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Compilation, Evaluation, and Selection of Physical−Chemical Property Data for Organochlorine Pesticides

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Accurate physical−chemical properties (aqueous solubility S_W, octanol−water partition coefficient K_{OW}, vapor pressure P, Henry's law constant H, octanol−air partition coefficient K_{OA}, octanol solubility S_O) and their temperature dependence are of fundamental importance for interpreting and simulating the environmental fate and transport of organochlorine pesticides (OCPs). A complete set of property data for 14 organochlorine chemicals is derived by evaluating, averaging, and regressing all measured values reported in the literature. The 14 chemicals are hexachlorobenzene (HCB), pentachlorobenzene (PeCB), *cis*-chlordane, *trans*-chlordane, 1,1,1-trichloro-2,2-bis-4-chlorophenyl-ethane (*p*,*p*′-DDT) and its metabolites 1,1-dichloro-2,2-bis-4-chlorophenyl-ethene (*p*,*p*′-DDE) and 1,1-dichloro-2,2-bis-4-chlorophenyl-ethylene (*p*,*p*′-DDD), heptachlor and its metabolite heptachlor epoxide, aldrin, dieldrin, endrin, α-endosulfan, and *β*-endosulfan. Properties for each individual chemical are adjusted to ensure thermodynamic consistency. That adjustment is sized according to, and is usually smaller than, the measurement uncertainty. Internal energies of phase transfer ΔU could be derived only for HCB and PeCB. The lack of property measurements as a function of temperature for the other chemicals prevents their ΔU values from being derived.

Introduction

Organochlorine pesticides (OCPs) were extensively used in agriculture from the 1950s to the 1970s. Some have been used longer than others, and some, such as lindane and endosulfan, are still in use. The OCPs comprise a diverse group of chemicals but tend to share certain characteristics and structural features. They typically have an aliphatic or aromatic cyclical structure, which is heavily substituted with chlorines. As a result, most OCPs are sparingly soluble and semivolatile. Early measurements detected OCPs in a wide range of environmental compartments, even in remote regions far from the original site of application.[1,2] Because of their high stability, OCPs can remain unchanged for a long time in the environment. Numerous investigations on OCPs have shown their continued and ubiquitous presence around the world (e.g., refs 3 and 4). Because of this persistence, phase distribution and transport processes tend to play a larger role in controlling their environmental fate and bioaccumulation behavior than for other more readily degradable substances.[5] Phase distribution and transport processes of pollutants in the environment are often quantified by using key physical−chemical properties such as the aqueous solubility S_W, vapor pressure P, octanol−water partition coefficient K_{OW}, Henry's law constant H, octanol−air partition coefficient K_{OA}, and solubility in octanol S_O. Assessment models predicting the fate and behavior of OCPs in the environment require these properties as input parameters.

Several OCPs, including HCB, DDT, chlordane, heptachlor, dieldrin, and endrin, are among the first persistent organic pollutants (POPs) to be subjected to global restrictions in the Stockholm Protocol.[6] That global treaty also allows for the nomination of additional chemicals if they fulfill a number of criteria related to toxicity, bioaccumulation, persistence, and long-range transport potential. Some of these criteria are based on physical−chemical property thresholds, in particular with respect to K_{OW} and vapor pressure. The protocol furthermore allows for the use of models in defining the attributes of candidate substances (e.g., in terms of the long-range transport potential), and physical−chemical properties are key input parameters for such models. Accurate and precise physical−chemical property data for the OCPs are thus required if they are to serve as benchmarks for defining the combination of properties that render a chemical a POP.

Considering that the OCPs are among the first detected and most widely studied organic pollutants, one might expect that their partitioning properties are well established. Indeed, a large number of studies have reported physical−chemical properties for the OCPs over the last several decades, and handbooks of property data compile long lists of property values.[7] However, the reported values often conflict with each other and may even range over several orders of magnitude. Using the water solubility and K_{OW} of *p*,*p*′-DDT and *p*,*p*′-DDE as an example, Pontolillo and Eganhouse[8] painstakingly documented reporting errors, multilevel referencing, and a common lack of information on precision as well as other problems in both original literature sources and property compilations, which are partly responsible for the intimidating degree of inconsistency. Another reason for the problems in identifying the true value of the partitioning properties of OCPs is the difficulty in reliably measuring S_W, H, and K_{OW} of sparingly soluble substances and P, H, and K_{OA} of semivolatile substances.[8]

Beyer et al.[9] suggested that the solution to this dilemma lies in taking advantage of the thermodynamic relationships between the physical−chemical descriptors of an organic chemical. The accuracy of a particular property

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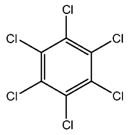
Table 1. Reported and Selected Physical−Chemical Properties for Hexachlorobenzene (HCB)

common name	hexachlorobenzene	t_M/°C	228.0	23
CAS registry no.	118-74-1		229.7	24
formula	C_6Cl_6		228.9	25
MW/g·mol^{-1}	284.8		228.7	26
			228.0	22
			231.9	27
		$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	44.77	23
			50.16	25
			49.73	26
			48.96	22
			47.23	27



Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
−15	0.0000022	0.00053	−3.28	generator column - GC	28	
−5	0.000024	0.0037	−2.43			
10	0.00026	0.023	−1.63			
25	0.0031	0.16	−0.78			
40	0.012	0.40	−0.40			
−30	0.0000026	0.0012	−2.91	gas saturation - GC	29	
−20	0.0000073	0.0022	−2.66			
−10	0.000032	0.0062	−2.20			
0	0.00010	0.013	−1.88			
10	0.00036	0.032	−1.50			
20	0.0011	0.068	−1.17			
30	0.0033	0.15	−0.83			
15	0.00053	0.039	−1.41	gas saturation - GC	30	
25	0.0025	0.13	−0.87			
35	0.0085	0.33	−0.48			
45	0.028	0.80	−0.10			
41.05	0.021	0.66	−0.18	gas saturation - GC	31	
50.16	0.055	1.4	0.13			
60.3	0.17	3.1	0.49			
70.3	0.45	6.6	0.82			
80.3	1.2	13	1.12			
90.4	2.8	25	1.40			
100.25	6.3	46	1.67			
10	0.00080	0.071	−1.15	gas saturation - GC	32	
20	0.0026	0.16	−0.79			
30	0.0081	0.36	−0.44			
40	0.023	0.76	−0.12			
50	0.061	1.5	0.18			
10	0.00028	0.025	−1.61	vapor pressure balance	32	
20	0.0011	0.069	−1.16			
30	0.0039	0.18	−0.76			
40	0.013	0.43	−0.37			
50	0.039	0.97	−0.01			
20	0.00046	0.029	−1.54	relative loss rate	33	
20	0.00074	0.046	−1.34	evaporation rate	34	calcd from the reported equation log(P_S/Torr) = − 5152.1/(T/K) + 12.237 (20 to 60) °C
40	0.0095	0.32	−0.50			
60	0.089	1.7	0.23			
96	3.4	28	1.44	Rodebush manometer	24	calcd from the reported equation log(P_S/mmHg) = −4793.6/(T/K) + 11.4 (96 to 124) °C
105	7.0	47	1.67			
115	15	82	1.91			
124	28	131	2.12			
114.4	133	741	2.87		35	
149.3	667	1993	3.30			
166.4	1333	3049	3.48			
185.7	2666	4616	3.66			
206	5333	7057	3.85			
219	7999	9016	3.96			
235.5		13332	4.12			
258.5		26664	4.43			
283.5		53329	4.73			
309.4		101325	5.01			
−30		0.00024	−3.62	GC - retention time	36	calcd from the reported equation log(P_L/Pa) = −3582/(T/K) + 11.11
0		0.0099	−2.00			
25		0.12	−0.90			
50		1.1	0.03			
75		6.6	0.82			
100		32	1.51			
125		130	2.11			
LDV at 25 °C		0.14	−0.85	linear regression		log(P_L/Pa) = −3530/(T/K) + 10.97
FAV at 25 °C		0.094	−1.03			R^2 = 0.974

Table 1. (Continued)

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
5	0.0000077	0.00082	−3.08	generator column - GC	37	
15	0.000012	0.00091	−3.04			
25	0.000019	0.0010	−3.00			
35	0.000030	0.0012	−2.94			
45	0.000049	0.0014	−2.85			
25	0.000018	0.00093	−3.03	generator column - GC	38	
25	0.000017	0.00087	−3.06	generator column - GC	39	
20	0.000019	0.0012	−2.93	generator column - GC	40	
25	0.000017	0.00092	−3.04	shake flask - UV	41	
23	0.000030	0.0017	−2.77	shake flask - UV	42	
22	0.000014	0.00081	−3.09	shake flask - GC	43	
23		0.0027	−2.57	shake flask - GC	44	
23	0.000018	0.0010	−2.99	shake flask - HPLC	45	
25	0.000018	0.00093	−3.03	SPME-GC	46	
25	0.000021	0.0011	−2.95	radioassay	47	
24	0.00035	0.019	−1.72	nethelometric	48	
23	0.015	0.0029	−2.54	RP-HPLC	49	
23	0.0045	0.00090	−3.05		49	
23	0.00048	0.000096	−4.02		49	
LDV at 25 °C		0.00096	−3.02	log mean of the values at 25 °C		
FAV at 25 °C		0.0014	−2.84			

Henry's Law Constant

t/°C	H/Pa·m^3·mol^{-1}	K_{AW}	log K_{AW}	method	ref	note
14.8	24	0.0099	−2.01	gas stripping - GC	50	
20.1	30	0.012	−1.91			
22.1	47	0.019	−1.72			
24.2	53	0.021	−1.67			
34.8	88	0.034	−1.46			
50.5	217	0.081	−1.09			
20	49	0.020	−1.70	gas stripping - GC	51	
25	172	0.069	−1.16	gas stripping - GC	19	
23	133	0.054	−1.27	gas stripping - GC	20	
23	172	0.070	−1.15			not used, seawater
25	24	0.0096	−2.02	thermodynamic method	52	
26	26	0.011	−1.98	EPICS - GC	53	
46	30	0.011	−1.95			
LDV at 25 °C	52	0.021	−1.68	log mean of the values at (20 to 26) °C		
FAV at 25 °C	65	0.026	−1.58			

Octanol−Water Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
5	5.5×10^5	5.74	shake flask - GC	54	
15	4.0×10^5	5.6			
25	2.9×10^5	5.46			
35	2.0×10^5	5.3			
45	1.5×10^5	5.17			
25	3.2×10^5	5.5	shake flask - GC	55	
25	3.2×10^5	5.5	shake flask - GC	56	
25	2.1×10^5	5.31	shake flask - GC	57	
25	5.4×10^5	5.73	shake flask - GC	58	
25	4.0×10^5	5.6	slow stirring - GC	59	
25	3.2×10^5	5.5	slow stirring - GC	60	
25	3.0×10^5	5.47	generator column - GC	39	
25	3.5×10^5	5.55	dialysis - HPLC	61	without ultrasonic agitation
25	4.0×10^5	5.6			with ultrasonic agitation
23	1.6×10^5	5.2	radioactive analysis	62	
23	2.0×10^5	5.3	GLC analysis		
22	1.0×10^5	5	shake flask - GC	63	
25	1.9×10^6	6.27	RP-HPLC	63	
25	5.6×10^5	5.75	RP-HPLC	64	
25	2.6×10^7	7.42	RP-HPLC	65	
25	8.3×10^6	6.92	RP-HPLC	66	
25	7.9×10^5	5.9	RP-HPLC	59	100% water
25	4.0×10^6	6.6			85% methanol + 15% water
25	3.0×10^6	6.47	RP-HPLC	67	
25	2.6×10^6	6.41	RP-HPLC	68	
23	1.7×10^5	5.23	RP-HPLC	69	
23	3.2×10^6	6.51	RP-HPLC	49	
23	1.5×10^6	6.18			
LDV at 25 °C	3.3×10^5	5.52	log mean of the values at 25 °C		
FAV at 25 °C	4.3×10^5	5.64			

Table 1. (Continued)

Octanol−Air
Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
5	1.2×10^8	8.09	generator column - GC	12	calcd from the reported equation log $K_{OA} = 2914/(T/\text{K}) - 2.39$ (5 to 25) °C
10	8.0×10^7	7.90			
15	5.3×10^7	7.72			
20	3.6×10^7	7.55			
25	2.4×10^7	7.38			
−10	4.2×10^8	8.63	generator column - GC	13	calcd from the reported equation log $K_{OA} = 3928/(T/\text{K}) - 6.3$ (−10 to 20) °C not used
0	1.2×10^8	8.08			
10	3.7×10^7	7.57			
20	1.3×10^7	7.10			
LDV at 25 °C	2.4×10^7	7.38	directly taken from the value at 25 °C		
FAV at 25 °C	1.6×10^7	7.21			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	8.5	942	2.97	slow stirring - GC	18	not used for the adjustment
12	11	884	2.95			
20	14	861	2.94			
25	15	800	2.90	shake flask - GC	70	

value can be evaluated by relating it to the values of other associated partitioning properties. They proposed a method to adjust literature-derived property values for one chemical such that they conform to the thermodynamic relationships linking them. Li et al.[10] further complemented that approach by developing a rigorous and transparent procedure for compiling and evaluating measured data from the literature, selecting literature-derived values through averaging or linear regression and making estimates of the uncertainty of these values. These uncertainty estimates determine the extent of relative adjustment applied in the adjustment algorithm. The procedure was applied to 16 PCB congeners, and the resulting set of data shows consistency not only among the various partitioning properties for one congener but also for one property across various congeners.[10] Recently, an internally consistent set of physical-chemical property data for α-, β-, and γ-hexachlorocyclohexane (HCH) was derived on the basis of all experimentally obtained values reported for these isomers in the literature.[11] The final adjusted values indicated that the partitioning behavior of α- and γ-HCH differs from that of β-HCH, which may result in substantially different environmental pathways for β-HCH.

The present work's objective was to use this same approach to derive an internally consistent property data set for 14 additonal OCPs, which makes use of all available measured data. These OCPs are HCB, PeCB, *cis*-chlordane, *trans*-chlordane, *p*,*p*′-DDT and its metabolites *p*,*p*′-DDE and *p*,*p*′-DDD, and heptachlor and its metabolites heptachlor epoxide, aldrin, dieldrin, endrin, α-endosulfan, and β-endosulfan. Property measurements for several other OCPs, namely, nonachlor, methoxychlor, and mirex, were found to be too limited to allow this procedure to be applied. Beyer et al.[9] already adjusted for consistency property values for six of the OCPs (*p*,*p*′-DDT, *p*,*p*′-DDE, *trans*-chlordane, *cis*-chlordane, PeCB, HCB) but had used starting values, which were not as rigorously selected as in the current study.

Methods

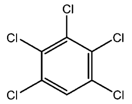
The principles and steps involved in the evaluation, selection, and adjustment procedure have been described previously[9,10] and will not be repeated here in detail. Briefly, the steps are as follows.

Deriving Property Values from Measurements Reported in the Literature. The *Chemical Abstracts Service Source Index* (CASSI) and other databases[7] are used to obtain and identify all of the published literature on measured physical−chemical properties for the chemicals of interest. Despite our efforts at comprehensiveness, it is likely that additional data sources exist that escaped our attention. To avoid multilevel referencing and reporting errors, only original data sources are considered; that is, no quoted values are included.[8] Although we may use handbooks to identify property values, we always consult the original sources to determine if the information is correct and available in the original publications. Values that refer to the same set of experiments, differ substantially from a cluster of other reported values, or are highly inconsistent with respect to the other property values for the same chemical are not used in the derivation of literature-derived values (LDVs). Data measured indirectly, such as those derived from chromatographic retention times, are included only if there are no directly measured data or the directly measured data are inconsistent with the other property data. Theoretically estimated values are excluded.

