volatility: k_H	
code	P_{L25}	Apl	Bpl	log S_{W25}	As	Bs	log K_{ow25}	Aow	Bow	Ah	Bh
CB1	1.11	10.29	3054.0	−1.738	0.786	753	4.673	4.715	12.64	9.50	2301.4
CB2	$8.04\cdot10^{-1}$	10.30	3099.7	−1.595	1.000	774	4.673	4.715	12.64	9.30	2325.9
CB3	$4.96\cdot10^{-1}$	10.32	3168.3	−2.147	1.083	963	4.673	4.715	12.64	9.24	2205.2
CB4	$3.75\cdot10^{-1}$	10.33	3207.9	−2.575	0.190	825	5.020	5.050	8.88	10.14	2383.4
CB5	$2.17\cdot10^{-1}$	10.36	3285.3	−2.346	0.671	900	5.115	5.050	−19.35	9.69	2385.8
CB6	$2.17\cdot10^{-1}$	10.36	3285.3	−2.063	0.410	737	5.020	5.050	8.88	9.95	2548.1
CB7	$1.61\cdot10^{-1}$	10.37	3327.5	−2.317	0.582	864	5.115	5.050	−19.35	9.79	2463.2
CB8	$1.54\cdot10^{-1}$	10.37	3333.7	−2.475	0.488	883	5.020	5.050	8.88	9.88	2450.4
CB9	$2.48\cdot10^{-1}$	10.35	3266.7	−2.298	0.509	837	5.115	5.050	−19.35	9.84	2429.6
CB10	$3.25\cdot10^{-1}$	10.34	3228.1	−2.405	0.180	771	5.115	5.050	−19.35	10.16	2457.3
CB11	$1.36\cdot10^{-1}$	10.38	3351.7	−2.331	0.624	881	5.020	5.050	8.88	9.76	2470.6
CB12	$1.30\cdot10^{-1}$	10.38	3358.5	−2.583	0.948	1053	5.115	5.050	−19.35	9.43	2305.9
CB13	$1.07\cdot10^{-1}$	10.39	3385.5	−2.038	0.708	819	5.020	5.050	8.88	9.68	2567.0
CB14	$1.36\cdot10^{-1}$	10.38	3351.7	−2.428	0.791	960	5.115	5.050	−19.35	9.59	2391.9
CB15	$8.19\cdot10^{-2}$	10.40	3423.8	−3.567	0.791	1300	5.020	5.050	8.88	9.61	2124.3
CB16	$8.11\cdot10^{-2}$	10.40	3425.1	−2.898	0.125	901	5.500	5.425	−22.33	10.28	2523.8
CB17	$5.92\cdot10^{-2}$	10.41	3469.9	−2.625	0.041	795	5.500	5.425	−22.33	10.37	2675.0
CB18	$9.14\cdot10^{-2}$	10.39	3408.2	−3.052	−0.032	900	5.500	5.425	−22.33	10.42	2507.9
CB19	$1.40\cdot10^{-1}$	10.38	3347.7	−3.452	−0.121	993	5.500	5.425	−22.33	10.50	2354.4
CB20	$4.13\cdot10^{-2}$	10.43	3520.9	−3.068	0.344	1017	5.500	5.425	−22.33	10.09	2503.6
CB21	$4.15\cdot10^{-2}$	10.43	3520.2	−3.751	0.506	1269	5.586	5.425	−48.13	9.92	2251.0
CB22	$3.43\cdot10^{-2}$	10.43	3547.3	−3.372	0.428	1133	5.500	5.425	−22.33	10.00	2414.2
CB23	$5.62\cdot10^{-2}$	10.41	3477.1	−3.057	0.235	982	5.586	5.425	−48.13	10.18	2495.6
CB24	$7.93\cdot10^{-2}$	10.40	3428.4	−3.211	0.172	1009	5.586	5.425	−48.13	10.23	2419.7
CB25	$3.68\cdot10^{-2}$	10.43	3537.2	−2.981	0.255	965	5.500	5.425	−22.33	10.18	2572.3
CB26	$4.08\cdot10^{-2}$	10.43	3522.5	−3.037	0.182	960	5.500	5.425	−22.33	10.25	2562.6
CB27	$7.78\cdot10^{-2}$	10.40	3431.0	−2.623	0.057	799	5.500	5.425	−22.33	10.34	2631.8
CB28	$2.27\cdot10^{-2}$	10.45	3606.1	−3.213	0.339	1059	5.500	5.425	−22.33	10.11	2547.1
CB29	$4.57\cdot10^{-2}$	10.42	3506.5	−3.456	0.329	1128	5.586	5.425	−48.13	10.09	2378.1
CB30	$6.08\cdot10^{-2}$	10.41	3466.0	−3.282	0.114	1013	5.586	5.425	−48.13	10.30	2453.3
CB31	$4.19\cdot10^{-2}$	10.43	3518.9	−3.265	0.266	1053	5.503	5.425	−23.45	10.16	2466.1
CB32	$5.78\cdot10^{-2}$	10.41	3473.2	−3.165	0.182	998	5.500	5.425	−22.33	10.23	2475.1
CB33	$4.42\cdot10^{-2}$	10.42	3511.4	−3.252	0.407	1091	5.500	5.425	−22.33	10.01	2420.4
CB34	$4.96\cdot10^{-2}$	10.42	3495.0	−3.179	0.130	987	5.500	5.425	−22.33	10.29	2508.3
CB35	$2.48\cdot10^{-2}$	10.45	3593.4	−3.336	0.621	1180	5.500	5.425	−22.33	9.83	2413.7
CB36	$2.92\cdot10^{-2}$	10.44	3570.2	−3.437	0.428	1152	5.500	5.425	−22.33	10.01	2418.0
CB37	$1.81\cdot10^{-2}$	10.46	3637.9	−3.614	0.705	1288	5.500	5.425	−22.33	9.76	2350.1
CB38	$2.96\cdot10^{-2}$	10.44	3568.2	−3.444	0.710	1238	5.586	5.425	−48.13	9.73	2329.8
CB39	$2.51\cdot10^{-2}$	10.45	3591.8	−3.533	0.428	1181	5.500	5.425	−22.33	10.02	2410.9
CB40	$1.37\cdot10^{-2}$	10.47	3677.0	−4.603	−0.016	1368	6.025	5.842	−54.52	10.49	2309.3
CB41	$1.27\cdot10^{-2}$	10.47	3687.8	−3.681	−0.397	979	5.854	5.842	−3.58	10.87	2708.8
CB42	$1.18\cdot10^{-2}$	10.48	3698.9	−3.986	−0.105	1157	6.025	5.842	−54.52	10.59	2541.6
CB43	$1.83\cdot10^{-2}$	10.46	3636.5	−3.622	−0.669	881	5.854	5.842	−3.58	11.13	2756.0
CB44	$1.49\cdot10^{-2}$	10.47	3665.3	−3.762	−0.178	1069	6.025	5.842	−54.52	10.65	2596.5
CB45	$3.13\cdot10^{-2}$	10.44	3560.1	−3.925	−0.731	952	5.854	5.842	−3.58	11.17	2608.0
CB46	$3.08\cdot10^{-2}$	10.44	3562.4	−4.553	−0.261	1280	6.025	5.842	−54.52	10.70	2282.9
CB47	$9.59\cdot10^{-3}$	10.49	3728.0	−3.719	−0.188	1053	6.025	5.842	−54.52	10.68	2675.2
CB48	$1.56\cdot10^{-2}$	10.47	3659.0	−4.010	−0.575	1024	5.854	5.842	−3.58	11.05	2634.8
CB49	$1.36\cdot10^{-2}$	10.47	3678.4	−3.952	−0.261	1100	6.025	5.842	−54.52	10.73	2578.0
CB50	$2.39\cdot10^{-2}$	10.45	3598.6	−3.629	−0.804	842	5.854	5.842	−3.58	11.25	2756.4
CB51	$2.25\cdot10^{-2}$	10.45	3606.8	−3.245	−0.350	863	6.025	5.842	−54.52	10.80	2743.6
CB52	$2.01\cdot10^{-2}$	10.46	3622.8	−4.122	−0.340	1128	6.025	5.842	−54.52	10.80	2495.0
CB53	$3.23\cdot10^{-2}$	10.44	3555.8	−4.281	−0.423	1150	6.025	5.842	−54.52	10.86	2405.5
CB54	$6.86\cdot10^{-2}$	10.40	3449.0	−5.145	−0.507	1383	6.025	5.842	−54.52	10.91	2066.0
CB55	$8.43\cdot10^{-3}$	10.49	3746.3	−4.092	−0.178	1167	5.854	5.842	−3.58	10.67	2579.1
CB56	$8.36\cdot10^{-3}$	10.49	3747.6	−4.394	0.266	1389	6.025	5.842	−54.52	10.22	2358.2
CB57	$1.01\cdot10^{-2}$	10.48	3720.4	−4.046	−0.449	1072	5.854	5.842	−3.58	10.93	2648.1
CB58	$9.40\cdot10^{-3}$	10.49	3731.0	−4.661	−0.010	1387	6.025	5.842	−54.52	10.50	2344.5
CB59	$1.44\cdot10^{-2}$	10.47	3670.5	−3.199	−0.554	789	5.854	5.842	−3.58	11.02	2881.9
CB60	$5.90\cdot10^{-3}$	10.51	3796.9	−4.765	−0.094	1393	5.854	5.842	−3.58	10.60	2404.4
CB61	$1.19\cdot10^{-2}$	10.48	3697.3	−4.228	−0.016	1256	5.957	5.842	−34.39	10.50	2441.3
CB62	$1.36\cdot10^{-2}$	10.47	3678.4	−4.010	−0.355	1090	5.957	5.842	−34.39	10.83	2588.6
CB63	$8.69\cdot10^{-3}$	10.49	3742.1	−4.083	−0.366	1108	5.854	5.842	−3.58	10.86	2633.7
CB64	$1.14\cdot10^{-2}$	10.48	3704.2	−4.049	−0.434	1078	5.854	5.842	−3.58	10.91	2626.3
CB65	$1.92\cdot10^{-2}$	10.46	3629.6	−4.021	−0.298	1110	5.957	5.842	−34.39	10.76	2519.6
CB66	$6.58\cdot10^{-3}$	10.50	3781.6	−4.715	0.178	1459	6.025	5.842	−54.52	10.32	2323.0
CB67	$9.10\cdot10^{-3}$	10.49	3735.5	−3.825	−0.355	1034	5.854	5.842	−3.58	10.85	2701.1
CB68	$8.07\cdot10^{-3}$	10.49	3752.5	−4.238	−0.099	1234	6.025	5.842	−54.52	10.59	2518.7
CB69	$1.10\cdot10^{-2}$	10.48	3708.3	−3.693	−0.674	900	5.854	5.842	−3.58	11.15	2808.1
CB70	$8.73\cdot10^{-3}$	10.49	3741.4	−4.455	0.225	1395	6.025	5.842	−54.52	10.27	2346.1
CB71	$1.33\cdot10^{-2}$	10.47	3682.0	−3.632	0.016	1088	6.025	5.842	−54.52	10.45	2594.5
CB72	$1.06\cdot10^{-2}$	10.48	3714.0	−4.381	−0.172	1255	6.025	5.842	−54.52	10.65	2459.3
CB73	$1.63\cdot10^{-2}$	10.46	3653.1	−3.984	−0.256	1112	6.025	5.842	−54.52	10.72	2541.6
CB74	$6.61\cdot10^{-3}$	10.50	3780.9	−4.506	−0.272	1263	5.854	5.842	−3.58	10.77	2518.4