The measured data are converted to appropriate and identical units and compiled in spreadsheets. If no exact experimental temperature is provided, then a temperature of 23 °C is assumed to apply. If the data are reported as a linear equation, then discrete values listed in tables are calculated for four or five temperatures that are either experimental temperatures indicated in the reference or temperatures in the environmentally relevant range. In some cases, values at low or high temperatures are calculated from an equation if it aids in the comparison with other measurements. Because the OCPs are solids at environmental temperatures, experimentally determined properties for the solid state were converted to those of the supercooled liquid. This is discussed in more detail below.

If measured values for a property exist at several temperatures, then a linear regression equation between the logarithm of all noneliminated data and the reciprocal absolute temperature is derived. The LDVs for the property at 25 °C are obtained from the regression equation, and the LDVs for the corresponding internal energy of phase transfer are calculated from the slope of the regression line. If measurements had been performed within only a fairly small temperature range (e.g., (20 to 25) °C) and measured data at 25 °C are close to each other, then the LDV at 25 °C is the logarithmic mean of the noneliminated values at

Table 2. Reported and Selected Physical−Chemical Properties for Pentachlorobenzene (PeCB)

common name	pentachlorobenzene	t_M/°C	84.6	23	
CAS registry no.	608-93-5	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	57.74	23	
formula	C_6HCl_5				
MW/g·mol^{-1}	250.3				

Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
30	0.55	1.9	0.28		71	
40	1.8	4.7	0.68			
50	5.3	11	1.05			
60	15	25	1.39			
30.3	0.39	1.4	0.13	pressure gauge	72	
40.3	1.2	3.1	0.49			
50.2	3.2	6.7	0.83			
60.2	8.5	14	1.15			
70.1	20	27	1.44			
80.0	47	52	1.71			
98.7		168	2.22			
108.7		285	2.45			
118.8		471	2.67			
128.9		756	2.88			
138.9		1189	3.08			
149.0		1821	3.26			
159.1		2731	3.44			
169.1		4010	3.60			
179.1		5751	3.76			
98.6		133	2.12		35	
129.7		667	2.82			
144.3		1333	3.12			
160		2666	3.43			
178.5		5333	3.73			
190.1		7999	3.90			
205.5		13332	4.12			
227		26664	4.43			
251.6		53329	4.73			
276		101325	5.01			
20	0.055	0.25	−0.60	relative loss rate	33	outlier
LDV at 25 °C		1.2	0.07	linear regression		log(P_L/Pa) = −3220/(T/K) + 10.87
FAV at 25 °C		1.0	0.01			R^2 = 0.997

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.0033	0.013	−1.88	generator column - GC	39	
22	0.00072	0.0031	−2.50	generator column - GC	73	
5	0.00058	0.0042	−2.37	generator column - GC	37	
15	0.0010	0.0054	−2.27			
25	0.0017	0.0067	−2.17			
35	0.0025	0.0075	−2.12			
45	0.0034	0.0081	−2.09			
25	0.0018	0.0071	−2.15	shake flask - GC	37	
25	0.0035	0.014	−1.86	shake flask - GC/MS	74	
25	0.0022	0.0090	−2.05	shake flask - UV	41	
25	0.0053	0.021	−1.67	shake flask - LSC	75	
22	0.0010	0.0046	−2.34	shake flask - GC	43	
23		0.0066	−2.18	shake flask - GC	44	
23	0.00088	0.0037	−2.43	shake flask - HPLC	45	
23	0.014	0.058	−1.23	RP-HPLC	49	not used, indirect
23	0.013	0.053	−1.27			
23	0.00035	0.0015	−2.82			
LDV at 25 °C		0.011	−1.96	log mean of the values at 25 °C		
FAV at 25 °C		0.014	−1.85			

Henry's Law Constant

t/°C	H/Pa·m^3·mol^{-1}	K_{AW}	log K_{AW}	method	ref	note
20	72	0.030	−1.53	gas stripping	51	
14.8	37	0.016	−1.81	gas stripping	50	
20.1	49	0.020	−1.69			
22.1	68	0.028	−1.56			
24.2	67	0.027	−1.57			
34.8	124	0.048	−1.31			
50.5	276	0.10	−0.99			
LDV at 25 °C	74	0.030	−1.52	linear regression		log K_{AW} = −2026/(T/K) + 5.27
FAV at 25 °C	72	0.029	−1.54			R^2 = 0.957

Table 2. (Continued)

Octanol−Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
5	1.6×10^5	5.20	shake flask - GC	54	
15	1.1×10^5	5.06			
25	8.7×10^4	4.94			
35	6.2×10^4	4.79			
45	4.6×10^4	4.66			
25	1.5×10^5	5.17	shake flask - GC	57	
25	1.6×10^5	5.20	shake flask - GC	56	
22	1.6×10^5	5.20	shake flask - GC	44	
25	8.7×10^4	4.94	shake flask - HPLC	64	
23	8.7×10^4	4.94	shake flask - LSC	75	
25	1.1×10^5	5.03	generator column - GC	39	
25	1.5×10^5	5.18	slow stirring - GC	58	
22	7.6×10^4	4.88	shake flask - GC	63	
25	1.5×10^5	5.18	RP-HPLC	64	
23	1.1×10^5	5.06	RP-HPLC	76	
23	4.9×10^5	5.69	RP-HPLC	77	
23	3.0×10^5	5.47	RP-HPLC	78	
18	1.3×10^6	6.12	RP-HPLC	66	
23	5.5×10^5	5.74	RP-HPLC	49	
LDV at 25 °C	1.2×10^5	5.08	log mean of the values at 25 °C		
FAV at 25 °C	1.6×10^5	5.19			

Octanol−Air
Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
−10	8.8×10^7	7.94	generator column - GC	13	calcd from the reported equation
0	2.7×10^7	7.43			$\log K_{OA} = 3722/(T/\text{K}) - 6.3$
5	1.5×10^7	7.18			(−10 to 20) °C
10	8.8×10^6	6.94			
20	3.1×10^6	6.50			
25	1.9×10^6	6.28			extrapolated
25	3.3×10^7	7.52	GC - retention time		Li, unpublished indirect, used anyhow
LDV at 25 °C	8.0×10^6	6.90	log mean of the values at 25 °C		
FAV at 25 °C	5.4×10^6	6.73			
Octanol Solubility					not found

25 °C. If there is an insufficient number of values at 25 °C or if data at 25 °C are scattered, then the LDV at 25 °C has to be derived using the logarithmic mean of the noneliminated values at (20 to 25) °C, assuming that in such cases the temperature dependence is minor compared to the uncertainty of the measurements. The arithmetic mean would give undue weight to higher values.

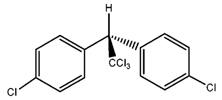
If property values for selected chemicals had been measured by only a single study, then the LDVs for the property and the corresponding internal energy of phase transfer are taken directly from the relevant studies. If there are multiple data sets from the same author or research group, then the latest data take precedence. For example, most of the LDVs for K_{OA}, except those for heptachlor epoxide and β-endosulfan, are taken from the study by Shoeib and Harner.[12] Harner and Mackay[13] had previously reported K_{OA} values for HCB and p,p'-DDT. The more recent values are higher and more consistent with other properties and are thus considered to be more reliable and served as LDVs.

Assigning Uncertainty Estimates to the Literature-Derived Values. For each LDV value of the six evaluated properties P_L, S_{WL}, K_{OW}, H or K_{AW}, K_{OA}, and S_{OL} of a particular chemical, a relative uncertainty estimate, u_X, is required to avoid the undue adjustment of a well-established property value to conform to a poorly characterized one.[9] To minimize ambiguity in deciding on the value of u_X for a property, a u_X value between 1 and 5 is assigned by comparing the size of the database, the technique employed in a measurement, the deviations between different literature data, and the general reliability of data reported by a particular research group. For example, a relatively large u_X, indicating high uncertainty, is assigned to properties for which few or no directly measured data exist (e.g., K_{AW} for most selected chemicals), whereas properties that had been measured directly several times with accepted techniques yielding comparable values would deserve a low u_X (e.g., P_L for HCB).

Adjusting the Literature-Derived Values to Conform to Thermodynamic Constraints. The LDVs were adjusted on the basis of their assigned uncertainties using the algorithm by Beyer et al.[9] This technique adjusts a set of physical−chemical property values in such a way that they conform to thermodynamic constraints yet deviate as little as possible from the original values. The adjusted values are referred to as final adjusted values (FAVs). Missing property values are calculated at the same time. For the selected chemicals, K_{OW} is assumed to be equal to S_{OL}/S_{WL} on the basis of the belief that for the OCPs the uncertainty caused by the effect of the mutual solubility of octanol and water on K_{OW} is less than that of experimentally measured data reported in the literature. Beyer et al.[9] provided a detailed account of the thermodynamic basis of the adjustment procedure and the equations on which it is based. A computer program with the algorithm is available from www.usf.uos.de/projects/elpos/download/adjust.en.html.

Conversion of Properties of the Solid to Those of the Supercooled Liquid. As mentioned above, the vapor pressure and solubility values reported for the solid phase

Table 3. Reported and Selected Physical−Chemical Properties for *p,p′*-DDT

common name	*p,p′*-DDT	t_M/°C	108.7	79	
CAS registry no.	50-29-3		109.8	27	
formula	$C_{14}H_9Cl_5$		108.9	22	
MW/g·mol^{-1}	354.5		111.7	16	
		$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	71.2	36	
			68.8	27	
			68.8	22	
			79.4	16	

Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
20	0.000029	0.00042	−3.38	gas saturation - HPLC	80	
25	0.000057	0.00067	−3.17			
30	0.00012	0.0012	−2.92			
40	0.00053	0.0037	−2.43			
50	0.0020	0.0099	−2.00			
60	0.0064	0.023	−1.63			
70	0.020	0.055	−1.26			
80	0.060	0.12	−0.90			
20	0.000020	0.00029	−3.54	gas saturation - GC	81	
30	0.000097	0.00095	−3.02			
40	0.00044	0.0031	−2.52			
0	0.00000050	0.000016	−4.79	gas saturation - GC	29	
10	0.0000025	0.000054	−4.27			
20	0.000017	0.00024	−3.61			
30	0.000081	0.00079	−3.10			
40	0.00038	0.0027	−2.58			
50.1	0.0020	0.0099	−2.00	gas saturation - GC	82	
60.1	0.0071	0.026	−1.59			
80.4	0.078	0.16	−0.80			
88.8	0.20	0.33	−0.48			
90.2	0.23	0.36	−0.44			
0	0.00000059	0.000019	−4.72	effusion manometer	83	
10	0.0000036	0.000076	−4.12			
20	0.000020	0.00028	−3.55			
30	0.000096	0.00094	−3.03			
40	0.00043	0.0029	−2.53			
50	0.0018	0.0088	−2.05			
60	0.0067	0.024	−1.61			
70	0.023	0.063	−1.20			
80	0.074	0.15	−0.81			
90	0.22	0.36	−0.44			
100	0.64	0.80	−0.10			
20	0.000043	0.00061	−3.21	relative loss rate	33	
20	0.000033	0.00047	−3.32		84	
20	0.000017	0.00024	−3.61	gas saturation - LSC	85	outlier
50	0.000063	0.00031	−3.51			
100	0.000090	0.00011	−3.95			
0		0.000016	−4.79	GC - retention time	36	calcd from the reported equation
25		0.00050	−3.30			log(P_L/Pa) = −4865/(T/K) + 13.02
50		0.0092	−2.03			
75		0.11	−0.95			
100		0.96	−0.02			
25		0.00083	−3.08	GC - retention time	86	BP-1 column
25		0.00047	−3.33			Apolane-87 column
LDV at 25 °C		0.00056	−3.25	linear regression		log(P_L/Pa) = −4666/(T/K) + 12.40
FAV at 25 °C		0.00048	−3.32			$R^2 = 0.995$

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.000014	0.00017	−3.77	generator column - GC	46	
23	0.0000088	0.00011	−3.95	shake flask - UV	42	
24	0.000015	0.00019	−3.73	shake flask - GC	87	
20	0.00011	0.0016	−2.79	shake flask - HPLC	88	
24	0.000011	0.00014	−3.86	shake flask - nephelometry	48	
25	0.000015	0.00018	−3.74	centrifuge - GC	55	
15	0.000048	0.00083	−3.08	shake flask - GC	89	particle size, 5 μm
25	0.000071	0.00083	−3.08			
35	0.00010	0.00086	−3.07			
45	0.00013	0.00074	−3.13			
15	0.0000071	0.00012	−3.91	shake flask - GC	89	not used, small particle size, 0.05 μm
25	0.000017	0.00020	−3.70			
35	0.000037	0.00030	−3.52			
45	0.000078	0.00045	−3.34			
15	0.0000028	0.000049	−4.31	shake flask - GC	89	not used, small particle size, 0.01 μm

Table 3. (Continued)

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.0000048	0.000056	−4.25			
35	0.0000073	0.000060	−4.22			
45	0.000011	0.000064	−4.19			
25	0.0000048	0.000056	−4.25	ultracentrigfugation - GC	90	outlier
25	0.000085	0.00100	−3.00	RP-HPLC	49	
2	0.0059	0.00016	−3.80	shake flask - radiometric	91	no isomer specified
25	0.037	0.00044	−3.36			no isomer specified
37.5	0.045	0.00035	−3.45			no isomer specified
23	0.0016	0.000020	−4.70	shake flask - GC	92	no isomer specified
25	0.0045	0.000053	−4.28	shake flask - LSC	93	no isomer specified
25	0.0023	0.000027	−4.57	generator column	94	no isomer specified
25	0.020	0.00023	−3.63	RP-HPLC	94	no isomer specified
LDV at 25 °C		0.00027	−3.56	log mean of the values at (20 to 25) °C		
FAV at 25 °C		0.00042	−3.37			

Henry's Law Constant

t/°C	H/Pa·m^3·mol^{-1}	K_{AW}	log K_{AW}	method	ref	note
25	1.3	0.00052	−3.28		84	
25	0.84	0.00034	−3.47	thermodynamic method	52	
22−24	0.86	0.00035	−3.46	wetted-wall column	95	not at 25 °C, used anyhow
23	1.3	0.00052	−3.28	fog chamber (drain)		
23	1.3	0.00054	−3.27	fog chamber (cyclone)		
LDV at 25 °C	1.1	0.00043	−3.37	log mean of the values at (23 to 25) °C		
FAV at 25 °C	1.1	0.00043	−3.37			

Octanol−Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	8.7×10^5	5.94	shake flask - GC	88	
25	2.3×10^6	6.36	shake flask - GC	55	
25	8.2×10^6	6.91	slow stirring - GC	58	
23	1.6×10^6	6.20	slow stirring - GC	59	average of four replicates
23	2.0×10^6	6.31	slow stirring - GC		
23	1.7×10^6	6.24	slow stirring - GC	60	
25	1.0×10^6	6.00	SPMD - GC	46	
25	4.0×10^5	5.60	RP-HPLC	65	
18	4.3×10^5	5.63	RP-HPLC	66	
25	2.4×10^6	6.38	RP-HPLC	76	
17	1.3×10^5	5.13	RP-HPLC	96	
23	3.2×10^5	5.50	RP-HPLC	97	
23	1.6×10^6	6.21	RP-HPLC	68	
23	2.8×10^5	5.44	RP-HPLC	67	
23	3.3×10^5	5.52	RP-HPLC	98	
23	3.9×10^5	5.59	RP-HPLC	85	
LDV at 25 °C	1.9×10^6	6.28	log mean of the values at (23 to 25) °C		
FAV at 25 °C	2.5×10^6	6.39			

Octanol−Air
Partition Coefficient

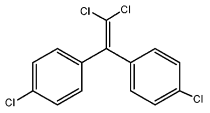
t/°C	K_{OA}	log K_{OA}	method	ref	note
5	8.3×10^{10}	10.92	generator column - GC	12	calcd from the reported equation
15	2.2×10^{10}	10.34			log $K_{OA} = 4603/(T/\text{K}) - 5.63$
25	6.4×10^9	9.81			(5 to 45) °C
35	2.0×10^9	9.31			
45	6.9×10^8	8.84			
−10	6.7×10^{11}	11.83	generator column - GC	13	calcd from the reported equation
0	1.9×10^{11}	11.28			log $K_{OA} = 3954/(T/\text{K}) - 3.2$
10	5.8×10^{10}	10.76			(−10 to 20) °C
20	1.9×10^{10}	10.29			not used
LDV at 25 °C	6.4×10^9	9.81	directly take the value at 25 °C		
FAV at 25 °C	5.4×10^9	9.73			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	76	2074		slow stirring - GC	18	not used for the adjustment
12	123	2403				
20	162	2306				
20	99	1404		shake flask - HPLC	88	

Table 4. Reported and Selected Physical−Chemical Properties for *p,p′*-DDE

common name	*p,p′*-DDE	t_M/°C	88.6	79
CAS registry no.	72-55-9		89.9	27
formula	$C_{14}H_8Cl_4$		87.3	22
MW/g·mol^{-1}	319		88.5	16
		$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	66.9	27
			65.3	22
			65.4	16



Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
15		0.00097	−3.01	GC - retention time	36	calcd from the reported equation
25		0.0033	−2.48			log(P_L/Pa) = −4554/(T/K) + 12.79
35		0.010	−1.99			used anyhow
45		0.030	−1.52			
30	0.00087	0.0040	−2.40	gas saturation - GC	81	
30	0.0017	0.0080	−2.10	gas saturation - GC	99	
30		0.0019	−2.73	GC - retention time	100	
25		0.0027	−2.57	GC - retention time	86	BP-1 column
25		0.0021	−2.68			Apolane-87 column
LDV at 25 °C		0.0033	−2.48	directly take the value at 25 °C		
FAV at 25 °C		0.0034	−2.47			

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
20	0.00013	0.00080	−3.10	shake flask - GC	101	
24	0.00020	0.0011	−2.94	shake flask - nephelometry	48	used anyhow
25	0.000044	0.00024	−3.62	generator column - GC	38	
15	0.00017	0.0013	−2.89	shake flask - GC	89	particle size, 5 μm
25	0.00038	0.0020	−2.69			
35	0.00074	0.0029	−2.54			
45	0.0014	0.0042	−2.38			
25	0.00013	0.00068	−3.17	shake flask - GC	89	not used, small particle size, 0.05 μm
25	0.000031	0.00017	−3.77			not used, small particle size, 0.01 μm
25	0.0000041	0.000022	−4.66	shake flask - LSC	47	outlier
23	0.0039	0.021	−1.68	RP-HPLC	49	
23	0.000074	0.00040	−3.40	RP-HPLC		
25	0.0000034	0.000018	−4.74	generator column	94	no isomer specified
25	0.000019	0.00010	−4.01	RP-HPLC		no isomer specified
LDV at 25 °C		0.00081	−3.09	log mean of the values at (20 to 25) °C		
FAV at 25 °C		0.00079	−3.10			

Henry’s Law Constant

t/°C	H/Pa·m^3·mol^{-1}	K_{AW}	log K_{AW}	method	ref	note
25	4.2	0.0017	−2.77	thermodynamic method	52	
23	123	0.05	−1.30	gas stripping - UV	20	not consistent with other properties
23	369	0.15	−0.82		20	not used, seawater
LDV at 25 °C	4.2	0.0017	−2.77	directly take the value at 25 °C		
FAV at 25 °C	4.2	0.0017	−2.77			

Octanol−Water Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	9.0×10^6	6.96	slow stirring	58	
23	6.8×10^5	5.83	RP-HPLC	69	
25	7.8×10^5	5.89	RP-HPLC	65	
18	1.2×10^6	6.09	RP-HPLC	66	
23	6.0×10^5	5.78	RP-HPLC	97	
23	1.9×10^6	6.29	RP-HPLC	49	
23	4.9×10^5	5.69	RP-HPLC	69	
23	4.3×10^5	5.63	RP-HPLC	94	no isomer specified
LDV at 25 °C	9.0×10^6	6.96	directly take the value at 25 °C		
FAV at 25 °C	8.6×10^6	6.93			

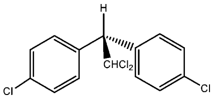
Octanol−Air Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
5	8.4×10^{10}	10.92	generator column - GC	12	calcd from the reported equation
15	1.9×10^{10}	10.28			log K_{OA} = 5116/(T/K) − 7.47
25	4.9×10^9	9.69			(5 to 35) °C
35	1.4×10^9	9.13			
LDV at 25 °C	4.9×10^9	9.69	directly take the value at 25 °C		
FAV at 25 °C	5.0×10^9	9.70			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	138	1546	3.19	slow stirring - GC	18	not used for the adjustment
12	138	1157	3.06			
20	200	1271	3.10			

Table 5. Reported and Selected Physical−Chemical Properties for *p,p′*-DDD

common name	*p,p′*-DDD	t_M/°C	109.2	27	
CAS registry no.	72-54-8		109.0	22	
formula	$C_{14}H_{10}Cl_4$	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	81.0	27	
MW/g·mol^{-1}	321		71.5	22	

Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
15		0.00028	−3.55	GC - retention time	36	calcd from the reported equation
25		0.00097	−3.01			log(P_L/Pa) = −4622/(T/K) + 12.49
35		0.0031	−2.51			
45		0.0092	−2.04			
30	0.000136	0.0015	−2.83	gas saturation - GC	81	
25		0.0016	−2.79	GC - retention time	86	BP-1 column
25		0.00062	−3.21			Apolane-87 column
LDV at 25 °C		0.00097	−3.01	directly take the value at 25 °C		
FAV at 25 °C		0.0012	−2.93			

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.000062	0.00083	−3.08	generator column - GC	38	
24	0.00050	0.0069	−2.16	shake flask - nephelometry	48	
15	0.00016	0.0031	−2.51	shake flask - GC	89	particle size, 5 μm
25	0.00028	0.0037	−2.43			
35	0.00047	0.0042	−2.37			
45	0.00075	0.0047	−2.32			
25	0.000047	0.00062	−3.21			not used, small particle size, 0.05 μm
25	0.000016	0.00021	−3.68			not used, small particle size, 0.01 μm
LDV at 25 °C		0.0028	−2.56	log mean of the values at (24 and 25) °C		
FAV at 25 °C		0.0023	−2.64			

Henry's Law Constant

t/°C	H/Pa·m^3·mol^{-1}	K_{AW}	log K_{AW}	method	ref	note
25	0.67	0.00027	−3.57	thermodynamic method	52	
LDV at 25 °C	0.67	0.00027	−3.57	directly take the value at 25 °C		
FAV at 25 °C	0.50	0.00020	−3.69			

Octanol−Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	1.6×10^6	6.217	slow stirring	58	
25	5.4×10^4	4.73	RP-HPLC	65	
18	1.0×10^5	5	RP-HPLC	66	from regression
23	6.6×10^4	4.82	RP-HPLC	97	
23	1.5×10^5	5.19	RP-HPLC	49	
LDV at 25 °C	1.6×10^6	6.22	directly take the value at 25 °C		
FAV at 25 °C	2.2×10^6	6.33			

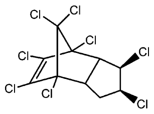
Octanol−Air
Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
5	1.3×10^{11}	11.11	generator column - GC	12	calcd from the reported equation
15	3.8×10^{10}	10.58			log K_{OA} = 4185/(T/K) − 3.94
25	1.2×10^{10}	10.10			(5 to 35) °C
35	4.4×10^9	9.64			
LDV at 25 °C	1.2×10^{10}	10.10	directly take the value at 25 °C		
FAV at 25 °C	1.1×10^{10}	10.03			

Octanol Solubility	not found

Table 6. Reported and Selected Physical−Chemical Properties for *cis*-Chlordane (CC)

common name	*cis*-chlordane	t_M/°C	104.1	14
CAS registry no.	5103−71−9		106.8	22
formula	C10 H6 Cl8	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	74.3	14
MW/g·mol^{-1}	409.8		60.9	22



Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
25		0.008	−2.10	gas saturation - GC		Rordorf, unpublished
50		0.11	−0.96			
75		0.98	0.01			
100		6.7	0.83			
125		36	1.56			
25		0.0047	−2.33	GC - retention time	36	calcd from the reported equation
50		0.061	−1.22			log(P_L/Pa) = −4284/(T/K) + 12.04
75		0.54	−0.27			
100		3.6	0.56			
125		19	1.28			
20		0.0029	−2.54	GC - AA	102	
25		0.0073	−2.14	GC - retention time		Li, unpublished
LDV at 25 °C		0.0080	−2.10	linear regression		log(P_L/Pa) = −4331/(T/K) + 12.43
FAV at 25 °C		0.0073	−2.14			R^2 = 1.000

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.00014	0.0015	−2.83	shake flask - GC	103	mixture of 3:1 cis/trans, used anyhow
24	0.000078	0.00084	−3.08	batch solubility	104	no isomer specified, used anyhow
25	0.0045	0.048	−1.32	generator column - GC	38	not consistent with other properties
LDV at 25 °C		0.0011	−2.96	log mean of the values at (24 and 25) °C		
FAV at 25 °C		0.0013	−2.89			

Henry's Law Constant

t/°C	H/Pa·m^3·mol^{-}1	K_{AW}	log K_{AW}	method	ref	note
25	4.9	0.0020	−2.71	gas stripping - GC	19	no isomer specified, used anyhow
22−24	8.4	0.0034	−2.47	wetted-wall column	95	τ-chlordane, used anyhow
23	5.4	0.0022	−2.66	fog chamber (drain)		
23	5.9	0.0024	−2.62	fog chamber (cyclone)		
23	89	0.036	−1.44	gas stripping - GC	20	not consistent with other properties
23	419	0.17	−0.77			not used, seawater
LDV at 25 °C	6.0	0.0024	−2.61	log mean of the values at (23 to 25) °C		
FAV at 25 °C	5.7	0.0023	−2.61			

Octanol−Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	1.3×10^6	6.10	slow stirring - GC	105	
25	6.0×10^2	2.78	shake flask - GC	103	not used, 3:1 *cis*-to *trans*-chlordane
23	1.2×10^5	5.08	RP-HPLC	97	no isomer specified
LDV at 25 °C	1.3×10^6	6.10	directly take the value at 25 °C		
FAV at 25 °C	1.6×10^6	6.20			

Octanol−Air
Partition Coefficient

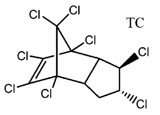
t/°C	K_{OA}	log K_{OA}	method	ref	note
5	1.4×10^{10}	10.14	generator column - GC	12	calcd from the reported equation
15	3.2×10^9	9.50			log K_{OA} = 5127/(T/K) − 8.29
25	8.1×10^8	8.91			(5 to 35) °C
35	2.2×10^8	8.35			
25	8.3×10^8	8.92	GC - retention time		Li, unpublished
LDV at 25 °C	8.1×10^8	8.91	directly take the value at 25 °C		
FAV at 25 °C	6.8×10^8	8.83			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	138	3483	3.54	slow stirring - GC	18	not used for the adjustment
12	151	2715	3.43			
20	209	2714	3.43			

Table 7. Reported and Selected Physical−Chemical Properties for *trans*-Chlordane (TC)

common name	*trans*-chlordane	t_M/°C	101.1	14
CAS registry no.	5103-74-2	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	75.4	14
formula	$C_{10}H_6Cl_8$			
MW/g·mol^{-1}	409.8			



Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
25		0.013	−1.89	gas saturation - GC		Rordorf, unpublished
50		0.16	−0.80			
75		1.4	0.15			
100		9.3	0.97			
125		48	1.68			
25		0.0066	−2.18	GC - retention time	36	calcd from the reported equation
50		0.082	−1.09			log(P_L/Pa) = −4216/(T/K) + 11.96
75		0.71	−0.15			
100		4.6	0.66			
125		23	1.37			
20		0.0039	−2.41	GC - AA	102	
25		0.0098	−2.01	GC - retention time		Li, unpublished
LDV at 25 °C		0.013	−1.89	linear regression		log(P_L/Pa) = −4238/(T/K) + 12.32
FAV at 25 °C		0.010	−1.99			R^2 = 1.000

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.00014	0.0014	−2.86	shake flask	103	mixture of 3:1 cis/trans, used anyhow
24	0.000078	0.00080	−3.10	batch solubility	104	no isomer specified, used anyhow
25	0.0045	0.046	−1.34	generator column - GC	38	not consistent with other properties
LDV at 25 °C		0.0011	−2.96	log mean of the values at (24 and 25) °C		
FAV at 25 °C		0.0015	−2.82			

Henry's Law Constant

t/°C	H/Pa·m^3·mol$^-$1	K_{AW}	log K_{AW}	method	ref	note
25	4.9	0.0020	−2.71	gas stripping - GC	19	no isomer specified, used anyhow
23	8.4	0.0034	−2.47	wetted-wall column	95	τ-chlordane, used anyhow
23	5.4	0.0022	−2.66	fog chamber (drain)		
23	5.9	0.0024	−2.62	fog chamber (cyclone)		
23	135	0.055	−1.26	gas stripping - GC	20	not consistent with other properties
23	566	0.23	−0.64			not used, seawater
LDV at 25 °C	6.0	0.0024	−2.62	log mean of the values at (23 and 25) °C		
FAV at 25 °C	6.8	0.0027	−2.56			

Octanol−Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	1.7 × 10^6	6.22	slow stirring	105	
25	6.0 × 10^2	2.78	shake flask	103	not used, 3:1 *cis*-to *trans*-chlordane
23	1.2 × 10^5	5.08	RP-HPLC	97	no isomer specified
LDV at 25 °C	1.7 × 10^6	6.23	directly take the value at 25 °C		
FAV at 25 °C	1.8 × 10^6	6.27			

Octanol−Air
Partition Coefficient

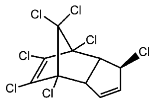
t/°C	K_{OA}	log K_{OA}	method	ref	note
5	1.2 × 10^{10}	10.08	generator column - GC	12	calcd from the reported equation
10	5.7 × 10^9	9.76			log K_{OA} = 5036/(T/K) − 8.03
15	2.8 × 10^9	9.45			(5 to 25) °C
20	1.4 × 10^9	9.15			
25	7.3 × 10^8	8.86			
25	5.9 × 10^8	8.77	GC - retention time		Li, unpublished
LDV at 25 °C	7.3 × 10^8	8.86	directly take the value at 25 °C		
FAV at 25 °C	6.7 × 10^8	8.83			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	204	4912	3.69	slow stirring - GC	18	not used for the adjustment
12	275	4699	3.67			
20	347	4274	3.63			

Table 8. Reported and Selected Physical−Chemical Properties for Heptachlor (HEPT)

common name	heptachlor	t_M/°C	93	14
CAS registry no.	76-44-8		98	15
formula	$C_{10}H_5Cl_7$	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	69.64	14
MW/g·mol^{-1}	373.4		70.96	15



Vapor Pressure

t/°C	P_s/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
25	0.021	0.16	−0.81	gas saturation - GC		Rordorf, unpublished
50	0.41	1.35	0.13			
75	5.1	8.38	0.92			
100		46	1.66			
125		320	2.51			
25		0.030	−1.52	GC - retention time	36	calcd from the reported equation
50		0.33	−0.48			log(P_L/Pa) = −3995/(T/K) + 11.88
75		2.5	0.41			
100		15	1.17			
125		70	1.85			
25		0.036	−1.44	GC - retention time		Li, unpublished
LDV at 25 °C		0.13	−0.87	linear regression		log(P_L/Pa) = −3870/(T/K) + 12.11
FAV at 25 °C		0.13	−0.87			R^2 = 0.996