Table 4. Continued

	vapor pressure: VPLEST			solubility in water: WATSOLU			log K_{ow}: TDLKOW			volatility: k_H	
code	P_{L25}	Apl	Bpl	log S_{W25}	As	Bs	log K_{ow25}	Aow	Bow	Ah	Bh
CB75	$8.05 \cdot 10^{-3}$	10.49	3752.8	−3.785	−0.590	952	5.854	5.842	−3.58	11.08	2800.4
CB76	$1.05 \cdot 10^{-2}$	10.48	3715.2	−4.618	−0.136	1336	5.854	5.842	−3.58	10.62	2378.8
CB77	$4.92 \cdot 10^{-3}$	10.51	3822.8	−5.535	0.548	1814	6.025	5.842	−54.52	9.96	2008.9
CB78	$5.83 \cdot 10^{-3}$	10.51	3798.6	−4.520	0.063	1366	5.854	5.842	−3.58	10.45	2432.3
CB79	$5.47 \cdot 10^{-3}$	10.51	3807.7	−4.685	0.266	1476	6.025	5.842	−54.52	10.24	2331.6
CB80	$7.05 \cdot 10^{-3}$	10.50	3771.8	−5.182	0.047	1559	6.025	5.842	−54.52	10.45	2212.8
CB81	$4.60 \cdot 10^{-3}$	10.52	3832.2	−5.031	0.104	1531	5.854	5.842	−3.58	10.42	2301.0
CB82	$2.59 \cdot 10^{-3}$	10.54	3913.9	−5.079	−0.460	1377	6.382	6.282	−29.74	11.00	2536.7
CB83	$3.27 \cdot 10^{-3}$	10.53	3880.9	−4.604	−0.732	1154	6.404	6.282	−36.40	11.26	2726.5
CB84	$5.92 \cdot 10^{-3}$	10.51	3796.6	−4.859	−0.794	1212	6.404	6.282	−36.40	11.30	2584.9
CB85	$1.99 \cdot 10^{-3}$	10.55	3951.5	−4.251	−0.549	1104	6.404	6.282	−36.40	11.10	2847.7
CB86	$3.37 \cdot 10^{-3}$	10.53	3876.3	−4.522	−0.962	1062	6.218	6.282	19.11	11.49	2814.8
CB87	$2.72 \cdot 10^{-3}$	10.54	3906.7	−4.951	−0.622	1291	6.404	6.282	−36.40	11.16	2616.0
CB88	$5.41 \cdot 10^{-3}$	10.51	3809.3	−4.278	−1.385	863	6.218	6.282	19.11	11.90	2946.8
CB89	$5.35 \cdot 10^{-3}$	10.51	3811.0	−4.630	−0.706	1170	6.404	6.282	−36.40	11.22	2641.0
CB90	$2.55 \cdot 10^{-3}$	10.54	3916.2	−4.270	−0.821	1028	6.404	6.282	−36.40	11.36	2887.8
CB91	$3.97 \cdot 10^{-3}$	10.52	3853.1	−4.364	−0.883	1038	6.404	6.282	−36.40	11.40	2815.4
CB92	$3.83 \cdot 10^{-3}$	10.52	3858.4	−4.343	−0.894	1028	6.404	6.282	−36.40	11.41	2830.1
CB93	$7.13 \cdot 10^{-3}$	10.50	3770.1	−4.531	−1.400	934	6.218	6.282	19.11	11.90	2836.6
CB94	$6.40 \cdot 10^{-3}$	10.50	3785.5	−4.545	−0.977	1064	6.404	6.282	−36.40	11.48	2721.7
CB95	$5.81 \cdot 10^{-3}$	10.51	3799.2	−4.715	−0.956	1121	6.404	6.282	−36.40	11.47	2678.6
CB96	$1.49 \cdot 10^{-2}$	10.47	3665.3	−4.881	−1.045	1144	6.404	6.282	−36.40	11.52	2521.5
CB97	$2.83 \cdot 10^{-3}$	10.54	3901.5	−4.611	−0.638	1185	6.404	6.282	−36.40	11.18	2716.8
CB98	$3.89 \cdot 10^{-3}$	10.52	3856.1	−4.666	−0.956	1106	6.404	6.282	−36.40	11.48	2750.0
CB99	$2.12 \cdot 10^{-3}$	10.55	3942.4	−4.353	−0.721	1083	6.404	6.282	−36.40	11.27	2859.6
CB100	$3.30 \cdot 10^{-3}$	10.53	3879.3	−4.495	−1.040	1030	6.404	6.282	−36.40	11.57	2849.1
CB101	$3.28 \cdot 10^{-3}$	10.53	3880.3	−4.540	−0.794	1117	6.404	6.282	−36.40	11.32	2763.6
CB102	$5.57 \cdot 10^{-3}$	10.51	3805.1	−4.454	−0.883	1065	6.404	6.282	−36.40	11.39	2740.6
CB103	$4.85 \cdot 10^{-3}$	10.52	3824.7	−4.398	−1.118	978	6.404	6.282	−36.40	11.64	2846.8
CB104	$1.02 \cdot 10^{-2}$	10.48	3719.2	−4.548	−1.191	1001	6.404	6.282	−36.40	11.67	2718.3
CB105	$1.37 \cdot 10^{-3}$	10.57	4003.8	−5.158	−0.100	1508	6.404	6.282	−36.40	10.67	2495.8
CB106	$2.04 \cdot 10^{-3}$	10.55	3947.5	−4.565	−0.753	1137	6.218	6.282	19.11	11.30	2810.9
CB107	$1.71 \cdot 10^{-3}$	10.56	3973.1	−4.808	−0.450	1300	6.404	6.282	−36.40	11.01	2673.6
CB108	$1.76 \cdot 10^{-3}$	10.56	3968.5	−5.131	−0.335	1430	6.404	6.282	−36.40	10.90	2538.4
CB109	$2.80 \cdot 10^{-3}$	10.54	3902.8	−4.381	−0.930	1029	6.218	6.282	19.11	11.47	2874.0
CB110	$2.60 \cdot 10^{-3}$	10.54	3913.3	−4.321	−0.518	1134	6.404	6.282	−36.40	11.06	2779.4
CB111	$2.11 \cdot 10^{-3}$	10.55	3943.0	−4.857	−0.727	1232	6.404	6.282	−36.40	11.28	2711.5
CB112	$3.63 \cdot 10^{-3}$	10.53	3865.9	−4.539	−1.186	1000	6.218	6.282	19.11	11.72	2866.3
CB113	$3.15 \cdot 10^{-3}$	10.53	3886.1	−4.314	−0.789	1051	6.404	6.282	−36.40	11.32	2835.2
CB114	$1.55 \cdot 10^{-3}$	10.56	3987.1	−4.722	−0.664	1210	6.218	6.282	19.11	11.22	2777.1
CB115	$1.92 \cdot 10^{-3}$	10.55	3956.4	−4.301	−1.087	958	6.218	6.282	19.11	11.64	2998.1
CB116	$4.08 \cdot 10^{-3}$	10.52	3849.2	−4.766	−1.254	1047	6.026	6.282	76.19	11.77	2802.2
CB117	$2.88 \cdot 10^{-3}$	10.54	3898.9	−5.359	−0.941	1317	6.218	6.282	19.11	11.48	2581.7
CB118	$1.47 \cdot 10^{-3}$	10.56	3994.6	−5.017	−0.361	1388	6.404	6.282	−36.40	10.92	2606.3
CB119	$1.93 \cdot 10^{-3}$	10.55	3955.4	−4.540	−0.674	1153	6.404	6.282	−36.40	11.22	2802.8
CB120	$1.72 \cdot 10^{-3}$	10.54	3953.7	−5.139	−0.674	1331	6.404	6.282	−36.40	11.21	2622.7
CB121	$2.54 \cdot 10^{-3}$	10.54	3916.9	−4.667	−0.951	1108	6.404	6.282	−36.40	11.49	2808.9
CB122	$1.81 \cdot 10^{-3}$	10.56	3964.6	−5.107	−0.262	1445	6.404	6.282	−36.40	10.82	2520.0
CB123	$1.37 \cdot 10^{-3}$	10.57	4003.8	−5.281	−0.345	1472	6.404	6.282	−36.40	10.92	2532.1
CB124	$2.00 \cdot 10^{-3}$	10.55	3950.5	−5.047	−0.418	1380	6.404	6.282	−36.40	10.97	2570.6
CB125	$3.16 \cdot 10^{-3}$	10.53	3885.5	−5.132	−0.507	1379	6.404	6.282	−36.40	11.04	2506.7
CB126	$1.18 \cdot 10^{-3}$	10.57	4025.6	−5.719	−0.058	1688	6.404	6.282	−36.40	10.63	2337.8
CB127	$1.33 \cdot 10^{-3}$	10.57	4008.7	−5.532	−0.256	1573	6.404	6.282	−36.40	10.83	2435.9
CB128	$5.20 \cdot 10^{-4}$	10.61	4141.6	−5.442	−0.371	1512	6.991	6.928	−18.77	10.98	2629.7
CB129	$8.13 \cdot 10^{-4}$	10.59	4078.3	−5.275	−0.945	1291	6.991	6.928	−18.77	11.54	2787.2
CB130	$7.05 \cdot 10^{-4}$	10.60	4098.5	−5.373	−1.065	1285	6.991	6.928	−18.77	11.67	2814.0
CB131	$1.06 \cdot 10^{-3}$	10.58	4040.3	−5.487	−1.368	1228	6.991	6.928	−18.77	11.95	2812.4
CB132	$1.04 \cdot 10^{-3}$	10.58	4043.6	−5.374	−1.133	1264	6.991	6.928	−18.77	11.71	2779.2
CB133	$9.33 \cdot 10^{-4}$	10.58	4058.6	−5.419	−1.337	1217	6.991	6.928	−18.77	11.92	2841.5
CB134	$1.32 \cdot 10^{-3}$	10.57	4009.7	−5.442	−1.384	1210	6.991	6.928	−18.77	11.95	2799.8
CB135	$1.48 \cdot 10^{-3}$	10.56	3993.3	−5.144	−1.405	1115	6.991	6.928	−18.77	11.97	2878.4
CB136	$3.47 \cdot 10^{-3}$	10.53	3872.4	−5.241	−1.467	1125	6.991	6.928	−18.77	12.00	2747.3
CB137	$5.40 \cdot 10^{-4}$	10.61	4136.4	−5.012	−1.034	1186	6.991	6.928	−18.77	11.64	2950.4
CB138	$5.36 \cdot 10^{-4}$	10.61	4137.4	−5.002	−0.971	1202	6.988	6.928	−17.90	11.58	2935.7
CB139	$8.55 \cdot 10^{-4}$	10.59	4071.1	−4.909	−1.311	1073	6.991	6.928	−18.77	11.90	2998.3
CB140	$8.37 \cdot 10^{-4}$	10.59	4074.0	−4.834	−1.410	1021	6.991	6.928	−18.77	12.00	3053.2
CB141	$8.28 \cdot 10^{-4}$	10.59	4075.6	−5.073	−1.107	1182	6.991	6.928	−18.77	11.70	2893.3
CB142	$1.48 \cdot 10^{-3}$	10.56	3993.3	−5.234	−1.854	1008	6.655	6.928	81.56	12.41	2985.5
CB143	$1.33 \cdot 10^{-3}$	10.57	4008.7	−5.065	−1.191	1155	6.991	6.928	−18.77	11.76	2853.5
CB144	$1.16 \cdot 10^{-3}$	10.57	4027.3	−4.843	−1.530	988	6.991	6.928	−18.77	12.10	3039.6
CB145	$2.67 \cdot 10^{-3}$	10.54	3909.7	−5.394	−1.614	1127	6.991	6.928	−18.77	12.15	2782.5
CB146	$7.11 \cdot 10^{-4}$	10.60	4097.2	−5.054	−1.243	1136	6.991	6.928	−18.77	11.84	2961.0
CB147	$1.15 \cdot 10^{-3}$	10.57	4028.9	−5.457	−1.473	1188	6.991	6.928	−18.77	12.04	2841.0
CB148	$1.03 \cdot 10^{-3}$	10.58	4044.9	−4.894	−1.554	996	6.991	6.928	−18.77	12.13	3049.0