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
15	0.00027	0.0028	−2.55	shake flask - GC	89	particle size, 5 μm
25	0.00048	0.0036	−2.45			
35	0.00084	0.0044	−2.35			
45	0.0013	0.0050	−2.30			
25	0.00033	0.0025	−2.61			not used, small particle size 0.05 μm
25	0.00008	0.00059	−3.23			not used, small particle size 0.01 μm
27	0.00015	0.0010	−2.99	shake flask - GC	106	not used, outlier
LDV at 25 °C		0.0035	−2.45	linear regression		log(S_{WL}/mol·m^{-3}) = −770/(T/K) + 0.13
FAV at 25 °C		0.0035	−2.45			R^2 = 0.990

Henry's Law Constant

t/°C	H/Pa·m^3·mol−1	K_{AW}	log K_{AW}	method	ref	note
25	30	0.012	−1.92	thermodynamic method	52	
25	150	0.060	−1.22	gas stripping - GC	19	not consistent with other properties
LDV at 25 °C	30	0.012	−1.92	directly take the value at 25 °C		
FAV at 25 °C	38	0.015	−1.81			

Octanol−Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	1.3 × 10^6	6.1	slow strirring - GC	105	
18	3.8 × 10^5	5.58	RP-HPLC	66	from regression
23	1.7 × 10^5	5.24	RP-HPLC	97	
23	2.8 × 10^5	5.44	RP-HPLC	69	
25	1.9 × 10^5	5.27	RP-HPLC	65	
LDV at 25 °C	1.3 × 10^6	6.10	directly take the value at 25 °C		
FAV at 25 °C	8.8 × 10^5	5.94			

Octanol−Air
Partition Coefficient

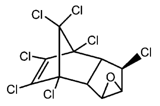
t/°C	K_{OA}	log K_{OA}	method	ref	note
5	3.0 × 10^8	8.47	generator column - GC	12	calcd from the reported equation
10	1.8 × 10^8	8.25			log K_{OA} = 3455/(T/K) − 3.95
15	1.1 × 10^8	8.04			(5 to 25) °C
20	6.9 × 10^7	7.84			
25	4.3 × 10^7	7.64			
25	4.3 × 10^7	7.64	GC - retention time		
LDV at 25 °C	4.3 × 10^7	7.64	directly take the value at 25 °C		
FAV at 25 °C	5.7 × 10^7	7.76			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	182	2960	3.47	slow stirring - GC	18	not used for the adjustment
12	219	2596	3.41			
20	234	2065	3.31			

Table 9. Reported and Selected Physical−Chemical Properties for Heptachlor Epoxide (HEPX)

common name	heptachlor epoxide	t_M/°C	166	14
CAS registry no.	1024-57-3		161.7	15
formula	$C_{10}H_5Cl_7O$	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	61.56	14
MW/g·mol^{-1}	389.2		55.62	15



Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
25		0.013	−1.88	GC - retention time		Li, unpublished
LDV at 25 °C		0.013	−1.88	directly taken		indirect, used anyhow
FAV at 25 °C		0.022	−1.65			

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.00090	0.024	−1.62	generator column - GC	38	
15	0.00028	0.011	−1.97	shake flask - GC	89	particle size, 5 μm
25	0.00051	0.014	−1.86			
35	0.00090	0.017	−1.77			
45	0.0015	0.021	−1.67			
25	0.00031	0.0082	−2.09			not used, small particle size, 0.05 μm
25	0.000064	0.0017	−2.77			not used, small particle size, 0.01 μm
27	0.000090	0.0022	−2.65	shake flask - GC	106	not used, small particle size, 0.05 μm
LDV at 25 °C		0.018	−1.74	log mean of the values at 25 °C		
FAV at 25 °C		0.013	−1.88			

Henry's Law Constant

t/°C	H/Pa·m^3·mol−1	K_{AW}	log K_{AW}	method	ref	note
25	2.1	0.00086	−3.07	thermodynamic method	52	
25	3.2	0.0013	−2.88	gas stripping - GC	19	not consistent with other properties
LDV at 25 °C	2.1	0.00086	−3.07	directly take the value at 25 °C		
FAV at 25 °C	1.7	0.00068	−3.17			

Octanol−Water Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	3.6×10^4	4.56	shake flask - GC	107	not consistent with other properties
23	2.5×10^5	5.4	RP-HPLC	69	indirect, used anyhow
LDV at 25 °C	2.5×10^5	5.4	directly taken		
FAV at 25 °C	2.6×10^5	5.42			

Octanol−Air Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
25	4.2×10^8	8.62	GC - retention time		Li, unpublished
LDV at 25 °C	4.2×10^8	8.62	directly take the value at 25 °C		indirect, used anyhow
FAV at 25 °C	3.9×10^8	8.59			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	87.10	5076	3.71	slow stirring - GC	18	not used for the adjustment
12	81.28	3468	3.54			
20	120.23	3820	3.58			

P_S, S_{WS}, and S_{OS} need to be converted to the properties of the supercooled liquid P_L, S_{WL}, and S_{OL}. This is done by using compound-specific entropy of fusion values, $\Delta_{fus}S$, and melting temperatures, $T_{M,}$ in eq 1:

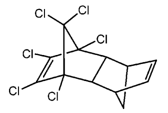
$$\frac{S_{WS}/\text{mol·m}^{-3}}{S_{WL}/\text{mol·m}^{-3}} = \frac{S_{OS}/\text{mol·m}^{-3}}{S_{OL}/\text{mol·m}^{-3}} = \frac{P_S/\text{Pa}}{P_L/\text{Pa}} = \exp\left[\frac{-\Delta_{fus}S/\text{J·K}^{-1}\text{·mol}^{-1}}{R/\text{J·K}^{-1}\text{·mol}^{-1}}\left(\frac{T_M/\text{K}}{T/\text{K}} - 1\right)\right] \qquad (1)$$

where R is the ideal gas constant and T is the experimental temperature in K. $\Delta_{fus}S$ can be calculated from the compound-specific enthalpy of fusion, $\Delta_{fus}H$, and T_M.

The literature search revealed that T_M values reported for a particular OCP can show large discrepancies. For example, T_M values compiled by Mackay et al.[7] are in the range of (70 to 109) °C for α-endosulfan and (108 to 213) °C for β-endosulfan. In addition, aldrin, dieldrin, heptachlor, and heptachlor epoxide have multiple phase transitions between the solid and liquid states. Different phase-transition energies are cited by different authors, referring to different articles. The molecules in an ideal crystal acquire both translational and rotational energy as they change from the solid to the liquid state and show only one melting temperature T_M.[14] However, for some OCPs,

Table 10. Reported and Selected Physical−Chemical Properties for Aldrin

common name	aldrin	t_M/°C	99	14
CAS registry no.	309-00-2		103.1	16
formula	$C_{12}H_8Cl_6$	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	52.17	14
MW/g·mol^{-1}	364.9		56.37	16



Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
35.3	0.063	0.25	−0.60	generator column - GC	108	
41	0.10	0.35	−0.45			
41.6	0.11	0.38	−0.42			
45.6	0.16	0.51	−0.29			
50.8	0.33	0.91	−0.04			
63.3	1.0	2.1	0.33			
70	2.2	4.0	0.60			
25	0.0081	0.043	−1.37	gas saturation - GC		Rordorf, unpublished
50	0.19	0.53	−0.27			
75	2.8	4.6	0.66			
100		29	1.46			
125		220	2.34			
20	0.0031	0.019	−1.73		109	outlier
30	0.0065	0.030	−1.52			
40	0.010	0.036	−1.45			
50	0.014	0.038	−1.41			
20	0.0010	0.0061	−2.22	relative loss rate	33	outlier
25		0.076	−1.12	GC - retention time	36	calcd from the reported equation
50		0.79	−0.10			log(P_L/Pa) = −3924/(T/K) + 12.04
75		5.9	0.77			
100		33	1.52			
125		153	2.18			
25		0.023	−1.64	GC - retention time	86	BP-1 column
25		0.033	−1.48			Apolane-87 column
LDV at 25 °C		0.061	−1.21	linear regression		log(P_L/Pa) = −4106/(T/K) + 12.56
FAV at 25 °C		0.064	−1.20			$R^2 = 0.990$

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.20	0.0029	−2.54	shake flask - UV	110	
35	0.39	0.0043	−2.36			
45	0.79	0.0068	−2.17			
15	0.11	0.0020	−2.69	shake flask - GC	89	particle size, 5 μm
25	0.18	0.0026	−2.58			
35	0.35	0.0039	−2.41			
45	0.60	0.0052	−2.28			
15	0.052	0.0010	−3.00	shake flask - GC	89	not used, small particle size, 0.05 μm
25	0.14	0.0020	−2.69			
35	0.24	0.0026	−2.58			
45	0.46	0.0039	−2.41			
15	0.0055	0.00011	−3.98	shake flask - GC	89	not used, small particle size, 0.01 μm
25	0.013	0.00019	−3.73			
35	0.030	0.00033	−3.48			
45	0.065	0.00056	−3.25			
27	0.027	0.00037	−3.43	shake flask - GC	106	outlier
25	0.017	0.00025	−3.61	generator column - GC	38	outlier
LDV at 25 °C		0.0029	−2.55	linear regression		log(S_{WL}/mol·m^{-3}) = −1480/(T/K) + 2.42
FAV at 25 °C		0.0027	−2.56			$R^2 = 0.948$

Henry's Law Constant

t/°C	H/Pa·m^3·mol$^-$1	K_{AW}	log K_{AW}	method	ref	note
25	50	0.020	−1.69	gas stripping - GC	19	
25	4.5	0.0018	−2.74	thermodynamic method	52	
LDV at 25 °C	15	0.0060	−2.22	log mean of the values at 25 °C		none above are consistent with other properties
FAV at 25 °C	23	0.0094	−2.03			

Octanol−Water
Partition Coefficient

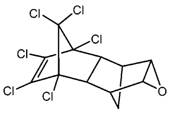
t/°C	K_{OW}	log K_{OW}	method	ref	note
25	3.1×10^6	6.50	slow stirring - GC	58	
20	2.5×10^7	7.4	RP-TLC	111	
23	5.5×10^5	5.74	RP-HPLC	97	
LDV at 25 °C	3.1×10^6	6.50	directly take the value at 25 °C		
FAV at 25 °C	1.7×10^6	6.24			

Octanol−Air
Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
5	9.2×10^8	8.96	generator column - GC	12	calcd from the reported equation
10	5.4×10^8	8.73			log K_{OA} = 3709/(T/K) − 4.37
15	3.2×10^8	8.50			(5 to 25) °C
20	1.9×10^8	8.28			
25	1.2×10^8	8.07			
25	2.0×10^8	8.31	GC - retention time		Li, unpublished
LDV at 25 °C	1.2×10^8	8.07	directly take the value at 25 °C		
FAV at 25 °C	1.8×10^8	8.26			

Octanol Solubility	not found

Table 11. Reported and Selected Physical−Chemical Properties for Dieldrin

common name	dieldrin	t_M/°C	175	14	
CAS registry no.	60-57-1		180	14	
formula	$C_{12}H_8Cl_6O$		180	15	
MW/g·mol^{-1}	380.9	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	45.69	14	
			52.04	14	
			54.37	15	

Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
35	0.0026	0.044	−1.35	generator column - GC	108	
38.2	0.0042	0.065	−1.19			
51.5	0.017	0.18	−0.74			
62.8	0.059	0.48	−0.32			
70	0.11	0.78	−0.11			
75.2	0.18	1.1	0.04			
20	0.00037	0.010	−2.00	gas saturation - GC	112	
30	0.00135	0.027	−1.58			
40	0.00452	0.067	−1.18			
25	0.00079	0.018	−1.74	gas saturation - GC		Rordorf, unpublished
50	0.018	0.20	−0.69			
75	0.25	1.5	0.18			
100	2.6	9.3	0.97			
125	19	43	1.63			
20	0.000387	0.010	−1.98		84	
20	0.00010	0.0028	−2.55		109	outlier
30	0.00019	0.0038	−2.42			
40	0.00037	0.0054	−2.27			
50	0.00071	0.0079	−2.10			
25		0.010	−2.00	GC - retention time	36	calcd from the reported equation
50		0.13	−0.88			log(P_L/Pa) = −4310/(T/K) + 12.46
75		1.2	0.08			
100		8.1	0.91			
125		43	1.63			
25		0.0053	−2.27	GC - retention time	86	BP-1 column
25		0.0060	−2.22			Apolane-87 column
LDV at 25 °C		0.016	−1.78	linear regression		log(P_L/Pa) = −3995/(T/K) + 11.62
FAV at 25 °C		0.014	−1.84			R^2 = 0.998

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.00053	0.012	−1.92	generator column - GC	38	
10	0.00025	0.0093	−2.03	slow stirring - GC	113	
15	0.00029	0.0091	−2.04			
20	0.00032	0.0086	−2.06			
25	0.00040	0.0092	−2.03			
30	0.00054	0.011	−1.97			
35	0.00064	0.011	−1.96			
40	0.00076	0.011	−1.95			
25	0.00066	0.015	−1.82	shake flask - UV	110	
35	0.0014	0.024	−1.62			
45	0.0026	0.034	−1.47			
25	0.00047	0.011	−1.96	shake flask - GC	92	particle size, 5 μm
27	0.00049	0.011	−1.98	shake flask - GC	106	
10	0.00021	0.0079	−2.10	shake flask - GC	114	
20	0.00037	0.0099	−2.00			
30	0.00053	0.010	−1.98			
15	0.00024	0.0075	−2.13	shake flask - GC	89	particle size, 5 μm
25	0.00051	0.012	−1.93			
35	0.0011	0.018	−1.75			
45	0.0017	0.022	−1.66			
15	0.00017	0.0054	−2.27	shake flask - GC	89	not used, small particle size, 0.05 μm
25	0.00039	0.0090	−2.04			
35	0.00071	0.012	−1.92			
45	0.0013	0.016	−1.79			
15	0.000026	0.00083	−3.08	shake flask - GC	89	not used, small particle size, 0.01 μm
25	0.000058	0.0013	−2.88			
35	0.00012	0.0021	−2.68			
45	0.00024	0.0030	−2.52			
25	0.00037	0.0084	−2.07	shake flask - GC	92	not used, small particle size, 0.4 μm
LDV at 25 °C		0.012	−1.94	linear regression		log(S_{WL}/mol·m^{-3}) = −1158/(T/K) + 1.94
FAV at 25 °C		0.013	−1.88			R^2 = 0.595

Table 11. (Continued)

Henry's Law Constant

t/°C	H/Pa·m^3·mol^{-1}	K_{AW}	log K_{AW}	method	ref	note
25	1.0	0.00041	−3.39	thermodynamic method	52	
25	5.9	0.0024	−2.63	gas stripping - GC	19	not consistent with other properties
20	3.2	0.0013	−2.89	gas stripping - UV	115	not consistent with other properties
LDV at 25 °C	1.0	0.00041	−3.39	directly take the value at 25 °C		
FAV at 25 °C	1.1	0.00044	−3.36			

Octanol−Water Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	2.5×10^5	5.40	slow stirring - GC	58	
25	3.4×10^4	4.54	slow stirring - GC	59	average of four measures not consistent with other properties
20	1.6×10^6	6.2	RP-TLC	111	
23	5.8×10^4	4.76	RP-HPLC	97	
18	3.2×10^4	4.51	RP-HPLC	66	
18	4.5×10^4	4.65			
LDV at 25 °C	2.5×10^5	5.40	directly taken		
FAV at 25 °C	3.1×10^5	5.48			

Octanol−Air Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
5	6.4×10^9	9.81	generator column - GC	12	calcd from the reported equation log $K_{OA} = 3790/(T/K) - 3.82$ (5 to 45) °C
15	2.2×10^9	9.33			
25	7.8×10^8	8.89			
35	3.0×10^8	8.48			
45	1.2×10^8	8.09			
25	1.0×10^9	9.02	GC - retention time		Li, unpublished
LDV at 25 °C	7.8×10^8	8.89	directly take the value at 25 °C		
FAV at 25 °C	6.9×10^8	8.84			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	91	4218	3.63	slow stirring - GC	18	not used for the adjustment
12	105	3665	3.56			
20	107	2882	3.46			

such as aldrin, dieldrin, β-endosulfan, heptachlor, and its metabolite heptachlor epoxide, a characteristic transition phase between the ordered solid phase and the liquid phase exists just below the melting points. In this rotator or plastic phase, the molecules are weakly ordered and behave as if they were in a liquid state. The phase-transfer process of such chemicals can be described as

$$\text{solid phase} \xrightarrow{T_{tr}(\Delta_{tr}H)} \text{transition phase} \xrightarrow{T_M(\Delta_M H)} \text{liquid phase}$$

and a temperature of transition T_{tr} from the solid to the rotator phase can then be observed. The existence of such an intermediate phase for aldrin, dieldrin, heptachlor, and β-endosulfan during their solid−liquid phase transition is clearly shown by endothermic peaks in their differential scanning calorimetry (DSC) curves.[15−17] During phase transfer from solid to liquid, chemicals that have characteristic rotator phases acquire only translational energy upon melting because they have already acquired rotational energy at a lower temperature.[14] The values of the melting entropies $\Delta_M S$ are usually small and equal to the gas constant R;[15] the sums of the energies of solid-rotator and rotator−liquid-phase transitions correspond to the energy of fusion:[14]

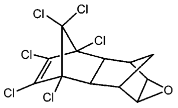
$$\Delta_{fus}H/\text{kJ·mol}^{-1} = \Delta_{tr}H/\text{kJ·mol}^{-1} + \Delta_M H/\text{kJ·mol}^{-1} \qquad (2)$$

$$\Delta_{fus}S/\text{J·mol}^{-1}\text{·K}^{-1} = \Delta_{tr}S/\text{J·K}^{-1}\text{·mol}^{-1} + \Delta_M S/\text{J·K}^{-1}\text{·mol}^{-1} = \frac{10^{-3}\Delta_{tr}H/\text{kJ·mol}^{-1}}{T_{tr}/\text{K}} + \frac{10^{-3}\Delta_M H/\text{kJ·mol}^{-1}}{T_M/\text{K}} \qquad (3)$$

The $\Delta_{fus}H$ and $\Delta_{fus}S$ values for aldrin, dieldrin, heptachlor, heptachlor epoxide, and β-endosulfan listed in Tables 8, 9, 11, 12, and 14 were calculated according to eqs 2 and 3 on the basis of T_{tr}, T_M, $\Delta_{tr}H$, and $\Delta_M H$ values found in the literature.[14−16] We believe that one reason for the large discrepancies in reported T_M values in the literature is that transition temperatures T_{tr} have been cited erroneously as melting temperatures T_M in some literature sources. In

Table 12. Reported and Selected Physical−Chemical Properties for Endrin

common name	endrin	t_M/°C	110.5	15
CAS registry no.	72-20-8		110.2	16
formula	$C_{12}H_8Cl_6O$	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	43.24	15
MW/g·mol^{-1}	380.9		40.73	16



Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
25		0.0052	−2.29	GC - retention time		Li, unpublished indirect, used anyhow
LDV at 25 °C		0.0052	−2.29	directly taken		
FAV at 25 °C		0.0031	−2.50			

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
25	0.00068	0.0030	−2.52	generator column - GC	38	
25	0.00060	0.0027	−2.57	shake flask - UV	110	
35	0.0010	0.0036	−2.45			
45	0.0013	0.0039	−2.41			
25	0.00068	0.0030	−2.52	shake flask - GC	92	particle size, 5 μm
15	0.00034	0.0019	−2.72	shake flask - GC	89	particle size, 5 μm
25	0.00066	0.0029	−2.53			
35	0.0011	0.0039	−2.40			
45	0.0016	0.0048	−2.32			
15	0.00024	0.0013	−2.88	shake flask - GC	89	not used, small particle size, 0.05 μm
25	0.00047	0.0021	−2.68			
35	0.00083	0.0030	−2.53			
45	0.0014	0.0040	−2.40			
15	0.000026	0.00015	−3.83	shake flask - GC	89	not used, small particle size, 0.01 μm
25	0.000064	0.00029	−3.54			
35	0.00015	0.00054	−3.26			
45	0.00032	0.00092	−3.04			
25	0.00050	0.0022	−2.65	shake flask - GC	92	not used, small particle size, 0.06 μm
LDV at 25 °C		0.0027	−2.57	linear regression		log(S_{WL}/mol·m^{-3}) = −1022/(T/K) + 0.86
FAV at 25 °C		0.0030	−2.53			$R^2 = 0.893$

Henry's Law Constant

t/°C	H/Pa·m^3·mol$^-$1	K_{AW}	log K_{AW}	method	ref	note
25	0.63	0.00026	−3.59	thermodynamic method	52	
LDV at 25 °C	0.64	0.00026	−3.59			
FAV at 25 °C	1.1	0.00043	−3.37	directly take the value at 25 °C		

Octanol−Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	1.6×10^5	5.20	slow stirring - GC	58	
23	3.6×10^4	4.56	RP-HPLC	69	
23	5.1×10^4	4.71	RP-HPLC	97	
LDV at 25 °C	1.6×10^5	5.20	directly take the value at 25 °C		
FAV at 25 °C	8.8×10^4	4.94			

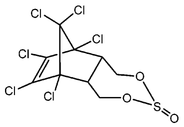
Octanol−Air
Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
5	1.6×10^9	9.20	generator column - GC	12	calcd from the reported equation
10	8.3×10^8	8.92			log K_{OA} = 4436/(T/K) − 6.75
15	4.4×10^8	8.64			(5 to 35) °C
20	2.4×10^8	8.38			
25	1.3×10^8	8.13			
30	7.6×10^7	7.88			
35	4.4×10^7	7.65			
25	1.2×10^9	9.09	GC - retention time		Li, unpublished
LDV at 25 °C	1.3×10^8	8.13	directly take the value at 25 °C		
FAV at 25 °C	2.1×10^8	8.32			

Octanol Solubility

t/°C	S_{OS}/mol·m^{-3}	S_{OL}/mol·m^{-3}	log(S_{OL}/mol·m^{-3})	method	ref	note
4	95	705	2.85	slow stirring - GC	18	not used for the adjustment
12	100	603	2.78			
20	115	572	2.76			

Table 13. Reported and Selected Physical−Chemical Properties for α-Endosulfan

common name	α-endosulfan	t_M/°C	106.8 (not used)	22	
CAS registry no.	959-98-8		85.9	17	
formula	$C_9H_6Cl_6O_3S$	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	26.32 (not used)	22	
MW/g·mol^{-1}	406.9		46.02	17	

Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
5		0.00058	−3.23	GC - retention time	36	calcd from the reported equation log(P_L/Pa) = −4201/(T/K) + 11.87 used anyhow
15		0.0020	−2.71			
25		0.0060	−2.22			
35		0.017	−1.76			
45		0.046	−1.33			
25		0.0086	−2.06	GC - retention time		Li, unpublished
LDV at 25 °C		0.0060	−2.22	directly take the value at 25 °C		
FAV at 25 °C		0.0044	−2.35			

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
20	0.0013	0.0043	−2.36	shake flask - GC	116	
25	0.0013	0.0040	−2.39	generator column - GC	38	
20	0.00016	0.0006	−3.25	liquid−liquid etraction-GC/MS	117	not consistent with other properties
LDV at 25 °C		0.0042	−2.38	log mean of the values at (20 and 25) °C		
FAV at 25 °C		0.0063	−2.20			

Henry's Law Constant

t/°C	H/Pa·m^3·mol^{-}1	K_{AW}	log K_{AW}	method	ref	note
25	0.72	0.00029	−3.54	thermodynamic method	52	
20	6.6	0.0027	−2.57	wetted- wall column	118	distilled water, not consistent with other properties
20	13	0.0053	−2.28		118	seawater
LDV at 25 °C	0.72	0.00029	−3.54	directly take the value at 25 °C		
FAV at 25 °C	0.70	0.00028	−3.55			

Octanol−Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	5.5×10^4	4.74	shake flask - GC	107	
25	6.8×10^3	3.83	shake flask - GC	119	not consistent with other properties
LDV at 25 °C	5.5×10^4	4.74	directly take the value at 25 °C		
FAV at 25 °C	8.7×10^4	4.94			

Octanol−Air
Partition Coefficient

t/°C	K_{OA}	log K_{OA}	method	ref	note
5	4.8×10^9	9.68	generator column - GC	12	calcd from the linear eq log K_{OA} = 4333/(T/K) − 5.9 (5 to 25) °C
10	2.5×10^9	9.40			
15	1.4×10^9	9.14			
20	7.6×10^8	8.88			
25	4.3×10^8	8.63			
25	6.8×10^8	8.83	GC - retention time		Li, unpublished
LDV at 25 °C	4.3×10^8	8.63	directly take the value at 25 °C		
FAV at 25 °C	3.1×10^8	8.49			

Octanol Solubility
not found

other cases, the true melting temperature T_M was not observed properly.

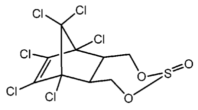
No articles reporting measured data for the melting point and the heat fusion of endrin have been found. Plato reported that endrin decomposes when it is heated to the melting point.[14] In a study by Ksiazczak and Nagata,[15] endrin showed an endothermic peak and a large exothermic peak during heating. The endothermic peak was assigned to a solid-rotator transition, and the exothermic peak was assigned to decomposition. In a DSC curve for endrin by Rodante et al.,[16] two endothermic peaks occur before endrin decomposes. The reported onset temperature and enthaly change of the first and larger of these two peaks are in agreement with the results by Ksiazczak and Nagata, but unfortunately, no thermodynamic information is provided for the second tiny peak. To convert its solid properties into those of the supercooled liquid, the melting temperature and entropy of fusion were estimated. T_{tr} was taken as the T_M value, and $\Delta_{fus}S$ was calculated from T_{tr} and $\Delta_{tr}H$ taken from the literature.[15,16]

Results and Discussion

The physical−chemical properties for 14 OCPs are compiled in Tables 1 to 14. At the top of each Table are

Table 14. Reported and Selected Physical–Chemical Properties for β-Endosulfan

common name	β-endosulfan	t_M/°C	213.1	15
CAS registry no.	33213-65-9	$\Delta_{fus}S$/J·K^{-1}·mol^{-1}	51.89	15
formula	$C_9H_6Cl_6O_3S$			
MW/g·mol^{-1}	406.9			



Vapor Pressure

t/°C	P_S/Pa	P_L/Pa	log(P_L/Pa)	method	ref	note
5		0.00040	−3.40	GC - retention time	36	calcd from the reported equation log(P_L/Pa) = −4306/(T/K) + 12.08 used anyhow
15		0.0014	−2.86			
25		0.0043	−2.36			
35		0.0013	−1.89			
45		0.0035	−1.45			
LDV at 25 °C		0.0043	−2.36	directly take the value at 25 °C		
FAV at 25 °C		0.0040	−2.40			

Aqueous Solubility

t/°C	S_{WS}/mol·m^{-3}	S_{WL}/mol·m^{-3}	log(S_{WL}/mol·m^{-3})	method	ref	note
20	0.0011	0.11	−0.96	shake flask - GC	116	
25	0.00069	0.057	−1.25	generator column - GC	38	
20	0.00028	0.028	−1.56	liquid–liquid extraction - GC/MS	117	not consistent with other properties
LDV at 25 °C		0.079	−1.10	log mean of the values at 20 and 25 °C		
FAV at 25 °C		0.089	−1.05			

Henry's Law Constant

t/°C	H/Pa·m^3·mol^{-1}	K_{AW}	log K_{AW}	method	ref	note
25	0.72	0.000016	−4.80	thermodynamic method	52	
20	6.6	0.000360	−3.44	wetted-wall column	118	distilled water, not consistent with other properties
20	13	0.000870	−3.06		118	seawater
LDV at 25 °C	0.040	0.000016	−4.80	directly take the value at 25 °C		
FAV at 25 °C	0.045	0.000018	−4.74			

Octanol–Water
Partition Coefficient

t/°C	K_{OW}	log K_{OW}	method	ref	note
25	6.0 × 10^4	4.78	shake flask - GC	107	
25	4.2 × 10^3	3.62	shake flask - GC	119	not consistent with other properties
LDV at 25 °C	6.0 × 10^4	4.78	directly take the value at 25 °C		
FAV at 25 °C	6.0 × 10^4	4.78			

Octanol–Air
Partition Coefficient
not found

Octanol Solubility
not found

Table 15. Literature-Derived Values (LDVs) and Assigned Uncertainty Estimates (*u*) for the Physical–Chemical Properties of 14 Organochlorine Pesticides at 25 °C

	P_L/Pa		S_{WL}/mol·m^{-3}		H/Pa·m^3·mol^{-1}		log K_{OW}		log K_{OA}	
compound	LDV	u_A	LDV	u_W	LDV	u_{AW}	LDV	u_{OW}	LDV	u_{OA}
HCB	0.14	1	0.00096	1	52	3	5.52	1	7.38	3
PeCB	1.2	1	0.011	2	74	3	5.08	1	6.90	3
p,p′-DDT	0.00056	1	0.00027	3	1.1	3	6.28	3	9.81	2
p,p′-DDE	0.0033	3	0.00081	3	4.2	5	6.96	5	9.69	3
p,p′-DDD	0.00097	3	0.0028	3	0.67	5	6.22	5	10.10	3
CC	0.0080	3	0.0011	5	6.0	5	6.10	4	8.91	3
TC	0.013	3	0.0011	5	6.0	5	6.22	4	8.86	3
HEPT	0.13	3	0.0035	2	30	5	6.10	4	7.64	3
HEPX	0.013	5	0.018	3	2.1	4	5.40	3	8.62	5
aldrin	0.061	1	0.0029	2	15	5	6.50	4	8.07	3
dieldrin	0.016	1	0.012	2	1.0	4	5.40	5	8.89	3
endrin	0.0052	5	0.0027	2	0.64	4	5.20	4	8.13	3
α-endo	0.0060	3	0.0042	5	0.72	4	4.74	4	8.63	3
β-endo	0.0043	3	0.079	5	0.040	4	4.78	4		

the data that are included in the derivation of the LDVs, including the experimental temperature, the method used, and the literature reference. For comparison and completeness, the data that are not included in the derivation of the LDVs are also listed, together with the reason for exclusion. The LDVs and FAVs at 25 °C for each property are given at the bottom of Tables 1 to 14. A summary of the LDVs for the 14 chemicals at 25 °C is presented in Table 15 along with the uncertainty estimates u_X assigned to each property. The corresponding FAVs and the required

Table 16. Internally Consistent Physical−Chemical Properties (Final Adjusted Values, FAV) at 25 °C and the Percent Required Adjustment (adj) for 14 Organochlorine Pesticides