Table 4. Continued

	vapor pressure: VPLEST			solubility in water: WATSOLU			log K_{ow}: TDLKOW			volatility: k_H	
code	P_{L25}	Apl	Bpl	log S_{W25}	As	Bs	log K_{ow25}	Aow	Bow	Ah	Bh
CB149	$1.15 \cdot 10^{-3}$	10.58	4029.5	−4.929	−1.311	1079	6.991	6.928	−18.77	11.89	2950.7
CB150	$2.17 \cdot 10^{-3}$	10.55	3938.7	−4.854	−1.624	963	6.991	6.928	−18.77	12.17	2975.6
CB151	$1.59 \cdot 10^{-3}$	10.56	3983.5	−5.080	−1.546	1054	6.991	6.928	−18.77	12.11	2929.9
CB152	$4.03 \cdot 10^{-3}$	10.52	3851.2	−5.299	−1.629	1094	6.991	6.928	−18.77	12.15	2757.0
CB153	$5.66 \cdot 10^{-4}$	10.60	4129.6	−5.221	−1.149	1214	6.991	6.928	−18.77	11.75	2915.3
CB154	$8.65 \cdot 10^{-4}$	10.59	4069.4	−4.815	−1.467	998	6.991	6.928	−18.77	12.06	3071.2
CB155	$1.57 \cdot 10^{-3}$	10.64	4005.0	−5.128	−1.786	997	6.991	6.928	−18.77	12.43	3008.5
CB156	$3.60 \cdot 10^{-4}$	10.62	4193.9	−5.678	−0.663	1495	6.991	6.928	−18.77	11.28	2698.5
CB157	$3.52 \cdot 10^{-4}$	10.62	4196.8	−6.087	−0.595	1637	6.991	6.928	−18.77	11.22	2559.5
CB158	$5.08 \cdot 10^{-4}$	10.61	4144.9	−5.324	−1.086	1264	6.991	6.928	−18.77	11.70	2881.4
CB159	$5.06 \cdot 10^{-4}$	10.61	4145.6	−5.826	−0.861	1480	6.991	6.928	−18.77	11.47	2665.3
CB160	$7.94 \cdot 10^{-4}$	10.59	4081.5	−5.199	−1.847	1000	6.655	6.928	81.56	12.44	3081.9
CB161	$7.19 \cdot 10^{-4}$	10.59	4095.6	−5.184	−1.363	1139	6.991	6.928	−18.77	11.95	2956.2
CB162	$4.34 \cdot 10^{-4}$	10.62	4167.4	−5.789	−0.783	1492	6.991	6.928	−18.77	11.40	2675.0
CB163	$7.59 \cdot 10^{-4}$	10.59	4088.0	−5.437	−1.102	1293	6.991	6.928	−18.77	11.69	2795.4
CB164	$7.24 \cdot 10^{-4}$	10.59	4094.6	−5.167	−0.929	1263	6.991	6.928	−18.77	11.52	2831.2
CB165	$8.69 \cdot 10^{-4}$	10.59	4068.8	−5.658	−1.311	1296	6.991	6.928	−18.77	11.90	2772.7
CB166	$5.59 \cdot 10^{-4}$	10.61	4131.5	−5.708	−1.373	1292	6.655	6.928	81.56	11.98	2839.2
CB167	$3.53 \cdot 10^{-4}$	10.62	4196.5	−5.592	−0.773	1437	6.991	6.928	−18.77	11.39	2759.5
CB168	$4.67 \cdot 10^{-4}$	10.61	4157.0	−5.312	−1.091	1258	6.991	6.928	−18.77	11.70	2898.7
CB169	$3.27 \cdot 10^{-4}$	10.63	4207.6	−6.882	−0.271	1971	6.991	6.928	−18.77	10.90	2236.6
CB170	$1.39 \cdot 10^{-4}$	10.66	4329.1	−5.966	−1.120	1445	7.359	7.384	7.56	11.78	2884.2
CB171	$1.92 \cdot 10^{-4}$	10.65	4283.1	−5.602	−1.543	1210	7.359	7.384	7.56	12.19	3073.1
CB172	$1.75 \cdot 10^{-4}$	10.65	4296.5	−5.841	−1.392	1327	7.359	7.384	7.56	12.04	2969.9
CB173	$3.30 \cdot 10^{-4}$	10.63	4206.3	−6.369	−1.674	1400	7.233	7.384	45.05	12.30	2806.4
CB174	$3.27 \cdot 10^{-4}$	10.63	4207.6	−5.755	−1.454	1282	7.359	7.384	7.56	12.08	2925.4
CB175	$2.73 \cdot 10^{-4}$	10.63	4232.8	−5.553	−1.815	1115	7.359	7.384	7.56	12.45	3118.3
CB176	$5.51 \cdot 10^{-4}$	10.61	4133.5	−5.321	−1.998	991	7.359	7.384	7.56	12.61	3142.8
CB177	$2.89 \cdot 10^{-4}$	10.63	4224.9	−6.002	−1.439	1361	7.359	7.384	7.56	12.07	2864.4
CB178	$3.32 \cdot 10^{-4}$	10.63	4205.3	−5.459	−1.789	1094	7.359	7.384	7.56	12.42	3111.0
CB179	$6.65 \cdot 10^{-4}$	10.60	4106.7	−5.556	−2.013	1056	7.359	7.384	7.56	12.61	3050.4
CB180	$1.40 \cdot 10^{-4}$	10.66	4327.8	−5.671	−1.141	1351	7.359	7.384	7.56	11.80	2977.2
CB181	$2.21 \cdot 10^{-4}$	10.64	4262.8	−5.572	−1.763	1136	7.233	7.384	45.05	12.40	3126.9
CB182	$1.95 \cdot 10^{-4}$	10.65	4281.2	−5.491	−1.611	1157	7.359	7.384	7.56	12.26	3124.4
CB183	$1.96 \cdot 10^{-4}$	10.65	4280.1	−5.318	−1.716	1074	7.359	7.384	7.56	12.37	3206.1
CB184	$4.67 \cdot 10^{-4}$	10.61	4157.0	−5.430	−2.034	1012	7.359	7.384	7.56	12.64	3144.6
CB185	$3.47 \cdot 10^{-4}$	10.62	4199.1	−5.768	−1.836	1172	7.233	7.384	45.05	12.46	3026.8
CB186	$7.26 \cdot 10^{-4}$	10.59	4094.3	−6.159	−1.919	1264	7.233	7.384	45.05	12.51	2830.3
CB187	$2.90 \cdot 10^{-4}$	10.63	4224.3	−5.408	−1.737	1095	7.359	7.384	7.56	12.37	3129.7
CB188	$5.50 \cdot 10^{-4}$	10.61	4133.8	−5.577	−2.050	1052	7.359	7.384	7.56	12.66	3082.2
CB189	$1.11 \cdot 10^{-4}$	10.67	4361.1	−6.338	−0.916	1617	7.359	7.384	7.56	11.59	2744.6
CB190	$1.44 \cdot 10^{-4}$	10.66	4323.9	−5.675	−1.397	1276	7.233	7.384	45.05	12.06	3048.4
CB191	$1.33 \cdot 10^{-4}$	10.66	4335.4	−5.549	−1.496	1208	7.233	7.384	45.05	12.16	3127.0
CB192	$1.72 \cdot 10^{-4}$	10.65	4298.4	−6.071	−1.669	1313	7.233	7.384	45.05	12.32	2985.8
CB193	$1.65 \cdot 10^{-4}$	10.66	4304.3	−5.898	−1.355	1354	7.359	7.384	7.56	12.02	2949.9
CB194	$4.74 \cdot 10^{-5}$	10.71	4481.4	−6.416	−1.397	1496	7.916	8.026	32.79	12.11	2985.0
CB195	$6.56 \cdot 10^{-5}$	10.69	4435.4	−6.341	−1.784	1359	7.784	8.026	72.19	12.47	3076.7
CB196	$6.64 \cdot 10^{-5}$	10.69	4433.7	−5.918	−1.810	1225	7.916	8.026	32.79	12.50	3208.9
CB197	$1.11 \cdot 10^{-4}$	10.67	4360.2	−5.856	−2.233	1080	7.916	8.026	32.79	12.90	3279.8
CB198	$8.04 \cdot 10^{-5}$	10.69	4406.6	−6.544	−1.909	1382	7.916	8.026	32.79	12.60	3024.6
CB199	$1.54 \cdot 10^{-4}$	10.66	4314.8	−6.284	−1.977	1284	7.784	8.026	72.19	12.64	3030.8
CB200	$1.35 \cdot 10^{-4}$	10.66	4333.4	−5.994	−1.972	1199	7.916	8.026	32.79	12.63	3134.1
CB201	$7.83 \cdot 10^{-5}$	10.69	4410.2	−6.038	−2.144	1161	7.784	8.026	72.19	12.83	3249.2
CB202	$1.88 \cdot 10^{-4}$	10.65	4286.1	−6.032	−2.264	1123	7.916	8.026	32.79	12.91	3162.7
CB203	$6.82 \cdot 10^{-5}$	10.69	4429.8	−5.653	−2.087	1063	7.784	8.026	72.19	12.78	3366.5
CB204	$1.07 \cdot 10^{-4}$	10.67	4365.4	−5.948	−2.682	974	7.784	8.026	72.19	13.35	3391.7
CB205	$4.24 \cdot 10^{-5}$	10.71	4497.4	−6.731	−1.585	1534	7.784	8.026	72.19	12.30	2963.3
CB206	$1.83 \cdot 10^{-5}$	10.75	4616.7	−7.408	−2.552	1448	8.071	8.416	103.00	13.30	3168.8
CB207	$3.08 \cdot 10^{-5}$	10.73	4542.5	−7.250	−2.975	1275	8.071	8.416	103.00	13.71	3268.0
CB208	$3.76 \cdot 10^{-5}$	10.72	4514.4	−6.946	−2.991	1179	8.071	8.416	103.00	13.71	3335.1
CB209	$9.77 \cdot 10^{-6}$	10.77	4705.5	−8.186	−2.948	1562	8.220	8.806	174.92	13.72	3143.6

[a] P_{L25} values were from Öberg.[29] Ah was calculated by eq 24 and Bh by eq 25.

WATSOLU to estimate solubility in water (eqs 12 and 13). The values of ΔS_f for the FATEMOD database (Table 2) were produced by SMLR, using 41 measured values as the training set (Table 7). With the significant predictors: constant, DB, L, and E, the regression equation was very well linear. The mean of all 209 values was 57.93 ± 6.12 with the range from 40.69 to 76.88. Training set ($N = 41$) statistics were: mean 58.20 ± 9.20 and range from 38.20 to 83.40. Thus, the range of predicted values (ΔS_{fpred}) was smaller than that of the measured ones. ANOVA produced an F value of 19.13 ($p = 1.17 \cdot 10^{-7}$), and the standard error (SE) of the predicted value was 0.536. The ΔS_{fpred} values and their standard deviations are listed in Table 2. The numbers from statistics (Tables 2 and 7) support strongly the conclusion of Hinckley et al.[34] that earlier use of an "average" ΔS_f value for all organic compounds (56.5 $J \cdot K^{-1} \cdot mol^{-1}$)[7,72] was obsolete because deviations between individual organic molecules were too large—also in the case of PCB congeners. The plot of predicted versus measured entropy of

Table 5. Degradation Rates (h^{-1}) and Half-Lives (h) at 25 °C of PCBs[a]

		degradation rates/h^{-1}			estimation results/h			values for FATEMOD/h			
code	nCl	Kp/air	Kp/solids	Kh/water	HL(1)	HL(2)	HL(3,4)	$HL_{25}(1)$	$HL_{25}(2)$	$HL_{25}(3)$	$HL_{25}(4)$
CB1	1	$6.93 \cdot 10^{-3}$	$1.39 \cdot 10^{-4}$	0	100	1471	5000	100	1500	5000	5000
CB2	1	$2.31 \cdot 10^{-3}$	$1.39 \cdot 10^{-4}$	0	300	4245	5000	300	4200	5000	5000
CB3	1	$3.47 \cdot 10^{-3}$	$1.39 \cdot 10^{-4}$	0	200	2885	5000	200	2900	5000	5000
CB4	2	$6.93 \cdot 10^{-3}$	$9.90 \cdot 10^{-5}$	0	100	1479	7000	100	1500	7000	7000
CB5	2	$3.47 \cdot 10^{-3}$	$9.90 \cdot 10^{-5}$	0	200	2917	7000	200	2900	7000	7000
CB6	2	$3.47 \cdot 10^{-3}$	$7.05 \cdot 10^{-5}$	0	200	2940	9833	200	2900	10000	10000
CB7	2	$4.62 \cdot 10^{-3}$	$9.90 \cdot 10^{-5}$	0	150	2203	7000	150	2200	7000	7000
CB8	2	$4.62 \cdot 10^{-3}$	$7.05 \cdot 10^{-5}$	0	150	2216	9833	150	2200	10000	10000
CB9	2	$3.47 \cdot 10^{-3}$	$9.90 \cdot 10^{-5}$	0	200	2917	7000	200	2900	7000	7000
CB10	2	$6.93 \cdot 10^{-3}$	$9.90 \cdot 10^{-5}$	0	100	1479	7000	100	1500	7000	7000
CB11	2	$2.31 \cdot 10^{-3}$	$5.47 \cdot 10^{-5}$	0	300	4396	12667	300	4400	13000	13000
CB12	2	$2.77 \cdot 10^{-3}$	$7.05 \cdot 10^{-5}$	0	250	3657	9833	250	3700	10000	10000
CB13	2	$2.77 \cdot 10^{-3}$	$9.90 \cdot 10^{-5}$	0	250	3621	7000	250	3600	7000	7000
CB14	2	$2.31 \cdot 10^{-3}$	$5.47 \cdot 10^{-5}$	0	300	4396	12667	300	4400	13000	13000
CB15	2	$3.47 \cdot 10^{-3}$	$5.47 \cdot 10^{-5}$	0	200	2953	12667	200	3000	13000	13000
CB16	3	$1.30 \cdot 10^{-3}$	$4.83 \cdot 10^{-5}$	0	534	7722	14333	530	7700	14000	14000
CB17	3	$1.72 \cdot 10^{-3}$	$4.83 \cdot 10^{-5}$	0	417	6078	14333	420	6100	14000	14000
CB18	3	$1.30 \cdot 10^{-3}$	$3.71 \cdot 10^{-5}$	0	534	7787	18667	530	7800	19000	19000
CB19	3	$2.30 \cdot 10^{-3}$	$6.93 \cdot 10^{-5}$	0	301	4383	10000	300	4400	10000	10000
CB20	3	$9.04 \cdot 10^{-4}$	$3.71 \cdot 10^{-5}$	0	767	11051	18667	770	11000	19000	19000
CB21	3	$1.09 \cdot 10^{-3}$	$6.93 \cdot 10^{-5}$	0	650	9155	10000	650	9200	10000	10000
CB22	3	$1.09 \cdot 10^{-3}$	$3.71 \cdot 10^{-5}$	0	650	9422	18667	650	9400	19000	19000
CB23	3	$9.04 \cdot 10^{-4}$	$6.93 \cdot 10^{-5}$	0	767	10685	10000	770	11000	10000	10000
CB24	3	$1.30 \cdot 10^{-3}$	$6.93 \cdot 10^{-5}$	0	534	7604	10000	530	7600	10000	10000
CB25	3	$1.09 \cdot 10^{-3}$	$3.01 \cdot 10^{-5}$	0	650	9482	23000	650	9400	23000	23000
CB26	3	$9.04 \cdot 10^{-4}$	$3.01 \cdot 10^{-5}$	0	767	11134	23000	770	11000	23000	23000
CB27	3	$1.30 \cdot 10^{-3}$	$3.71 \cdot 10^{-5}$	0	534	7787	18667	530	7800	19000	19000
CB28	3	$1.37 \cdot 10^{-3}$	$3.01 \cdot 10^{-5}$	0	533	7814	23000	530	7800	23000	23000
CB29	3	$1.09 \cdot 10^{-3}$	$6.93 \cdot 10^{-5}$	0	650	9155	10000	650	9200	10000	10000
CB30	3	$1.72 \cdot 10^{-3}$	$6.93 \cdot 10^{-5}$	0	417	6005	10000	420	6000	10000	10000
CB31	3	$1.09 \cdot 10^{-3}$	$3.01 \cdot 10^{-5}$	0	650	9482	23000	650	9500	23000	23000
CB32	3	$1.72 \cdot 10^{-3}$	$3.71 \cdot 10^{-5}$	0	417	6118	18667	420	6100	19000	19000
CB33	3	$1.09 \cdot 10^{-3}$	$3.71 \cdot 10^{-5}$	0	650	9422	18667	650	9400	19000	19000
CB34	3	$9.04 \cdot 10^{-4}$	$3.01 \cdot 10^{-5}$	0	767	11134	23000	770	11000	23000	23000
CB35	3	$7.97 \cdot 10^{-4}$	$3.01 \cdot 10^{-5}$	0	883	12755	23000	880	13000	23000	23000
CB36	3	$6.93 \cdot 10^{-4}$	$2.54 \cdot 10^{-5}$	0	1000	14471	27333	1000	14000	27000	27000
CB37	3	$9.36 \cdot 10^{-4}$	$3.01 \cdot 10^{-5}$	0	766	11120	23000	770	11000	23000	23000
CB38	3	$7.97 \cdot 10^{-4}$	$6.93 \cdot 10^{-5}$	0	883	12170	10000	880	12000	10000	10000
CB39	3	$7.97 \cdot 10^{-4}$	$2.54 \cdot 10^{-5}$	0	883	12831	27333	880	13000	27000	27000
CB40	4	$3.47 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	2000	27273	20000	2000	27000	20000	20000
CB41	4	$3.96 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	1750	25000	35000	1750	25000	35000	35000
CB42	4	$3.96 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	1750	24138	20000	1750	24000	20000	20000
CB43	4	$3.47 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	2000	28378	35000	2000	28000	35000	35000
CB44	4	$3.47 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2000	28846	50000	2000	29000	50000	50000
CB45	4	$4.62 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	1500	20930	20000	1500	21000	20000	20000
CB46	4	$4.62 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	1500	20930	20000	1500	21000	20000	20000
CB47	4	$4.62 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	1500	21845	50000	1500	22000	50000	50000
CB48	4	$3.96 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	1750	25000	35000	1750	25000	35000	35000
CB49	4	$3.96 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	1750	25362	50000	1750	25000	50000	50000
CB50	4	$5.54 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	1250	18103	35000	1250	18000	35000	35000
CB51	4	$5.54 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	1250	18103	35000	1250	18000	35000	35000
CB52	4	$3.47 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2000	28846	50000	2000	29000	50000	50000
CB53	4	$4.62 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	1500	21575	35000	1500	22000	35000	35000
CB54	4	$6.93 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	1000	14286	20000	1000	14000	20000	20000
CB55	4	$3.08 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	2250	30337	20000	2250	30000	20000	20000
CB56	4	$3.08 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	2250	31711	35000	2250	32000	35000	35000
CB57	4	$2.77 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2500	35714	50000	2500	36000	50000	50000
CB58	4	$2.77 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2500	35714	50000	2500	36000	50000	50000
CB59	4	$3.47 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	2000	28378	35000	2000	28000	35000	35000
CB60	4	$3.47 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	2000	28378	35000	2000	28000	35000	35000
CB61	4	$3.08 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	2250	30337	20000	2250	30000	20000	20000
CB62	4	$3.96 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	1750	24138	20000	1750	24000	20000	20000
CB63	4	$3.08 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2250	32297	50000	2250	32000	50000	50000
CB64	4	$3.96 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	1750	25000	35000	1750	25000	35000	35000
CB65	4	$3.96 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	1750	24138	20000	1750	24000	20000	20000
CB66	4	$3.47 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2000	28846	50000	2000	29000	50000	50000
CB67	4	$3.08 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2250	32297	50000	2250	32000	50000	50000
CB68	4	$3.08 \cdot 10^{-4}$	$1.07 \cdot 10^{-5}$	0	2250	32621	65000	2250	33000	65000	65000
CB69	4	$3.96 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	1750	25362	50000	1750	25000	50000	50000
CB70	4	$3.08 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2250	32297	50000	2250	32000	50000	50000
CB71	4	$3.96 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	1750	25000	35000	1750	25000	35000	35000
CB72	4	$3.08 \cdot 10^{-4}$	$1.07 \cdot 10^{-5}$	0	2250	32621	65000	2250	33000	65000	65000
CB73	4	$3.47 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2000	28846	50000	2000	29000	50000	50000
CB74	4	$3.47 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2000	28846	50000	2000	29000	50000	50000