	P_L/Pa		S_{WL}/mol·m^{-3}		H/Pa·m^3·mol^{-1}		log K_{OW}		log K_{OA}		S_{OL}/mol·m^{-3}
compound	FAV	adj/%	FAV	adj/%	FAV	adj/%	FAV	adj/%	FAV	adj/%	FAV
HCB	0.094	−33	0.0014	49	65	26	5.64	30	7.21	−32	618
PeCB	1.0	−13	0.014	31	72	−4	5.19	30	6.73	−33	2212
p,p′-DDT	0.00048	−14	0.00042	55	1.1	0	6.39	30	9.73	−16	1053
p,p′-DDE	0.0034	3	0.00079	−3	4.2	0	6.93	−5	9.70	3	6830
p,p′-DDD	0.0012	20	0.0023	−16	0.50	−25	6.33	31	10.03	−15	4986
CC	0.0073	−9	0.0013	16	5.7	−6	6.20	25	8.83	−15	2017
TC	0.010	−19	0.0015	43	6.8	13	6.27	11	8.83	−8	2783
HEPT	0.13	0	0.0035	0	38	28	5.94	−30	7.76	31	3099
HEPX	0.022	69	0.013	−27	1.7	−21	5.42	4	8.59	−7	3466
aldrin	0.064	4	0.0027	−4	23	55	6.24	−45	8.26	57	4720
dieldrin	0.014	−12	0.013	14	1.1	8	5.48	22	8.84	−11	4027
endrin	0.0031	−40	0.0030	11	1.1	64	4.94	−44	8.32	54	262
α-endo	0.0044	−26	0.0063	51	0.70	−2	4.94	58	8.49	−29	546
β-endo	0.0040	−9	0.089	13	0.045	13	4.78		9.53		5357

Table 17. Sample Calculation for Obtaining Internally Consistent Final Adjusted Values (FAV) of Hexachlorobenzene

	P_L/Pa	S_A/mol·m^{-3}	S_{WL}/mol·m^{-3}	K_{AW}	K_{OW}	K_{OA}	ϵ_1	ϵ_2
LDV	0.14	0.000056	0.00096	0.021	3.3 × 10^5	2.4 × 10^7		
log LDV	−0.855	−4.249	−3.018	−1.678	5.522	7.384	−0.448	0.183
u_X		1	1	3	2	3		
δ_X (eq 7)		−0.090	−0.090	−0.269				
δ_X (eq 8)				0.069	0.046	0.069		
δ_X (final)		−0.174	−0.174	−0.100	0.113	0.170		
log FAV		−4.423	−2.845	−1.578	5.635	7.214	0.000	0.000
FAV	0.093	0.000039	0.0014	0.026	4.3 × 10^5	1.6 × 10^7		

Table 18. Literature-Derived Values (LDV) and Assigned Uncertainty Estimates (*u*) for the Internal Phase-Transfer Energies of Hexa- and Pentachlorobenzene

	ΔU_A/kJ·mol^{-1}		ΔU_W/kJ·mol^{-1}		ΔU_{AW}/kJ·mol^{-1}		ΔU_{OW}/kJ·mol^{-1}		ΔU_{OA}/kJ·mol^{-1}	
compd	LDV	u_A	LDV	u_W	LDV	u_{AW}	LDV	u_{OW}	LDV	u_{OA}
HCB	67.59[a]	1	9.50[c]	3	47.70[d]	3	−24.40[e]	3	−75.50[f]	3
PeCB	61.65[b]	1	12.10[c]	3	40.60[d]	3	−22.80[e]	3	−71.25[f]	3

[a] Regression of log(P_L/Pa) vs 1/(*T*/K) using data from refs 24 and 28−34. [b] Regression of log(P_L/Pa) vs 1/(*T*/K) using data from refs 35, 71, and 72. [c] Derived from data given in ref 37. [d] Derived from data given in derived form from data given in ref 50. [e] Derived from data given in ref 54. [f] Derived from data given in ref 13.

Table 19. Internally Consistent Final Adjusted Values (FAV) of the Energies of Phase Transfer for Hexa- and Pentachlorobenzene and Percent Required Adjustment (adj)

	ΔU_A/kJ·mol^{-1}		ΔU_W/kJ·mol^{-1}		ΔU_{AW}/kJ·mol^{-1}		ΔU_{OW}/kJ·mol^{-1}		ΔU_{OA}/kJ·mol^{-1}		ΔU_O/kJ·mol^{-1}
compd	FAV	adj/%	FAV	adj/%	FAV	adj/%	FAV	adj/%	FAV	adj/%	FAV
HCB	65.69	−3	15.20	60	50.49	6	−24.70	1	−75.20	−0.4	−9.51
PeCB	60.22	−2	16.39	35	43.83	8	−25.11	10	−68.94	−3	−8.72

percentage adjustment for the 14 chemicals are listed in Table 16.

LDVs could be derived for all properties, except for the solubility in octanol. Also, no measured K_{OA} for *β*-endosulfan could be found during our literature search. One study[18] reported S_{OS} for most of the investigated chemicals, but these data are inconsistent with other measured properties. Although the measured S_{OS} data were not used in the adjustment algorithm, they are still included in the Tables. All S_{OL} values and the K_{OA} of *β*-endosulfan in Table 16 are calculated from the other properties using thermodynamic constraints.

When deriving LDVs for the solubility of the chlordanes, the measured S_{WS} value from Warner[19] had to be applied to both cis and trans isomers because of the lack of isomer-specific measurements. Liquid-phase solubility S_{WL} values were then calculated according to eq 1 using isomer-specific T_M and $\Delta_{fus}S$ values. The LDVs for the Henry's law constant *H* of the cis and trans isomers of chlordane are also identical. Although isomer-specific *H* values for *cis*- and *trans*-chlordane had been reported by Atlas et al.,[20] those data are not consistent with other property measurements. Nevertheless, it is encouraging to see good consistency between the five LDVs for the two isomers, which points to accurate measurements and suggests that the real solubility and *H* values are likely close to the LDV values.

Property Values at 25 °C. The physical−chemical properties for most OCPs are difficult to measure accurately. The variability of the literature data listed in Tables 1 to 14 gives an approximate indication of the considerable uncertainty of these values. The measured data for the water solubility of the OCPs shows especially large discrepancies (Figure 1). However, the literature-derived values for the 14 OCPs are reasonably consistent. In general, most properties needed to be adjusted by less than 30% to achieve consistency. Out of 70 property values for 14 OCPs, 8 required adjustments are higher than 50%; and the maximum adjustment to the LDVs at 25 °C is 69%. The required adjustments thus occur normally well within the range of the measured values (i.e., no FAV falls outside the range of reported literature values). This indicates that the procedure applied in the selection of the LDVs is successful in selecting already reasonably consistent property values.

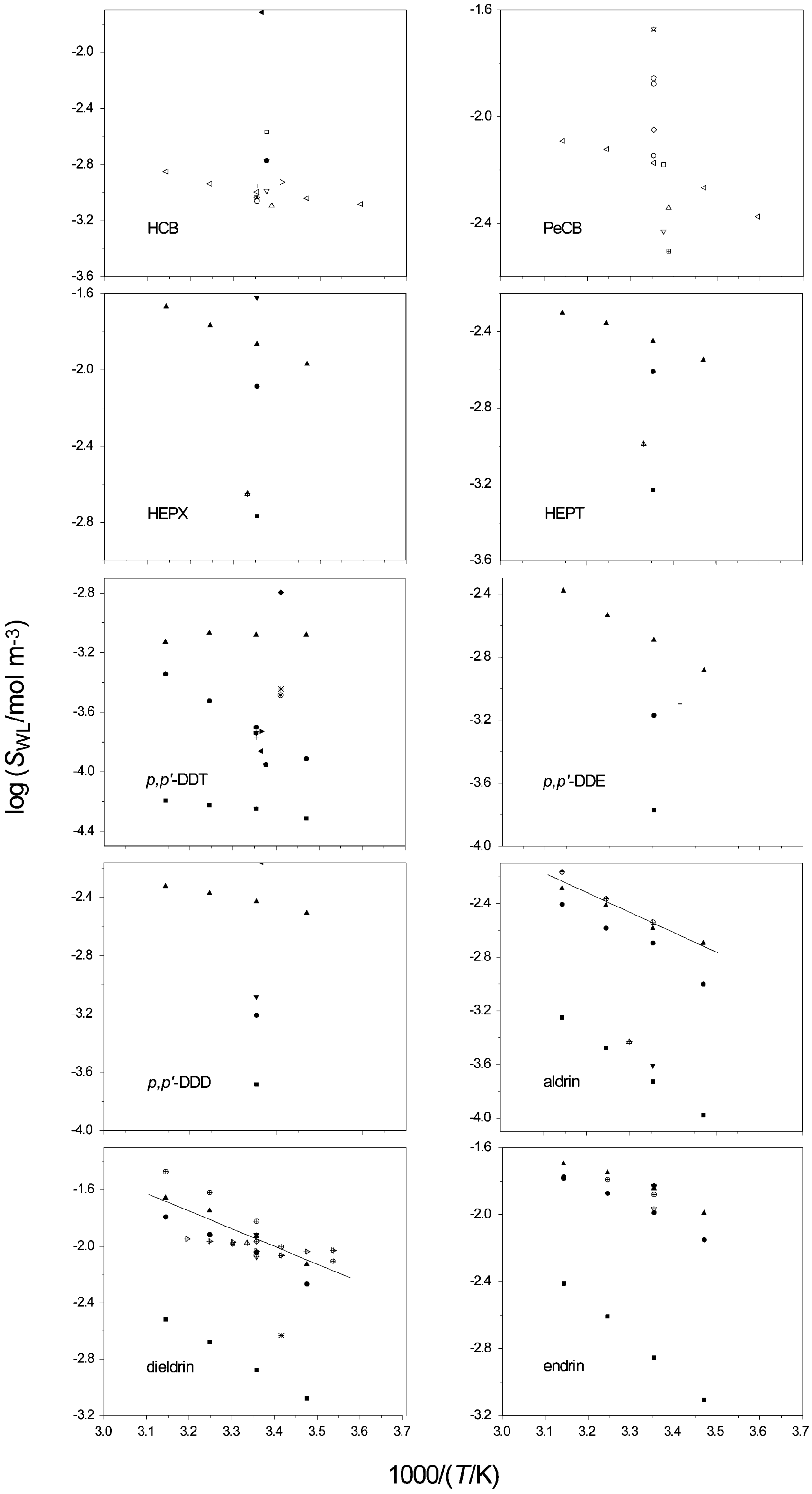


Figure 1. Relationships between the logarithm of the water solubility (log S_{WL}/ mol·m^{-3}) and the reciprocal absolute temperature [1/(*T*/K)] for hexachlorobenzene (HCB), pentachlorobenzene (PeCB), heptachlor (HEPT), and heptachlor epoxide (HEPX), *p*,*p*′-DDT, *p*,*p*′-DDE, *p*,*p*′-DDD, aldrin, dieldrin, and endrin based on data from Shiu et al. (open, left-pointing triangle);[37] Weil et al. (▼);[38] Miller et al. (○);[39] Hashimoto et al. (open, right-pointing triangle);[40] Yalkowsky et al. (◇);[41] Patton (⬟);[42] Konemann (△);[43] Chiou (⬢);[44] Li and Yalkowsky (▽);[45] Paschke et al. (×);[46] Metcalf et al. (|);[47] Hollifield (black, left-pointing triangle);[48] Chiou (⬣);[55] Opperhuizen et al. (open square with cross);[73] Boyd et al. (⬠);[74] Banerjee (☆);[75] Atkins and Eggleton (∗);[84] Webster et al. (⊙);[85] Chiou et al. (black, right-pointing triangle);[87] Ellgehausen et al. (◆);[88] Biggar and Riggs, 0.01 *μ*m (■), 0.05 *μ*m (●), and 5 *μ*m (▲);[89] Biggar (★);[90] Robeck et al., 0.06 *μ*m (open, downward-pointing traingle with cross), 5 *μ*m (open diamond with cross);[92] Chiou et al. (−);[101] Park and Bruce (open, upward-pointing triangle with cross);[106] Richardson and Miller (⊕);[110] Eye (open, right-pointing triangle with cross);[113] and Bowman and Sans (open hexagon with cross).[114]

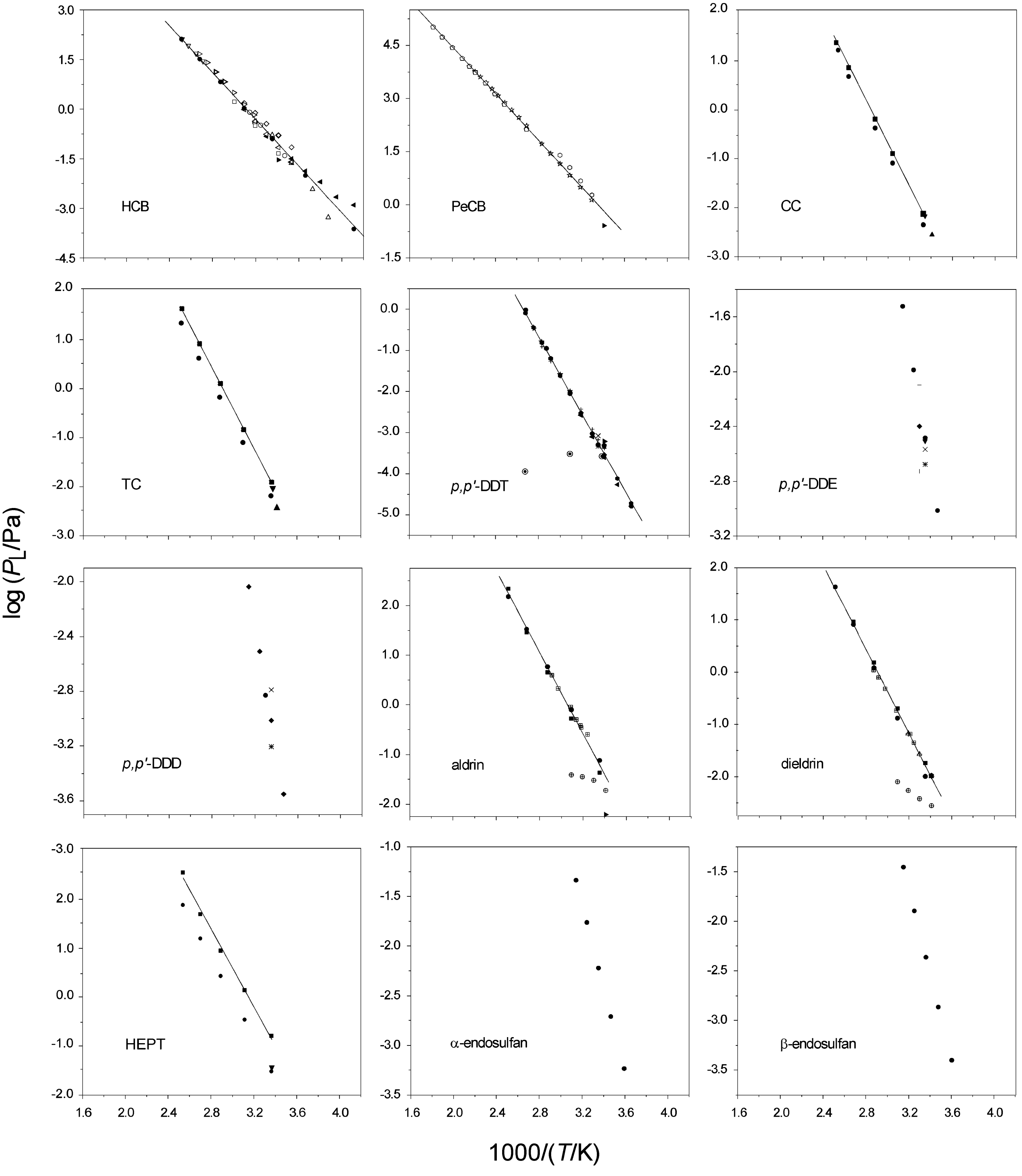


Figure 2. Relationships between the logarithm of the liquid vapor pressure (log P_L/Pa) and the reciprocal absolute temperature [1/(*T*/K)] for hexachlorobenzene (HCB), pentachlorobenzene (PeCB), *cis*-chlordane (CC), *trans*-chlordane (TC), *p,p'*-DDT, *p,p'*-DDE, *p,p'*-DDD, aldrin, dieldrin, heptachlor (HEPT), α-endosulfan, and *β*-endosulfan based on data from Sears and Hopke (▽);[24] Liu and Dickhut (△);[28] Wania et al. (black, left-pointing triangle);[29] Farmer et al. (○);[30] Rordorf et al. (open, right-pointing triangle);[31] OECD (◇);[32] Dobbs and Cull (black, right-pointing triangle);[33] Gückel et al. (□);[34] Stull et al. (⌂);[35] Hinckley et al. (●);[36] Rordorf (⬡);[71] Polednicek et al. (☆);[72] Rothman (+);[80] Spencer and Cliath (◆);[81] Dickinson (★);[82] Atkins and Eggleton (⬟),[84] Webster et al. (⊙);[85] Bidleman, BP-1 (×); Apolane-87 (∗);[86] Westcott et al. (−);[99] Westcott and Bidleman (|);[100] Bidleman et al. (▲);[102] Grayson and Fosbraey (open square with cross);[108] Porter (open hexagon with cross);[109] Spencer and Cliath (open, upward-pointing triangle with cross);[112] Li, unpublished (▼); and Rordorf, unpublished (■).