Table 5. Continued

		degradation rates/h^{-1}			estimation results/h			values for FATEMOD/h			
code	nCl	Kp/air	Kp/solids	Kh/water	HL(1)	HL(2)	HL(3,4)	$HL_{25}(1)$	$HL_{25}(2)$	$HL_{25}(3)$	$HL_{25}(4)$
CB75	4	$4.62 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	1500	21845	50000	1500	22000	50000	50000
CB76	4	$3.08 \cdot 10^{-4}$	$1.98 \cdot 10^{-5}$	0	2250	31711	35000	2250	32000	35000	35000
CB77	4	$2.77 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2500	35714	50000	2500	36000	50000	50000
CB78	4	$2.52 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2750	39100	50000	2750	39000	50000	50000
CB79	4	$2.52 \cdot 10^{-4}$	$1.07 \cdot 10^{-5}$	0	2750	39576	65000	2750	40000	65000	65000
CB80	4	$2.31 \cdot 10^{-4}$	$8.66 \cdot 10^{-6}$	0	3000	43373	80000	3000	43000	80000	80000
CB81	4	$2.77 \cdot 10^{-4}$	$1.39 \cdot 10^{-5}$	0	2500	35714	50000	2500	36000	50000	50000
CB82	5	$3.47 \cdot 10^{-4}$	$2.45 \cdot 10^{-5}$	0	1900	26704	28250	2000	27000	28000	28000
CB83	5	$3.15 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	2100	29786	36500	2300	30000	37000	37000
CB84	5	$3.85 \cdot 10^{-4}$	$2.45 \cdot 10^{-5}$	0	1650	23384	28250	2800	23000	28000	28000
CB85	5	$3.85 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1700	24365	36500	2800	24000	37000	37000
CB86	5	$4.33 \cdot 10^{-4}$	$2.45 \cdot 10^{-5}$	0	1450	20688	28250	1600	21000	28000	28000
CB87	5	$3.47 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1900	27090	36500	2000	27000	37000	37000
CB88	5	$4.33 \cdot 10^{-4}$	$2.45 \cdot 10^{-5}$	0	1450	20688	28250	1600	21000	28000	28000
CB89	5	$4.33 \cdot 10^{-4}$	$2.45 \cdot 10^{-5}$	0	1450	20688	28250	1600	21000	28000	28000
CB90	5	$3.47 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	1900	27339	44750	2000	27000	45000	45000
CB91	5	$4.33 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1450	20919	36500	1600	21000	37000	37000
CB92	5	$3.15 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	2100	30088	44750	2300	30000	45000	45000
CB93	5	$3.85 \cdot 10^{-4}$	$2.45 \cdot 10^{-5}$	0	1650	23384	28250	1800	23000	28000	28000
CB94	5	$3.85 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	1650	23870	44750	1800	24000	45000	45000
CB95	5	$3.85 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1650	23680	36500	1800	24000	37000	37000
CB96	5	$4.95 \cdot 10^{-4}$	$2.45 \cdot 10^{-5}$	0	1200	17267	28250	1200	17000	28000	28000
CB97	5	$3.47 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1900	27090	36500	2000	27000	37000	37000
CB98	5	$4.33 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1450	20919	36500	1600	21000	37000	37000
CB99	5	$3.85 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	1700	24567	44750	1800	25000	45000	45000
CB100	5	$4.95 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	1250	18240	44750	1300	18000	45000	45000
CB101	5	$3.47 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	1900	27339	44750	2000	28000	45000	45000
CB102	5	$4.33 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	1450	21067	44750	2600	21000	45000	45000
CB103	5	$4.33 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1450	20919	36500	1600	21000	37000	37000
CB104	5	$5.78 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1000	14600	36500	1100	15000	37000	37000
CB105	5	$3.15 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	2150	30456	36500	2300	30000	37000	37000
CB106	5	$3.15 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	2150	30456	36500	2300	30000	37000	37000
CB107	5	$2.89 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	2350	33491	44750	2500	33000	45000	45000
CB108	5	$2.89 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	2350	33491	44750	2500	33000	45000	45000
CB109	5	$3.47 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1900	27090	36500	2000	27000	37000	37000
CB110	5	$3.47 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1900	27090	36500	2000	27000	37000	37000
CB111	5	$2.67 \cdot 10^{-4}$	$1.31 \cdot 10^{-5}$	0	2550	36494	53000	2700	36000	53000	53000
CB112	5	$3.15 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	2100	29786	36500	2300	30000	37000	37000
CB113	5	$3.15 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	2100	30088	44750	2300	30000	44750	44750
CB114	5	$3.15 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	2150	30456	36500	2300	30000	37000	37000
CB115	5	$3.85 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1700	24365	36500	1800	24000	37000	37000
CB116	5	$3.47 \cdot 10^{-4}$	$3.47 \cdot 10^{-5}$	0	1900	26027	20000	2000	26000	20000	20000
CB117	5	$3.47 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1900	27090	36500	2000	27000	37000	37000
CB118	5	$3.15 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	2150	30772	44750	2300	31000	45000	45000
CB119	5	$3.85 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	1700	24567	44750	1800	25000	45000	45000
CB120	5	$2.89 \cdot 10^{-4}$	$1.31 \cdot 10^{-5}$	0	2350	33753	53000	2500	34000	53000	53000
CB121	5	$3.47 \cdot 10^{-4}$	$1.31 \cdot 10^{-5}$	0	1900	27514	53000	2000	28000	53000	53000
CB122	5	$2.89 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	2350	33118	36500	2500	33000	36500	36500
CB123	5	$3.15 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	2150	30772	44750	2300	31000	45000	45000
CB124	5	$2.89 \cdot 10^{-4}$	$1.55 \cdot 10^{-5}$	0	2350	33491	44750	2500	33000	45000	45000
CB125	5	$3.47 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	1900	27090	36500	2000	27000	37000	37000
CB126	5	$2.67 \cdot 10^{-4}$	$1.90 \cdot 10^{-5}$	0	2600	36407	36500	2800	36000	37000	37000
CB127	5	$2.48 \cdot 10^{-4}$	$1.31 \cdot 10^{-5}$	0	2800	39892	53000	3000	40000	53000	53000
CB128	6	$1.07 \cdot 10^{-4}$	$1.66 \cdot 10^{-5}$	0	5800	76369	41667	2000	76000	42000	42000
CB129	6	$1.03 \cdot 10^{-4}$	$1.66 \cdot 10^{-5}$	0	6500	84343	41667	2300	84000	42000	42000
CB130	6	$1.03 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	6500	87725	58333	2300	88000	58333	58333
CB131	6	$1.40 \cdot 10^{-4}$	$1.66 \cdot 10^{-5}$	0	5100	68158	41667	2800	68000	42000	42000
CB132	6	$1.40 \cdot 10^{-4}$	$1.66 \cdot 10^{-5}$	0	5100	68158	41667	2800	68000	42000	42000
CB133	6	$1.00 \cdot 10^{-4}$	$9.24 \cdot 10^{-6}$	0	7200	98540	75000	2500	99000	75000	75000
CB134	6	$1.35 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	5800	79132	58333	2000	79000	58000	58000
CB135	6	$1.35 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	5800	79132	58333	2000	79000	58000	58000
CB136	6	$2.04 \cdot 10^{-4}$	$1.66 \cdot 10^{-5}$	0	4400	59696	41667	2500	60000	42000	42000
CB137	6	$1.07 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	5800	79132	58333	2000	79000	58000	58000
CB138	6	$1.07 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	5800	79132	58333	2000	79000	58000	58000
CB139	6	$1.46 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	4400	61371	58333	2500	61000	58000	58000
CB140	6	$1.46 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	4400	61371	58333	2500	61000	58000	58000
CB141	6	$1.03 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	6500	87725	58333	2300	88000	58000	58000
CB142	6	$1.40 \cdot 10^{-4}$	$2.77 \cdot 10^{-5}$	0	5100	63538	25000	1800	64000	25000	25000
CB143	6	$1.40 \cdot 10^{-4}$	$1.66 \cdot 10^{-5}$	0	5100	68158	41667	1800	88000	42000	42000
CB144	6	$1.40 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	5100	70349	58333	1800	70000	58000	58000
CB145	6	$2.17 \cdot 10^{-4}$	$1.66 \cdot 10^{-5}$	0	3700	50974	41667	1300	51000	42000	42000
CB146	6	$1.03 \cdot 10^{-4}$	$9.24 \cdot 10^{-6}$	0	6500	89724	75000	2300	90000	75000	75000
CB147	6	$1.40 \cdot 10^{-4}$	$1.19 \cdot 10^{-5}$	0	5100	70349	58333	1800	70000	58000	58000
CB148	6	$1.40 \cdot 10^{-4}$	$9.24 \cdot 10^{-6}$	0	5100	71629	75000	1800	72000	75000	75000

Table 5. Continued

		degradation rates/h^{-1}			estimation results/h			values for FATEMOD/h			
code	nCl	Kp/air	Kp/solids	Kh/water	HL(1)	HL(2)	HL(3,4)	HL_{25}(1)	HL_{25}(2)	HL_{25}(3)	HL_{25}(4)
CB149	6	$1.40\cdot10^{-4}$	$1.19\cdot10^{-5}$	0	5100	70349	58333	1800	70000	58000	58000
CB150	6	$2.17\cdot10^{-4}$	$1.19\cdot10^{-5}$	0	3700	52190	58333	1300	52000	58000	58000
CB151	6	$1.35\cdot10^{-4}$	$1.19\cdot10^{-5}$	0	5800	79132	58333	2000	79000	58000	58000
CB152	6	$2.04\cdot10^{-4}$	$1.66\cdot10^{-5}$	0	4400	59696	41667	1500	60000	42000	42000
CB153	6	$1.07\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	5800	80755	75000	2000	81000	75000	75000
CB154	6	$1.46\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	4400	62343	75000	1500	62000	75000	75000
CB155	6	$2.31\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	3000	43269	75000	1000	43000	75000	75000
CB156	6	$8.40\cdot10^{-5}$	$1.19\cdot10^{-5}$	0	7200	96134	58333	2500	96000	58000	58000
CB157	6	$8.40\cdot10^{-5}$	$1.19\cdot10^{-5}$	0	7200	96134	58333	2500	96000	58000	58000
CB158	6	$1.07\cdot10^{-4}$	$1.19\cdot10^{-5}$	0	5800	79132	58333	2000	79000	58000	58000
CB159	6	$8.20\cdot10^{-5}$	$9.24\cdot10^{-6}$	0	7900	107207	75000	2800	110000	75000	75000
CB160	6	$1.03\cdot10^{-4}$	$1.66\cdot10^{-5}$	0	6500	84343	41667	2300	84000	42000	42000
CB161	6	$1.03\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	6500	89724	75000	2300	90000	75000	75000
CB162	6	$8.20\cdot10^{-5}$	$9.24\cdot10^{-6}$	0	7900	107207	75000	2800	110000	75000	75000
CB163	6	$1.03\cdot10^{-4}$	$1.19\cdot10^{-5}$	0	6500	87725	58333	2300	89000	58333	58333
CB164	6	$1.03\cdot10^{-4}$	$1.19\cdot10^{-5}$	0	6500	87725	58333	2300	88000	58333	58333
CB165	6	$1.00\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	7200	98540	75000	2500	99000	75000	75000
CB166	6	$1.07\cdot10^{-4}$	$1.66\cdot10^{-5}$	0	5800	76369	41667	2000	76000	42000	42000
CB167	6	$8.40\cdot10^{-5}$	$9.24\cdot10^{-6}$	0	7200	98540	75000	2500	99000	75000	75000
CB168	6	$1.07\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	5800	80755	75000	2000	81000	75000	75000
CB169	6	$6.93\cdot10^{-5}$	$9.24\cdot10^{-6}$	0	8600	115730	75000	3000	120000	75000	75000
CB170	7	$9.24\cdot10^{-5}$	$9.24\cdot10^{-6}$	0	6500	89724	75000	7900	90000	75000	75000
CB171	7	$1.32\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	4750	67006	75000	5800	67000	75000	75000
CB172	7	$8.15\cdot10^{-5}$	$5.78\cdot10^{-6}$	0	7375	104220	120000	8900	100000	120000	120000
CB173	7	$1.11\cdot10^{-4}$	$2.31\cdot10^{-5}$	0	5625	71053	30000	6800	71000	30000	30000
CB174	7	$1.11\cdot10^{-4}$	$2.31\cdot10^{-5}$	0	5625	71053	30000	6800	71000	30000	30000
CB175	7	$1.11\cdot10^{-4}$	$5.78\cdot10^{-6}$	0	5625	80597	120000	6800	81000	120000	120000
CB176	7	$1.73\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	3875	55269	75000	4700	55000	75000	75000
CB177	7	$1.11\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	5625	78488	75000	6800	78000	75000	75000
CB178	7	$9.56\cdot10^{-5}$	$5.78\cdot10^{-6}$	0	6500	92490	120000	7900	92000	120000	120000
CB179	7	$1.39\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	4750	67006	75000	5800	67000	75000	75000
CB180	7	$9.24\cdot10^{-5}$	$5.78\cdot10^{-6}$	0	6500	92490	120000	7900	92000	120000	120000
CB181	7	$1.32\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	4750	67006	75000	5800	67000	75000	75000
CB182	7	$1.32\cdot10^{-4}$	$5.78\cdot10^{-6}$	0	4750	68537	120000	5800	68000	120000	120000
CB183	7	$1.32\cdot10^{-4}$	$5.78\cdot10^{-6}$	0	4750	68537	120000	5800	69000	120000	120000
CB184	7	$2.31\cdot10^{-4}$	$5.78\cdot10^{-6}$	0	3000	43902	120000	3600	44000	120000	120000
CB185	7	$1.73\cdot10^{-4}$	$9.24\cdot10^{-6}$	0	3875	55269	75000	4700	55000	75000	75000
CB186	7	$1.73\cdot10^{-4}$	$2.31\cdot10^{-5}$	0	3875	51476	30000	4700	51000	30000	30000
CB187	7	$1.11\cdot10^{-4}$	$5.78\cdot10^{-6}$	0	5625	80597	120000	6800	81000	120000	120000
CB188	7	$1.73\cdot10^{-4}$	$5.78\cdot10^{-6}$	0	3875	56307	120000	4700	56000	120000	120000
CB189	7	$7.11\cdot10^{-5}$	$5.78\cdot10^{-6}$	0	8250	115789	120000	10000	120000	120000	120000
CB190	7	$9.24\cdot10^{-5}$	$9.24\cdot10^{-6}$	0	6500	89724	75000	7900	90000	75000	75000
CB191	7	$9.24\cdot10^{-5}$	$5.78\cdot10^{-6}$	0	6500	92490	120000	7900	92000	120000	120000
CB192	7	$8.15\cdot10^{-5}$	$5.78\cdot10^{-6}$	0	7375	104220	120000	8900	100000	120000	120000
CB193	7	$8.15\cdot10^{-5}$	$5.78\cdot10^{-6}$	0	7375	104220	120000	8900	100000	120000	120000
CB194	8	$2.31\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	26000	335484	160000	30000	340000	160000	160000
CB195	8	$3.47\cdot10^{-5}$	$1.73\cdot10^{-5}$	0	18000	186207	40000	21000	190000	40000	40000
CB196	8	$3.47\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	18000	242697	160000	21000	240000	160000	160000
CB197	8	$6.93\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	10000	141176	160000	12000	140000	160000	160000
CB198	8	$3.47\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	20000	266667	160000	23000	270000	160000	160000
CB199	8	$6.93\cdot10^{-5}$	$1.73\cdot10^{-5}$	0	12000	138462	40000	14000	140000	40000	40000
CB200	8	$6.93\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	12000	167442	160000	14000	170000	160000	160000
CB201	8	$3.47\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	20000	266667	160000	23000	270000	160000	160000
CB202	8	$6.93\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	14000	193103	160000	16000	190000	160000	160000
CB203	8	$3.47\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	18000	242697	160000	21000	240000	160000	160000
CB204	8	$6.93\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	10000	141176	160000	12000	140000	160000	160000
CB205	8	$2.31\cdot10^{-5}$	$4.33\cdot10^{-6}$	0	26000	335484	160000	30000	340000	160000	160000
CB206	9	$2.77\cdot10^{-5}$	$3.85\cdot10^{-6}$	0	28000	363462	180000	30000	360000	180000	180000
CB207	9	$4.62\cdot10^{-5}$	$3.85\cdot10^{-6}$	0	10000	142105	180000	11000	140000	180000	180000
CB208	9	$3.96\cdot10^{-5}$	$3.85\cdot10^{-6}$	0	11000	155497	180000	12000	160000	180000	180000
CB209	10	$2.31\cdot10^{-5}$	$3.47\cdot10^{-6}$	0	50000	600000	200000	50000	590000	200000	200000

[a] For definition of the variables and estimation of their values see Abbreviations section, Table 1, and eqs 35 to 40 in the end of the Section 2 (Materials and Methods).

fusion values is illustrated in Figure 1. The small deviations of predicted and measured ΔS_f values and their significant linear correlation ($R = 0.780$, $p = 1.88\cdot10^{-9}$) clearly suggest that the present SMLR-predicted entropy of fusion values of PCBs are quite suitable for model use. By using ΔS_{fpred} values (Table 2), conversions (eqs 8 to 10) and WATSOLU results (eqs 12 and 13) will be improved related to use of the same default melting entropy for all PCBs.

Temperature Corrections to Physical Properties. In Table 4, temperature coefficients for the properties, liquid state vapor pressure (log P_L), solubility in water (log S_W), and octanol−water partition (log K_{OW}) are listed together with reference values log P_{L25}, log S_{W25}, and log K_{OW25}. Temperature coefficients of the volatility (Henry's law constant k_H as log $k_H = Ah - Bh/T$) determined by eqs 24 and 25 are also listed in Table 4. The k_H value of the modeled substance is computed automatically in each run of FATEMOD by P_L/S_W.

Validation of the coefficients for the logarithms of P_L, S_W, K_{OW}, and k_H in Table 4 was done by comparisons of their model-

Table 6. WATSOLU Tests for Influence of (10 and 20) °C Uncertainty in the Estimated[15] Values of Mp

	WATSOLU input data					WATSOLU test results			deviation % from first Mp		
code	Mp/°C	ΔS_f	KaccW	V_b	DB	As	Bs	S_{W25}/mmol·m^{-3}	in S_{W25}	in As	in Bs
CB6	**36**	50.35	38	189.8	18.12	−0.187	831.2	1.0600	0.0	0.00	0.00
CB6	46	50.35	38	189.8	18.12	−0.187	857.5	0.8640	18.5	0.00	−3.16
CB6	56	50.35	38	189.8	18.12	−0.187	883.8	0.7060	33.4	0.00	−6.33
CB13	**51**	56.07	38	189.8	18.12	0.112	967.5	0.7360	0.0	0.00	0.00
CB13	61	56.07	38	189.8	18.12	0.112	996.8	0.5870	20.2	0.00	−3.03
CB13	71	56.07	38	189.8	18.12	0.112	1026.1	0.4680	36.4	0.00	−6.06
CB17	**35**	53.58	33	204.7	17.68	−0.571	892.6	0.2720	0.0	0.00	0.00
CB17	45	53.58	33	204.7	17.68	−0.571	920.5	0.2190	19.5	0.00	−3.13
CB17	55	53.60	33	204.7	17.68	−0.571	948.5	0.1770	34.9	0.00	−6.26
CB27	**46**	53.88	33	204.7	17.68	−0.556	928.3	0.2140	0.0	0.00	0.00
CB27	56	53.88	33	204.7	17.68	−0.556	956.5	0.1720	19.6	0.00	−3.04
CB27	66	53.88	33	204.7	17.68	−0.556	984.6	0.1390	35.0	0.00	−6.06
CB51	**45**	57.41	30	219.6	17.30	−0.923	998.3	0.0536	0.0	0.00	0.00
CB51	55	57.41	30	219.6	17.30	−0.923	1028.3	0.0425	20.7	0.00	−3.01
CB51	65	57.41	30	219.6	17.30	−0.923	1058.2	0.0337	37.1	0.00	−6.00
CB59	**42**	53.47	30	219.6	18.08	−1.129	905.5	0.0683	0.0	0.00	0.00
CB59	52	53.47	30	219.6	18.08	−1.129	933.4	0.0550	19.5	0.00	−3.08
CB59	62	53.47	30	219.6	18.08	−1.129	961.3	0.0444	35.0	0.00	−6.16

Table 7. Example of Output from the SMLR Regression Equation for Determination of the Entropy of Fusion (ΔS_f) Values of all PCBs from Measured Values of 41 Congeners[12–16]

		F to enter 0.05	
model summary		F to remove 0.10	
R	*R* square	AdjRSq	StdEEst
0.327	0.107	0.084	8.804
0.636	0.405	0.373	7.283
0.780	0.608	0.576	5.988

predictors: (constant), DB
predictors: (constant), DB, *L*
predictors: (constant), DB, *L*, *E*
Dependent Variable: measured ΔS_f

ANOVA	SumSq	df	mean Sq	*F*	sig.
regression	362	1	362	4.67	$3.68\cdot10^{-2}$
residual	3023	39	78		
total	3385	40			
regression	1369	2	685	12.91	$5.27\cdot10^{-5}$
residual	2015	38	53		
total	3385	40			
regression	2058	3	686	19.13	$1.17\cdot10^{-7}$
residual	1327	37	36		
total	3385	40			

predictors (constant), DB
predictors (constant), DB, *L*
predictors (constant), DB, *L*, *E*
Dependent Variable: measured ΔS_f, Std Error Pred Value: 0.536

coefficients (a)	UnstCoeff B	std. error	StCoeff β	*t*	sig.
(constant)	155.15	44.87		3.46	$1.33\cdot10^{-3}$
DB	−5.42	2.51	−0.327	−2.16	$3.68\cdot10^{-2}$
(constant)	222.62	40.22		5.54	$2.47\cdot10^{-6}$
DB	−11.59	2.51	−0.700	−4.62	$4.36\cdot10^{-5}$
L	4.94	1.13	0.661	4.36	$9.64\cdot10^{-5}$
(constant)	168.97	35.26		4.79	$2.68\cdot10^{-5}$
DB	**−7.94**	**2.23**	**−0.480**	**−3.57**	$\mathbf{1.02\cdot10^{-3}}$
L	**18.37**	**3.20**	**2.457**	**5.74**	$\mathbf{1.43\cdot10^{-6}}$
E	**−65.05**	**14.84**	**−1.981**	**−4.38**	$\mathbf{9.31\cdot10^{-5}}$

based values with their independent experimental and QSPR-derived values.

Log P_L Temperature Correction Coefficients (Apl and Bpl by VPLEST Calculation). These were validated by comparison of the input values[29] of log P_{L25} to VPLEST with those calculated from GC-based coefficients[36] (Figure 2). The two-tailed Pearson correlation coefficient was $R = 0.986$ with $p = 8\cdot10^{-140}$ for $N = 180$. Secondly, the temperature dependence of P_L from (0 to 30) °C curves from VPLEST and from GC-based estimation[36] were compared (Figure 3). Comparisons validate VPLEST as a convenient QSPR program for P_L determination with reasonable accuracy for modeling the environmental fate of PCBs at various environmental temperatures. Quantitative values in the VPLEST algorithm are specified by input P_L[29] and curvature on K_F from structure.[28] Evidently, P_L values from VPLEST and ref 36 are near enough for all PCB congeners to allow either set to be safely used in modeling. While VPLEST produced data for all 209 PCB congeners, it is recommended as useful material to compute internally consistent values, e.g., for the partition coefficient K_{AW} (volatility, dimensionless k_H).

Water Solubility. Estimations of the water solubility of PCB congeners have been done in many laboratories, but they have mainly been limited to values at 25 °C or "room temperature". Our aim was to study a Clausius−Clapeyron type of equation (eq 11) for S_W over the environmental temperature range (from (−2 to +30) °C).[3,7,8] Some temperature dependence estimations of solubility of PCBs have been done,[15,38,41] but only for a too limited number of congeners for proper validation. However, wide validation between independently evaluated log S_{W25} values was feasible. We compared our WATSOLU-derived values with eight other sets with correlation and principal components analyses (PCA; Table 8 and Figure 4). These eight independent S_{W25} value sets were obtained from the literature (refs 15, 22, 39 to 41, 47, 85, and 88). The sets consisted of 58 to 209 congeners. Figure 4 shows variable loadings PC1loa and PC2loa as arrows in the PCA diagram. The nearest arrows indicate the closest similarity of PCB patterns. The WATSOLU arrow is located nearest to the experimental values cited in ref 39, and the next nearest are patterns from three sets of QSPR predicted values.[39,47,85,88] This result indicates that the algorithm of WATSOLU is successful for log S_{W25} values of all PCB congeners.

Temperature Correction Coefficients of log K_{OW}. These have been given in very few reports[7,9,46,87]—only one (ref 46) contained experimental temperature dependence data for three PCB congeners. No literature data were found about the temperature dependence of K_{OW} for major PCBs with nCl > 4. Validation was possible with literature sets of K_{OW25} only. We found nine sets of log K_{OW25} values[21,22,39,41,47,48,84,85,88] comparable in correlation by "pair-wise exclusion of missing values" (*N* from 16 to 209 pairs). Five sets[21,22,41,47,88] and TDLKOW were useful for PCA by allowed "listwise exclusion" (*N* from 153 to 209; Table 9 and Figure 5). Predicted values ($N = 154$) of Ruelle[21] and QSPR values ($N = 209$) of Abraham and Al-Hussaini[22] showed the most similar patterns with the TDLKOW

Table 8. Correlations and PCA of the log S_{W25} Sets

		(39/cited)	(39)	(47, 88)	(22)	(41)	(40)	(15)	(85)
two-tailed Pearson correl.	Ref.->	EXPER	RuelleKess	HawkerEq	AbrAlHus	BrodBall	Patil	AbrYalkows	PuriETal
WATSOLU (this work)	*R*	0.967	0.982	0.982	0.940	0.879	0.941	0.933	0.981
	p	$1.21\cdot10^{-44}$	$3.24\cdot10^{-46}$	$3.24\cdot10^{-46}$	$1.50\cdot10^{-98}$	$1.12\cdot10^{-50}$	$9.31\cdot10^{-67}$	$1.48\cdot10^{-93}$	$1.19\cdot10^{-41}$
	N	74	63	63	209	154	140	209	58
EXPER cited in 38	*R*		0.967	0.967	0.930	0.872	0.915	0.948	0.959
	p		$3.46\cdot10^{-37}$	$3.46\cdot10^{-37}$	$5.46\cdot10^{-33}$	$1.57\cdot10^{-21}$	$1.62\cdot10^{-20}$	$1.18\cdot10^{-37}$	$3.02\cdot10^{-32}$
	N		62	62	74	66	50	74	58

Total Variance Explained

	Initial Eigenvalues		
component	total	% of var	cum %
1	8.62	**95.76**	95.76
2	0.18	**2.03**	97.78
3	0.08	0.86	98.65
4	0.06	0.66	99.31
5	0.04	0.46	99.77
6	0.01	0.17	99.94

Extraction Method: Principal Component Analysis

ref	variable loadings:	PC1loa	PC2loa
(47, 88)	Hawker Equation	0.991	−0.070
(39)	Ruelle, Kessering	0.991	−0.070
(85)	Puri et al.	0.990	−0.072
(22)	Abraham, Al-Husssaini	0.989	0.081
rhis work	**WATSOLU**	0.987	−0.128
(40)	Patil	0.987	0.097
(15)	Abramowitz, Yalkowsky	0.974	−0.008
(39/cited)	**EXPER**	0.960	−0.151
(41)	Brodsky, Ballschmiter	0.935	0.335

Table 9. Correlations and PCA of the log K_{OW25} Sets

		(21/cited)	(21)	(47, 88)	(22)	(41)	(48)	(84)	(84)
two-tailed Pearson correl.	Ref->	RuelleExper	RuellePred	HawConn	AbrAlHuss	BrodBall	Kong et al.	Li, LDV	Li, FAV
TDLKOW	*R*	0.931	0.993	0.925	0.989	0.908	0.962	0.974	0.978
This work	*p*	$2.96\cdot10^{-68}$	$6.72\cdot10^{-141}$	$7.65\cdot10^{-89}$	$1.05\cdot10^{-174}$	$7.31\cdot10^{-59}$	$3.54\cdot10^{-12}$	$1.97\cdot10^{-10}$	$5.62\cdot10^{-11}$
	N	154	154	209	209	153	21	16	16