The LDVs and FAVs for the properties of α-endosulfan presented here are slightly different from those reported previously.[21] The previous data were obtained by using a default value for $\Delta_{fus}S$ because Donnely's value was judged to be unreasonably low.[22] Since then, an experimentally determined $\Delta_{fus}S$ for α-endosulfan by Rodante et al.[17] has

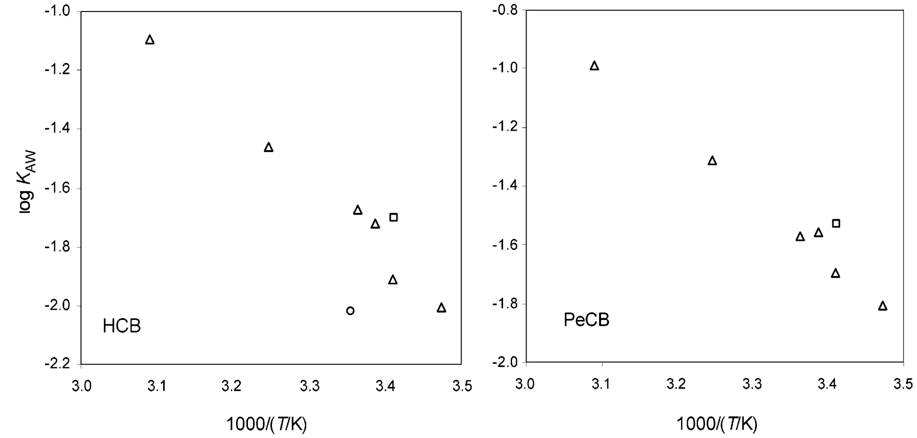


Figure 3. Relationships between the logarithm of the air−water partition coefficient (log K_{AW}) and the reciprocal absolute temperature [1/(*T*/K)] for HCB and PeCB based on 10 data points from Hulscher (△);[50] Oliver (□);[51] and Altschuh (○).[52]

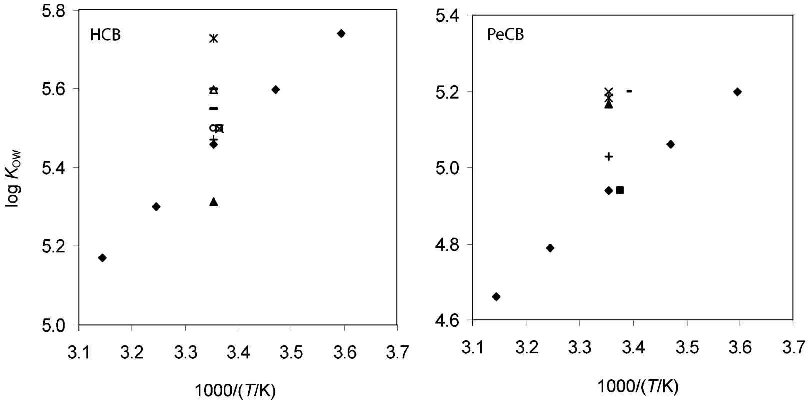


Figure 4. Relationships between the logarithm of the octanol−water partition coefficient (log K_{OW}) and the reciprocal absolute temperature [1/(*T*/K)] for HCB and PeCB based on data from Miller et al. (+);[39] Chiou (-);[44] Bahadur et al. (◆);[54] Chiou and Schmedding (□);[55] Pereira et al. (×);[56] Watarai et al. (▲);[57] De Bruijn (*);[58] Brook et al. (△);[59] Toll et al. (○);[60] Andersson and Schrader (−)[61]; and Banerjee et al. (■).[75]

been located and was used in this study. This should lead to smaller errors in the calculated liquid properties of α-endosulfan.

Specimen Calculation of the Final Adjustment. To apply the adjustment algorithm by Beyer et al.,[9] all properties need to be converted either into solubilities in units of mol·m^{-3} or into a dimensionless partition coefficient. The solubility in air, S_A, can be derived from the supercooled vapor pressure using

$$S_A/\text{mol}\cdot\text{m}^{-3} = \frac{n/\text{mol}}{V/\text{m}^3} = \frac{P_L/\text{Pa}}{(R/\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})(T/\text{K})} \quad (4)$$

According to Cole and Mackay,[120] the properties S_A, S_{WL}, K_{AW}, K_{OW}, and K_{OA} can be related through two constraining equations

$$\log K_{AW} = \log (S_A/\text{mol}\cdot\text{m}^{-3}) - \log (S_{WL}/\text{mol}\cdot\text{m}^{-3}) \quad (5)$$

$$\log K_{AW} = \log K_{OW} - \log K_{OA} \quad (6)$$

The deviation ϵ from the ideal relationship caused by experimental errors is expressed as

$$\log K_{AW}^{LDV} - \log (S_A^{LDV}/\text{mol}\cdot\text{m}^{-3}) + \log (S_{WL}^{LDV}/\text{mol}\cdot\text{m}^{-3}) = \epsilon_1 \quad (7)$$

$$\log K_{AW}^{LDV} - \log K_{OW}^{LDV} + \log K_{OA}^{LDV} = \epsilon_2 \quad (8)$$

The goal when obtaining FAVs is to adjust the LDVs by factors δ_X such that eqs 5 and 6 are fully satisfied; that is, the deviations derived from eqs 9 and 10 are equal to zero.

$$(\log K_{AW}^{LDV} - \delta_{AW}) - [\log (S_A^{LDV}/\text{mol}\cdot\text{m}^{-3}) + \delta_A] + [\log (S_{WL}^{LDV}/\text{mol}\cdot\text{m}^{-3}) - \delta_{WL}] = 0 \quad (9)$$

$$(\log K_{AW}^{LDV} - \delta_{AW}) - (\log K_{OW}^{LDV} + \delta_{OW}) + (\log K_{OA}^{LDV} - \delta_{OA}) = 0 \quad (10)$$

Therefore,

$$\log (S_A^{FAV}/\text{mol}\cdot\text{m}^{-3}) = \log (S_A^{LDV}/\text{mol}\cdot\text{m}^{-3}) + \delta_A \quad (11)$$

$$\log (S_{WL}^{FAV}/\text{mol}\cdot\text{m}^{-3}) = \log (S_{WL}^{LDV}/\text{mol}\cdot\text{m}^{-3}) - \delta_{WL} \quad (12)$$

$$\log K_{AW}^{FAV} = \log K_{AW}^{LDV} - \delta_{AW} \quad (13)$$

$$\log K_{OW}^{FAV} = \log K_{OW}^{LDV} + \delta_{OW} \quad (14)$$

$$\log K_{OA}^{FAV} = \log K_{OA}^{LDV} - \delta_{OA} \quad (15)$$

The adjustment factor δ_X for each property is calculated on the basis of the assigned uncertainty u_X.

$$\delta_X = \epsilon \frac{u_X}{\sum u_X} \quad (16)$$

Beyer et al.[9] proposed two approaches to derive the FAVs.

One approach is to apply iterations. Equations 7 and 8 are used to derive ϵ_1 and ϵ_2 and δ_X for one property (i.e., K_{AW}), and the properties are adjusted separately using both equations. The adjusted properties are then used to derive new ϵ and δ_X values. By repeating this iteration, the properties will converge to a set (FAVs) that is consistent with both eqs 7 and 8. The second approach also first deduces different ϵ and δ_X values separately according to eqs 7 and 8. For the property that occurs in both equations (i.e., K_{AW}), the mean adjustment factor is calculated and applied to both equations. The δ_X values for the remaining properties (i.e., S_A and S_{WL}) in the constraining equation are then adjusted again on the basis of their uncertainties to account for the remaining error in the equation. The deviations between the two approaches have been discussed by Beyer et al.,[9] and the same adjusted properties were obtained for PCB 15 when applying both methods.

As an example, HCB is used to illustrate the second approach of obtaining consistent values (FAVs) for P_L, S_{WL}, K_{AW}, K_{OW}, and K_{OA} from their LDVs (Table 1). The properties used in the adjustment algorithm are presented in Table 17. Inserting the LDVs of HCB into eqs 7 and 8, we find that ϵ_1 and ϵ_2 are $-$ 0.448 and 0.183, respectively. On the basis of eq 16, the δ_X value of each property is derived separately according to ϵ_1 and ϵ_2 and listed in Table 15. The δ_{AW} values of log K_{AW} are -0.269 (eq 7) and 0.069 (eq 8). The LDV of log K_{AW} is thus corrected by the mean (-0.100) of -0.269 and 0.069. The δ_A and δ_{WL} for eq 9 are then modified according to the uncertainties of S_A and S_{WL} to account for the remaining error of ϵ_1 (-0.348); δ_{OW} and δ_{OA} are deduced accordingly. All final δ_X values are listed in Table 17. Substituting the LDV and the final δ_X of each property into eqs 9 and 10 satisfies both equations. The logarithm of FAV for each property is thus obtained using eqs 11 to 15.

Energies of Phase Transfer. Because of the lack of measured temperature-dependence data for most investigated chemicals, the LDVs of the internal energies of phase transfer, ΔU, could be derived only for HCB and PeCB. These values are presented in Table 18 together with their origin and uncertainty estimate. The FAVs for the ΔU values and the required percentage of adjustment are given in Table 19. Plots of the logarithm of the measured data for a property versus reciprocal absolute temperature are shown in Figures 1 to 4. In general, the measured temperature dependence of the properties for HCB and PeCB is in good agreement. The required adjustments to the energies of phase transfer ΔU are usually less than 10%; only the measured temperature dependence of the water solubilities ΔU_W needed to be adjusted by a higher percentage (Table 19). Compared to the other energies of phase transition, the absolute value of ΔU_W is small. This makes the relative adjustment of ΔU_W appear to be large, even though the absolute adjustment of ΔU_W is not much larger than that of the other phase-transfer energies.

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Literature Cited

(1) George, J. L.; Frear, D. E. H. Pesticides in the Antarctic. *J. Appl. Ecol.* **1966**, *3*, 155−167.
(2) Bidleman T. F.; Olney C. E. Chlorinated hydrocarbons in the Sargasso Sea atmosphere and surface water. *Science* **1974**, *183*, 516−518.
(3) Halsall, C. J. Investigating the occurrence of persistent organic pollutants POPs in the Arctic: their atmospheric behavior and interaction with the seasonal snow pack. *Environ. Pollut.* **2004**, *128*, 163−175.
(4) Meijer, S. N.; Ockenden, W. A.; Steinnes, E.; Corrigan, B. P.; Jones, K. C. Spatial and Temporal Trends of POPs in Norwegian and UK Background Air: Implications for Global Cycling. *Environ. Sci. Technol.* **2003**, *37*, 454−461.
(5) Wania F.; Mackay D. The evolution of mass balance models of persistent organic pollutant fate in the environment. *Environ. Pollut.* **1999**, *100*, 223−40.
(6) United Nations Environment Programme, UNEP, North American regional report, regionally based assessment of persistent toxic substances. Global Environment Facility, United Nations, 2002.
(7) Mackay, D.; Shiu, W. Y.; Ma, K. C. *Physical-Chemical Properties and Environmental Fate Handbook*; Chapman & Hall/CRCnet Base: Boca Raton, FL, 2000.
(8) Pontolillo, J.; Eganhouse, R. P. *The Search for Reliable Aqueous Solubility S_w and Octanol-Water Partition Coefficient K_{OW} Data for Hydrophobic Organic Compounds: DDT and DDE as a Case Study*; U.S. Geological Survey Water-Resources Investigation Report 01-4201: 2001.
(9) Beyer, A.; Wania, F.; Gouin, T.; Mackay, D.; Matthies, M. Selecting internally consistent physicochemical properties of organic compounds. *Environ. Toxicol. Chem.* **2002**, *21*, 941−953.
(10) Li, N.; Wania, F.; Lei, Y. D.; Daly, G. L. A comprehensive and critical compilation, evaluation, and selection of physical-chemical property data for selected polychlorinated biphenyls. *J. Phys. Chem. Ref. Data* **2003**, *32*, 1545−1590.
(11) Xiao, H.; Li, N.; Wania, F. Compilation, Evaluation, and Selection of Physical-Chemical Property Data for α-, β-, and γ-Hexachlorocyclohexane. *J. Chem. Eng. Data* **2004**, *49*, 173−185.
(12) Shoeib, M.; Harner, T. Using measured octanol-air partition coefficients to explain environmental partitioning of organochlorine pesticides. *Environ. Toxicol. Chem.* **2002**, *21*, 984−990.
(13) Harner, T.; Mackay, D. Measurement of octanol-air partition coefficients for chlorobenzenes, PCBs, and DDT. *Environ. Sci. Technol.* **1995**, *29*, 1599−1606.
(14) Plato, C. Differential Scanning Calorimetry as a General Method for Determining Purity and Heat of Fusion of High-Purity Organic Chemicals. Application to 64 Compounds. *Anal. Chem.* **1972**, *44*, 1531−1534.
(15) Ksiazczak, A.; Nagata, I. Crystal-plastic and plastic−liquid phase transitions, and purity determination. *Thermochim. Acta* **1995**, *254*, 31−39.
(16) Rodante, F.; Marrosu, G.; Catalani, G. Thermal analysis and kinetic study of decomposition processes of some pesticides. *J. Therm. Analysis* **1992**, *38*, 2669−2682.
(17) Rodante, F.; Vecchio, S.; Catalani, G.; Guidotti, M. Thermal analysis and nonisothermal kinetic study of some pesticides. Part II, chlorinate ferivatives. *J. Therm. Anal. Calorim.* **2002**, *60*, 605−622.
(18) Niimi, A. J. Solubility of organic chemicals in octanol triolein and cod liver oil and relationships between solubility and partition coefficients. *Water Res.* **1991**, *25*, 1515−1521.
(19) Warner, H. P.; Cohen, J. M.; Ireland, J. C. *Determination of Henry's Law Constants of Selected Priority Pollutants*; EPA/600/D-87/229; NTIS PB87-212684; U.S. Environmental Protection Agency: Cincinnati, OH, 1987.
(20) Atlas, E. L.; Foster, R.; Giam, C. S. Air−Sea Exchange of High Molecular Weight Organic Pollutants: Laboratory Studies. *Environ. Sci. Technol.* **1982**, *16*, 283−286.
(21) Muir, D. C. G.; Teixeira, C.; Wania, F. Empirical and modeling evidence of regional atmospheric transport of currently used pesticides. *Environ. Toxicol. Chem.* **2004**, *23*, 2421−2432.
(22) Donnelly, J. R.; Drewes, L. A.; Johnson, R. L.; Munslow, W. D.; Knapp, K. K. Purity and heat of fusion data for environmental standards as determined by differential scanning calorimetry. *Thermochim. Acta* **1990**, *167*, 155−187.
(23) Miller, M. M.; Ghodbane, S.; Wasik, S. P.; Tewari, Y. B.; Martire, D. E. Aqueous Solubilities, Octanol/Water Partition Coefficients, and Entropies of Melting of Chlorinated Benzenes and Biphenyls. *J. Chem. Eng. Data* **1984**, *29*, 184−190.
(24) Sears, G. W.; Hopke, E. R. Vapor Pressures of nAphthalene, Anthracene, and Hexachlorobenzene in a Low-Pressure Region. *J. Am. Chem. Soc.* **1949**, *71*, 1632−1634.
(25) Sabbah, R.; An, X. W. Thermodynamic analysis of chlorobenzenes. *Thermochim. Acta* **1991**, *179*, 81−88.
(26) Sabbah, R.; El Watik, L. New reference materials for the calibration temperature and energy of differential thermal analysers and scanning calorimeters. *J. Therm. Analysis* **1992**, *38*, 855−863.
(27) Plato, C.; Glasgow, A. R., Jr. Differential scanning calorimetry as a general method for determining the purity and heat of fusion of high-purity organic chemicals. Application to 95 compounds. *Anal. Chem.* **1969**, *41*, 330−336.
(28) Liu, K.; Dickhut, R. M. Saturation vapor pressures and thermodynamic properties of benzene and selected chlorinated benzenes at environmental temperatures. *Chemosphere* **1994**, *29*, 581−589.