Total Variance Explained

	initial eigenvalues		
component	total	% of var.	cum. %
1	5.7681	96.14	96.14
2	0.1458	2.43	98.56
3	0.0586	0.98	99.54
4	0.0174	0.29	99.83
5	0.0089	0.15	99.98
6	0.0012	0.02	100

Extraction Method: Principal Components Analysis

reports included		loading matrix	
ref		PC1loa	PC2loa
this work	**TDLKOW**	0.981	-0.178
(21/cited)	**Ruelle Experim.**	0.971	0.123
(21)	**Ruelle Predicted**	0.987	-0.152
(47, 88)	**Hawker, Connell**	0.984	0.098
(22)	**Abraham, Al-Hussaini**	0.992	-0.115
(41)	**Brodsky, Ballschmiter**	0.967	0.230

Table 10. Mean Concentrations and YSM in Salmon[90,91] [a]

code -->	CB77	CB126	CB169	CDF77	CDF94	CDF114	TotPCB	
year	$ng\cdot g^{-1}$ lw	$ng\cdot g^{-1}$ lw	$ng\cdot g^{-1}$ lw	$ng\cdot g^{-1}$ lw	$ng\cdot g^{-1}$ lw	$ng\cdot g^{-1}$ lw	$\mu g\cdot g^{-1}$ lw	
1988	22.20	1.77	0.00	0.030	0.0000	0.000	6.00	
1989	11.80	1.46	0.55	0.175	0.0000	0.170	6.45	
1990	5.70	2.84	0.34	0.158	0.0206	0.145	3.45	
1991	14.40	4.85	0.79	0.140	0.0333	0.287	4.77	
1992	20.39	3.97	0.40	0.143	0.0208	0.167	2.54	
N	40	40	40	40	40	40	73	
Code -->	CB77	CB126	CB169	CDF77	CDF94	CDF114	TotPCB	
FTEF/WHO	0.0001	0.005	0.00005	0.05	0.05	0.5	< 0.000005	YSM
FTEQ	$pg\cdot g^{-1}$ lw	$pg\cdot g^{-1}$ lw	$pg\cdot g^{-1}$ lw	$pg\cdot g^{-1}$ lw	$pg\cdot g^{-1}$ lw	$pg\cdot g^{-1}$ lw	$pg\cdot g^{-1}$ lw	%
1988	2.22	8.85	0.00	1.50	0.00	0.00	0.030	3.30
1989	1.18	7.30	0.03	8.75	0.00	85.00	0.032	24.00
1990	0.57	14.20	0.02	7.90	1.03	72.50	0.017	2.07
1991	1.44	24.25	0.04	7.00	1.67	143.50	0.024	26.73
1992	2.04	19.85	0.02	7.15	1.04	83.50	0.013	75.29
trend[90]	nonsign	increase $p < 0.001$	nonsign	nonsign	increase $p < 0.01$	increase $p < 0.05$	decrease $p < 0.001$	increase $p < 0.001$

[a] Toxic equivalents to fish: FTEQs from FTEFs of WHO.[92]

results. Although the slope of the log−linear temperature equation by TDLKOW was small (Bow from −54.5 to 174.9), the temperature dependence of log K_{OW} was clear and varied as negative or positive for different PCB congeners (see Table 4). While log K_{OW25} patterns from TDLKOW and five other independent patterns of a large number of congeners at 25 °C were quite similar (Figure 5), we suggest to keep the present TDLKOW derived values in use. While the observed temperature dependence of K_{OW} of PCBs is low, use of the widely established values at 25 °C or log K_{OW} from our Aow and Bow values by eq 16 cannot cause any significant differences to the PEC predictions by the model.

Table 11. Sensitivity Analysis: For Emission to Baltic Proper at 10 °C for CB156 Emission 100 g·h^{-1} Modeled by FATEMOD with Database (Tables 4 and 5) Values of $HL_{25}(2)$ and Bs and Their Values Raised or Lowered 50 % and Raised 100 %

	$HL(2)_{25}$	added	FATEMOD	modeled	devA(1,2,3)-A0	devTests A(i)	relative error ratios	
Test	h	%	$HL(2)_{10}$/h	conc./ng·L^{-1}	ng·L^{-1}	$HL(2)_{10}$ case %	case	ratio
A0	96000	0	235700	0.0132604		0.00		
A1	144000	50	352139	0.0132680	0.0000076	0.057	B1/A1	130.6
A2	192000	100	469519	0.0132723	0.0000119	0.090	B2/A2	84.4
A3	48000	−50	117379	0.0132366	−0.0000238	−0.179	B3/A3	131.9
		added	FATEMOD	modeled	devB(1,2,3)-B0	devTests B(i)		
Test	Bs	%	S_{W10}/mol·m^{-3}	conc/ng·L^{-1}	ng·L^{-1}	S_{W10} case %		
B0	1495	0	$1.14 \cdot 10^{-6}$	0.014260			mean	115.6
B1	2242.5	50	$2.61 \cdot 10^{-9}$	0.013193	0.001067	7.48		
B2	2990	100	$5.99 \cdot 10^{-12}$	0.013180	0.001080	7.57		
B3	747.5	−50	$4.98 \cdot 10^{-4}$	0.017636	−0.003376	−23.67		

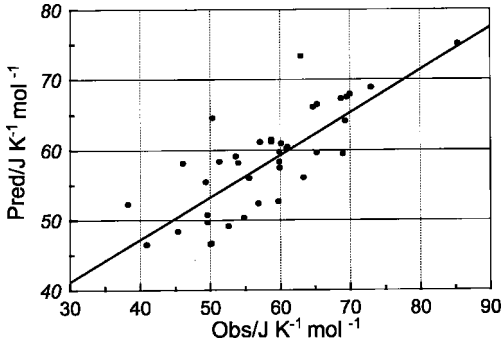

Figure 1. SMLR-predicted ΔS_f values plotted against 41 measured (Obs) values from the literature.[13–16]

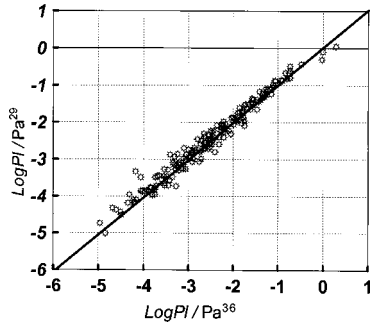

Figure 2. log P_{L25}/Pa values of all PCBs estimated by Öberg with 260 molecular descriptors,[29] which were input values for VPLEST (y-axis), compared to GC-based values of Falconer and Bidleman at the x-axis.[36] The two-tailed Pearson correlation coefficient between log P_{L25} values (in refs 36 and 29) was $R = 0.986$ and $p = 8 \cdot 10^{-140}$ with $N = 180$.

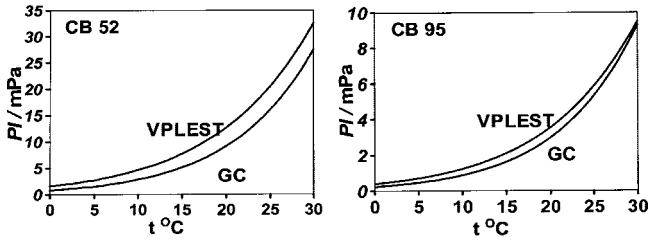

Figure 3. Comparison of temperature dependence of the liquid state vapor pressures P_L of two PCB congeners by two independent methods: VPLEST computing (this work) and determination on GC basis by Falconer and Bidleman.[36]

Henry's Law Constant. The ratio $k_H = P_L/S_W$ was used for PCBs. This needs no more validation for environmental fate modeling after P_L and S_W estimates were shown to be satisfactory. For a visual example of temperature dependences of P_L, S_W, k_H, and K_{OW}, curves of physical behavior of CB126 are illustrated in Figure 6. Volatility H (= k_H, Henry's law constant)

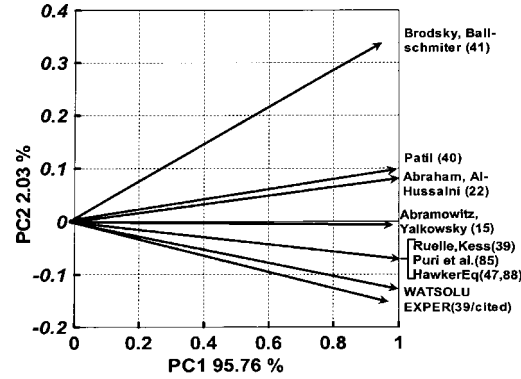

Figure 4. PCA loadings as arrows from nine sets of log S_{W25} values of PCBs. The patterns are most equal between the sets having arrows close to each other. Correlations and PCA results are shown in Table 8.

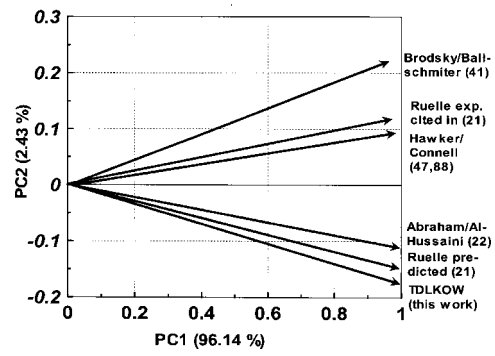

Figure 5. PCA loadings as arrows from six sets of log K_{OW25} values of PCBs. The patterns are most equal between the sets having arrows close to each other. Correlations and PCA results are shown in Table 9.

rose most steeply with temperature. S_W and P_L also rose with T, but K_{OW} decreased slightly by increasing T. Our K_{OW} trials have shown both effects of T (for musks).[8]

Degradation Rates and Half-Lives of PCBs. Episode of YSM in Baltic Salmon. Because the highly chlorinated PCBs are extremely persistent in the environment, validation of their half-life estimates by direct follow-up analyses is not practical. A feasible validation can be achieved indirectly from case studies where both analyses and modeling of environmental fate are used. One example of such a case was the episodic yolk sac mortality (YSM) of the fry among some Baltic salmon populations initially observed in 1974.[89] We performed a five-year study from 1988 to 1992 on Simojoki River (flowing to the Bay of Bothnia in Finland) salmon and their fry.[90,91] Trends of annual means of the analyzed total and coplanar PCBs (CB77, CB126, and CB169) and toxic tetra- and pentachloro dibenzofurans (CDF77, CDF94, and CDF114) in salmon lipid compared

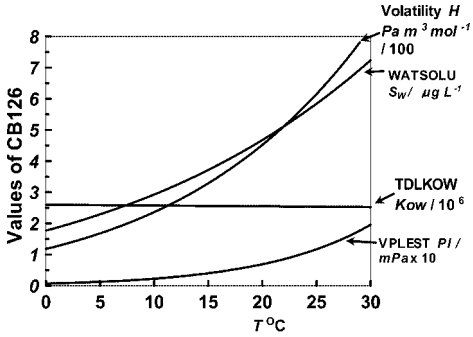

Figure 6. Temperature dependences of four physical properties of CB126 from (0 to +30) °C estimated by Clausius−Clapeyron type equations (4, 11, 16, and 23) from the temperature dependence coefficients for the FATEMOD database (Table 4).

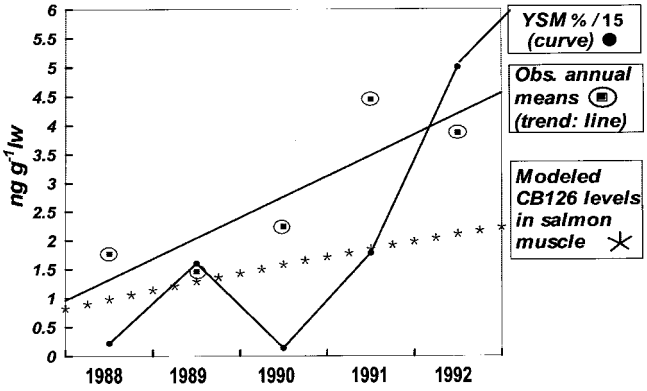

Figure 7. Trends in Simojoki River salmon: YSM (circles and curve) of juveniles of Simojoki River salmon.[90,91] Observed annual means CB126 in lipid of the mother salmon[90,91] (rounded filled squares and trend line). Modeled (FATEMOD and consecutive reactions kinetics[101] in this work) levels in lipid including calculated BAF of truly dissolved POPs in water.[102] See Table 10 for numeric values of YSM and annual CB126 means.

to the YSM are presented in Table 10. Figure 7 illustrates the observed and modeled levels of the most toxic CB126 compared to YSM. The major toxicants causing YSM appeared to be compounds CB126 and 2,3,4,7,8-PeCDF (CDF114). Similar episodes in fish populations were reproduced in the laboratory on juvenile fish[93,94] and on rats[95] with exposures to 2,3,7,8-tetra-CDD ("dioxin") and related compounds. Juvenile fish mortality was established to be caused from thiamine (vitamin) deficiency.[95–98] We believe that exposure to dioxin-like toxicants caused low thiamine levels in the body of female salmon and, consequently, to their eggs. When residual thiamine was fully consumed, the yolk-sac juvenile died from convulsions (like humans in "beri-beri" disease). This phenomenon was predictable by analyses of thiamine contents in fish and eggs. YSM was cured by adding thiamine to a bath of the yolk sac juveniles or injecting it into the fry.[97]

Our analyses during the years 1988 to 1992 of Simojoki River salmon produced a trend of total PCBs (as Clophen A60) to be significantly decreasing. In contrast, trends of YSM, 2,3,4,7,8-PeCDF, and CB126 were significantly increasing (Table 10). To explain these trends, FATEMOD modeling followed by photolysis kinetics and bioaccumulation estimates were applied. The Simojoki salmon were feeding over winter and spring in the southern part of the Baltic Sea, most intensively in the 40 m high-surface water column at Baltic Proper. Some surveys of PCBs in Baltic Sea water solution and suspension were known from Schulz-Bull et al.[99,100] The PCB congener patterns in these studies deviated from those of PCB formulations stored in darkness. In the latter, highly chlorinated mono-*ortho*-chlorine

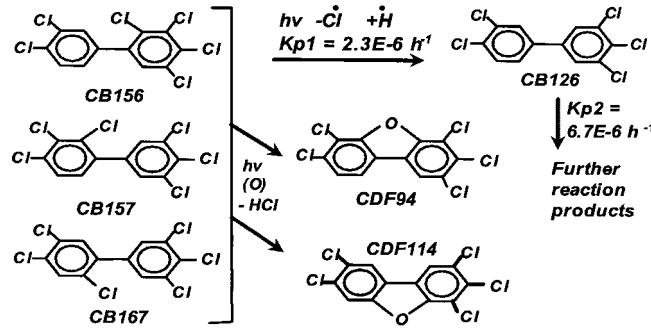

Figure 8. Possible formation of the toxic CB126 from three mono-ortho chlorinated hexa-CB's in assumed leakage of PCB oil into Baltic Proper to explain the increasing trends of CB126 levels and YSM. Kp1 is the sun irradiation induced photodegradation rate in water at 10 °C—nearly equal in size for CBs 156, 157, and 167. It is calculated from Kp/air value (Table 5) using Kp/15 and temperature correction via eq 32. Kp2 for the consecutive reaction series[101] is approximated from the sunshine photolysis rate and the less dominating biodegradation rate by eq 28 of intermediate CB126. The observed increasing trends of CDF94 and CDF114 could be assumed to take place by an oxidative photolysis from mono-ortho hexa-CBs 156, 157, and 167. However, mechanism and rate of these reactions are yet unknown.

substituted congeners, e.g., CB156, CB157, and CB167, were stable. However, in air or water columns of the environment, sunlight irradiation could cause their fast degradation to CB126 as the primary product (Figure 8). Other products from CB156, CB157, and CB167 could include toxic PeCDFs formed by a direct oxidative metabolism. These observations indicate some leaks of PCB transformer oil into Baltic Proper.

Fish toxic equivalents (FTEQ) calculated from our analysis results of Simojoki salmon (annual means, Table 10) indicated that the most probable pollutants behind YSM were CB126 and 2,3,4,7,8-PeCDF (CDF114). Toxic loads (FTEQ values) were high and the increasing trends very significant for CB126 and CDF114. Also, two other PCBs, 2,3,7,8-TeCDF (CDF83) and 1,2,3,7,8-PeCDF (CDF94), showed increasing but less significant trends in salmon. In contrast, the total PCB trend (Table 10) was very significantly decreasing in Simojoki River salmon during 1988 to 1992 like generally in Baltic biota.[90,91]

Our results about the role of CB126 in the YSM episode of Simojoki River salmon were obtained by modeling using compound properties now evaluated (this work). Firstly, FATEMOD level 3 concentrations in water were modeled from default emissions to Baltic Proper. The fate of the SUM of CB156, 157, and 167 (4000 kg) and CB126 (200 kg) in 1 h to the whole area was first modeled. Then, a kinetic calculation of consecutive reactions[101] from three hexaCB's to CB126 allowed the model to increase the latter in the studied episode time (Figure 8). Bioaccumulation (BAF_{10} = 77 290 000) of CB126 from 10 °C water to "piscivore" salmon was calculated using the statistical model of Voutsas et al.[102] to get modeled annual means in salmon. Results from this model chain were compared to the observed annual mean concentrations in Simojoki River salmon and YSM of their fry[91] (Table 10 and Figure 7). The results of the comparisons support our half-life estimates (Table 5). Also, water concentrations in level 3 (steady state) validated correctness of the compound properties at 10 °C. The most surprising result was an indication of the origin of toxic Te- and PeCDF's from reactions of PCBs in the environment. These CDF congeners have been found to be abundant in environmental samples, especially in Baltic Sea biota,[103] but relatively low in most known emissions.[104]

Sensitivity Analysis of HL(2) and Bs Values of CB156 (Table 11). The $HL_{25}(2)$ (96 000 h; Table 5) value based on the minimum and maximum in each congener group and relative photolysis rates[73–78] of CB156 was taken as the starting half-life value in a test where the influence of added or subtracted relative error of (50 and 100) % was modeled by FATEMOD in Baltic Proper at 10 °C. The resulting concentrations were compared with similarly modeled concentrations with the values (starting from 1495; Table 4) of Bs, the temperature dependence coefficient for water solubility (derived by WATSOLU). The relative error in Bs caused a concentration change 84- to 132-fold related to that in $HL_{25}(2)$ (Table 11). This result indicates that use of rounded approximates as HL values as reference half-lives of reactions of the highly chlorinated biphenyls is well justified due to their negligible sensitivity. But instead, errors in parameters for physical properties can more readily destroy accuracy of fate modeling of these POPs.

4. Conclusions

Parameters for modeling the environmental fate for all PCB congeners were estimated with sufficient accuracy and internal consistency for use in PEC predictions for risk estimations, especially considering the influence of ambient temperature. New effective methods for temperature corrections with automatic algorithms ON LINE for estimation of liquid state vapor pressure (P_L), solubility in water (S_W), volatility (k_H), lipophilicity (K_{OW}), and degradation half-lives (HL(i)) were developed. Preliminary statistical comparisons of these data with previous independent data at 25 °C were successful. However, final validation of their values requires more experimental and theoretical research because only indirectly derived vapor pressure values at different environmental temperatures were available for all PCB congeners for comparisons with the present thermodynamically derived values. According to the available comparisons with literature and independently derived values and analyzed episodes in the environment, the present new data can be used as improved interim tools in the management of hazards from PCB pollution. Parameters evaluated for 209 PCBs in this study can be considered internally consistent. It is not necessary to evaluate more parameters and their temperature dependency. Fugacity models like FATEMOD can be programmed to compute the other values needed to obtain all necessary data for computing PEC values at various temperatures and geographic and weather conditions. Especially, the half-lives of tetra- to decaCBs in the environment are, in general, so long that they cannot be validated accurately. This situation, however, does not make their mass balance modeling unreliable as a predictive tool because the environmental fate of PCBs depends more on their physical properties.

Abbreviations

ANOVA	analysis of variance
CASRN	Chemical Abstract's Service Registry Number
CB	Chlorobiphenyl
CDD	Chlorodibenzo-*p*-dioxin
CDF	Chlorodibenzofuran
DSC	differential scanning calorimeter
ESF	European Science Foundation
FTEF	fish toxic equivalent factor
FTEQ	toxic equivalent to fish
GC	gas chromatography
MD	molecular descriptor
MOD	mobile order and disorder thermodynamics
POP	persistent organic pollutant
QSAR	quantitative structure−activity relationship
QSPR	quantitative structure−property relationship
R	overall correlation
RP-HPLC	reversed phase - high performance liquid chromatography
SE	standard error
SMLR	stepwise multiple linear regression
YSM	yolk sac mortality
WHO	World Health Organization

***Symbol*/Unit**	**Explanation**
vAcc(i)	number of active proton acceptor sites
B	hydrogen bond basicity
BAF_{10}	bioaccumulation factor at 10°C
boh	coefficient for primary, secondary, or tertiary OH (1,2 or 2.9, respectively)
CN	square root of the number of chlorine atoms
DB/MPa$^{1/2}$	solubility parameter, DB = SUM(Fdi)/Vb
vDon(i)	number of active proton donating sites
μ/D	Dipole moment
E/dm^3·mol^{-1}/10	excess molar refraction
F_{di}	dispersion component of the molar attraction (from ref 20)
ΔG_V/J·mol^{-1}	free enthalpy of vaporization or Gibbs function
k_H/Pa·m^3·mol^{-1}	volatility log k_H = Ah − Bh/T (or $k_H = P_L/S_W$): = Henry's law constant
HL(i)/h	half-life for reaction in compartments Air(i = 1), Water(2), Soil/Plants(3), and Sediment(4)
ΔH_f/J·mol^{-1}	enthalpy of fusion
IP/eV	ionization potential; polarizabiliy
KaccO(i)	stability constants for proton acceptor groups in *n*-octanol
KaccW(i)	stability constants for proton acceptor groups in water
Kb/h^{-1}	biodegradation rate
KdonO(i)	stability constants for proton donator groups in *n*-octanol
KDonW(i)	stability constants for proton donator groups in water
Kh/h^{-1}	hydrolysis rate
K_{ow}	lipophility logK_{ow} = Aow − Bow/T (log octanol−water partition coefficient)
Kp/h^{-1}	photodegradation rate
L	log gas to hexadecane partition coefficient at 298 K
MAXO	greatest value of KAccO(i) or KDonO(i) for solute in *n*-octanol
MAXW	greatest value of KAccW(i) or KDonW(i) in water
Mp/°C	melting point in degree Celsius
Nchch	number of −CH=CH− combinations (from 0 to 7)
nCl	number of chlorine atoms (from 1 to 10)
Nm	number of chlorine atoms in meta position (from 0 to 4)
No	number of chlorine atoms in ortho position (from 0 to 4)
Np	number of chlorine atoms in para position (from 0 to 2)
PEC	predicted environmental concentration
Phen	nonsubstituted phenyl ring (−C_6H_5; 0 or 1)
pK_a	−log acid dissociation constant
P_L/Pa	(subcooled) liquid state vapor pressure: log P_L = Apl − Bpl/T

PNEC	predicted no-effect concentration
R/J·K^{-1}·mol^{-1}	gas constant
Ro	threshold risk level to harmful effect: (Ro = PEC/PNEC)
S	solute dipolarity/polarizability
ΔS_f/J·K^{-1}·mol^{-1}	entropy of fusion
ΔS_{fpred}	entropy of fusion from SMLR estimation
S_W/mol·m^{-3}	solubility in water: log S_W = As − Bs/T
T/K	temperature in Kelvin
T_f/K	melting point in Kelvin
TSAplan/10^{-20}m^2	total surface area for planar molecules
V/mol·dm^{-3}/100	McGovan volume
V_b/cm^3·mol^{-1}	liquid state molar volume
WM/g·mol^{-1}	weight of the molecule

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