(29) Wania, F.; Shiu, W. Y.; Mackay, D. Measurement of the Vapor Pressure of Several Low-Volatility Organochlorine Chemicals at Low Temperatures with a Gas Saturation Method. *J. Chem. Eng. Data* **1994**, *39*, 572−577.

(30) Farmer, W. J.; Yang, M. S.; Letey, J.; Spencer, W. F. Hexachlorobenzene: Its vapor presure and vapor phase diffuson in soil. *Soil Sci. Soc. Am. J.* **1980**, *44*, 676−680.

(31) Rordorf, B. F.; Sarna, L. P.; Webster, G. R. B. Vapor pressure determination for several polychlorodioxins by two gas saturation methods. *Chemosphere* **1986**, *15*, 2073−2076.

(32) *OECD Test Guideline No 4: Vapour pressure curve*; Report No. 104, 1981.

(33) Dobbs, A. J.; Cull, M. R. Volatilisation of chemicals - Relative loss rates and the estimation of vapor pressures. *Environ. Pollut. B* **1982**, *3*, 289−298.

(34) Gückel, W.; Kastel, R.; Lewerenz, J.; Synnatschke, G. A method for determining the volatility of active ingredients used in plants protection. Part III: The temperature relationship between vapour pressure and evaporation rate. *Pestic. Sci.* **1982**, *13*, 161−168.

(35) Stull, D. R. Vapor Pressure of Pure Substances: Organic Compounds. *Ind. Eng. Chem.* **1947**, *39*, 517−550.

(36) Hinckley, D. A.; Bidleman, T. F.; Foreman, W. T.; Tuschall, J. R. Determination of Vapor Pressures for Nonpolar and Semipolar Organic Compounds from Gas Chromatographic Retention Data. *J. Chem. Eng. Data* **1990**, *35*, 232−237.

(37) Shiu, W. Y.; Wania, F.; Hung, H.; Mackay, D. Temperature Dependence of Aqueous Solubility of Selected Chlorobenzenes, Polychlorinated Biphenyls, and Dibenzofuran. *J. Chem. Eng. Data* **1997**, *42*, 293−297.

(38) Weil, L.; Dure, G.; Quentin, K.-E. Solubility in water of insecticide chlorinated hydrocarbons and polychlorinated biphenyls in view of water pollution. *Wasser-Abwasserforsch.* **1974**, *7*, 169−175.

(39) Miller, M. M.; Wasik, S. P.; Huang, Shiu, W. Y.; Mackay, D. Relationships between Octanol−Water Partition Coefficient and Aqueous Solubility. *Environ. Sci. Technol.* **1985**, *19*, 522−529.

(40) Hashimoto, Y.; Tokura, K.; Ozaki, K.; Strachan, W. M. J. A comparison of water solubilities by the flask and micro-column methods. *Chemosphere* **1982**, *11*, 991−1001.

(41) Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. Solubility and Partitioning. III: The Solubility of Halobenzenes in Water. *Ind. Eng. Chem. Fundam.* **1979**, *18*, 351−353.

(42) Patton, J. S.; Stone, B.; Papa, C.; Abramowitz, R. Solubility of fatty acid and other hydrophobic molecules in liquid trioleoylglcerol. *J. Lipid Res.* **1984**, *25*, 189−197.

(43) Könemann, W. H.; Musch, A. Quantitative structure-activity relationships in fish toxicity studies. Part 1: Relationship for 50 industrial pollutants. *Toxicology* **1981**, *19*, 209−221.

(44) Chiou, C. T. Partition Coefficients of Organic Compounds in Lipid−Water Systems and Correlations with Fish Bioconcentration Factors. *Environ. Sci. Technol.* **1985**, *19*, 57−62.

(45) Li, A.; Yalkowsky, S. H. Solubility of organic solutes in ethanol/water mixtures. *J. Pharm. Sci.* **1994**, *83*, 1735−1740.

(46) Paschke, A.; Popp, P.; Schüürmann, G. Water solubility and octanol/water partitioning of hydrophobic chlorinated organic substances determined by using SPME/GC. *Fresenius' J. Anal. Chem.* **1998**, *360*, 52−57.

(47) Metcalf, R. L.; Kapoor, I. P.; Lu, P.-Y.; Schuth, C. K.; Sherman, P. Model ecosystem studies of the environmental fate of six organochlorine pesticides. *Environ. Health Perspect.* **1973**, *4*, 35−44.

(48) Hollifield, H. C. Rapid nephelometric estimate of water solubility of highly insoluble organic chemicals of environmental interest. *Bull. Environ. Contam. Toxicol.* **1979**, *23*, 579−586.

(49) Chin, Y.; Weber, W. J.; Voice, T. C. Determination of partition coefficient and aqueous solubilities by reverse phase chromatography-II. *Water. Res.* **1986**, *20*, 1443−1450.

(50) ten Hulscher, Th. E. M.; van der Velde, L. E.; Bruggeman, W. A. Temperature dependence of Henry's law constants for selected chlorobenzenes, polychlorinated biphenyls and polycyclic aromatic hydrocarbons. *Environ. Toxicol. Chem.* **1992**, *11*, 1595−1603.

(51) Oliver, B. G. Desorption of chlorinated hydrocarbons from spiked and anthropogenically contaminated sediments. *Chemosphere* **1985**, *14*, 1087−1106.

(52) Altschuh, J.; Brüggemann, R.; Santl, H.; Eichinger, G.; Piringer, O. G. Henry's law constants for a diverse set of organic chemicals: Experimental determination and comparison of estimation methods. *Chemosphere* **1999**, *39*, 18711−1887.

(53) Hansen, K. C.; Zhou, Z.; Yaws, C. L.; Aminabhavi, T. M. Determination of Henry's Law Constants of Organics in Dilute Aqueous Solutions. *J. Chem. Eng. Data* **1993**, *38*, 546−550.

(54) Bahadur, N. P.; Shiu, W. Y.; Boocock, D. G. B.; Mackay, D. Temperature Dependence of Octanol−Water Partition Coefficient for Selected Chlorobenzenes. *J. Chem. Eng. Data*, **1997** *42*, 685−688.

(55) Chiou, C. T.; Schmedding, D. W. Partitioning of Organic Compounds in Octanol−Water Systems. *Environ. Sci. Technol.* **1982**, *16*, 4−10.

(56) Pereira, W. E.; Rostad, C. E.; Chiou, C. T.; Brinton, T. I.; Barber, L. B.; Demcheck, D. K.; Demas, C. R. Contamination of Estuarine Water, Biota, and Sediment by Halogenated Organic Compounds: A Field Study. *Environ. Sci. Technol.* **1988**, *22*, 772−778.

(57) Watarai, H.; Tanaka, M.; Suzuki, N. Determination of Partition Coefficient of Halobenzenes in Heptane/Water and 1-Octanol/Water Systems and Comparison with the Scaled Particle Calculation. *Anal. Chem.* **1982**, *54*, 702−705.

(58) De Bruijn, J.; Busser, F.; Seinen, W.; Hermens, J. L. M. Determination of octanol/water partition coefficients for hydrophobic organic chemicals with the 'slow-stirring' method. *Environ. Toxicol. Chem.* **1989**, *8*, 499−512.

(59) Brooke, D. N.; Dobbs, A. J.; Williams, N. Octanol/water partitioning coefffcient P: measure, estimation, and interpretation, particularly for chemicals with $P > 10^5$. *Ecotoxicol. Environ. Saf.* **1986**, *11*, 251−260.

(60) Tolls, J.; Bodo, K.; De Felip, E.; Dujardin, R.; Kim, Y. H.; Moeller-Jensen, L.; Mullee, D.; Nakajima, A.; Paschke, A.; Pawliczek, J.; Tadeo, J.-L.; Tognucci, A.; Webb, J.; Zwijzen, A. C. Slow-Stirring Method for Determining the *n*-Octanol/Water Partition Coefficient P_{ow} for Highly Hydrophobic Chemicals: Performance Evaluation in a Ring Test. *Environ. Sci. Technol.* **2003**, *22*, 1051−1057.

(61) Andersson, J. T.; Schrader, W. A Method for Measuring 1-Octanol−Water Partitioning Coefficient. *Anal. Chem.* **1999**, *71*, 3610−3614.

(62) Platford, R. F.; Carey, J. H.; Hale, E. J. The environmental significance of surface films: Part 1 - octanol-water partition coefficients for DDT and hexachlorobenzene. *Environ. Pollut. B* **1982**, *3*, 125−128.

(63) Könemann, W. H.; Zelle, R.; Busser, F. Determination of log P_{oct} values of chloro-substituted benzenes, toluenes and anilines by high-performance liquid chromatography of ODS-silica. *J. Chromatogr.* **1979**, *178*, 559−565.

(64) Garst, J. E.; Wilson, W. C. Accurate, wide-range, automated, high-performance liquid chromatographic method for the estimation of octanol/water partition coefficients I: Effect of chromatographic conditions and procedure variables on accuracy and reproducibility of the method. *J. Pharm. Sci.* **1984**, *73*, 1616−1623.

(65) McDuffie, B. Estimation of octanol/water partition coefficients for organic pollutants using reverse-phase HPLC. *Chemosphere* **1981**, *10*, 73−83.

(66) De Kock, A. C.; Lord, D. A. A simple procedure for determining octanol−water partition coefficients using reversed phase high performance liquid chromatography RPHPLC. *Chemosphere* **1987**, *16*, 133−142.

(67) Burkhard, L. P.; Kuehl, D. W.; Veith, G. D. Evaluation of reversed phase liquid chromatography/mass spectrometry for estimation of n-octanol/water partition coefficients of organic chemicals. *Chemosphere* **1985**, *14*, 1551−1560.

(68) Eadsforth, C. V. Application of reverse-phase HPLC for the determination of partition coefficients. *Pestic. Sci.* **1986**, *17*, 311−325.

(69) Gobas, F. A. P. C.; Lahittete, J. M.; Garofalo, G.; Shiu, W. Y.; Mackay, D. A novel method for measuring membrane-water partition coefficients of hydrophobic organic chemicals: comparison with 1-octanol-water partitioning. *J. Pharm. Sci.* **1988**, *77*, 265−272.

(70) Veith, G. D.; Austin, N. M.; Morris, R. T. A rapid method for estimation log P for organic chemicals. *Water Res.* **1979**, *13*, 43−47.

(71) Rordorf, B. F. Thermodynamic and thermal properties of polychlorinated compounds: The vapor pressures and flow tube kinetics of 10 dibenzo-para-dioxines. *Chemosphere* **1985**, *14*, 885−892.

(72) Polednicek, M.; Guetachew, T.; Ruzicka, V.; Rohac, V.; Zabransky, M. Vapor pressure and sublimation pressures of dichlorobenzenes 1,2-, 1,3-, 1,4- trichlorobenzenes 1,2,3- and 1,3,5- and pentachlorobenzene. *J. Phys. Chem. Data* **1996**, *2*, 41−50.

(73) Opperhuizen, A.; Velde, E. W. V. D.; Gobas, F. A. P. C.; Liem, D. A. K.; Steen, J. M. D.; Hutzinger, O. Relationship between bioconcentration in fish and steric factors of hydrophobic chemicals. *Chemosphere* **1985**, *14*, 1871−1896.

(74) Boyd, E. M.; Meharg, A. A.; Wright, J.; Killham, K. Toxicity of chlorobenzenes to a lux-marked terrestrial bacterium, pseudomonas fluorescens. *Environ. Toxicol. Chem.* **1998**, *17*, 2134−2140.

(75) Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. Water Solubility and Octanol/Water Partition Coefficients of Organics. Limitations of the Solubility−Partition Coefficient Correlation. *Environ. Sci. Technol.* **1980**, *14*, 1227−1229.

(76) Hammers, W. E.; Meurs, G. J.; De Ligny, C. L. Correlations between liquid chromatographic capacity ratio data on lichrosorb RP-18 and partition coefficients in the octanol−water system. *J. Chromatogr.* **1982**, *247*, 1−13.

(77) Bruggeman, W. A.; Van der Steen, J. M. D.; Hutzinger, O. Reversed-phase thin-layer chromatography of polynuchlear aromatic hydrocarbons and chlorinated biphenyls. Relationship with hydrophobicity as measured by aqueous solubility and octanol−water partition coefficient. *J. Chromatogr.* **1982**, *238*, 335−346.

(78) Doucette, W. J.; Andren, A. W. Estimation of octanol/water partition coefficients: Evaluation of six methods for highly hydrophobic aromatic hydrocarbons. *Chemosphere* **1988**, *17*, 345−359.

(79) Haller, H. L.; Bartlett, P. D.; Drake, N. L.; Newman, M. S.; Christol, S. J.; Eaker, C. M.; Hayes, R. A.; Kilmer, G. W.; Magerlein, B.; Mueller, G. P.; Schneider, A.; Wheatley, W. The Chemical Composition of Technical DDT. *J. Am. Chem. Soc.* **1945**, *67*, 1591−1602.

(80) Rothman, A. M. Low Vapor Pressure Determination by the Radiotracer Transpiration Method. *J. Agric. Food Chem.* **1980**, *28*, 1225−1228.

(81) Spencer, W. F.; Cliath, M. M. Volatility of DDT and related compounds. *J. Agric. Food Chem.* **1972**, *20*, 645−649.

(82) Dickinson, W. The vapour pressure of 1: 1:*p: p′* dichorodiphenyl trichloroethane D. D. T. *Trans. Faraday Soc.* **1956**, *52*, 31−35.

(83) Balson, E. W. Studies in vapour pressure measurement, part lll. An effusion manometer sensitive to 5×10^{-6} millimetres of mercury: vapour pressure of D. D. T. and other slightly volatile substances. *Trans. Faraday Soc.* **1947**, *43*, 54−60.

(84) Atkins D. H. F.; Eggleton, A. E. J. *Studies of Atmospheric Wash-Out and Deposition of γ-BHC, Dieldrin and p,p′-DDT Using Radio-Labelled Pesticides*; International Atomic Energy Agency: Vienna, 1971; pp 521−533.

(85) Webster, G. R. B.; Fricoan, K. J.; Sarna, L. P.; Muir, D. C. G. Environmental fate modelling of chlorodioxins: Determination of physical constants. *Chemosphere* **1985**, *14*, 609−622.

(86) Bidleman, T. F. Estimation of Vapour Pressures for Nonpolar Organic Compounds by Capillary Gas Chromatography *Anal. Chem.* **1984**, *56*, 2490−2496.

(87) Chiou, C. T.; Malcolm, R. L.; Brinton, T. I.; Kile, D. E. Water Solubility Enhancement of Some Organic Pollutants and Pesticides by Dissolved Humic and Fulvic Actids. *Environ. Sci. Technol.* **1986**, *20*, 502−508.

(88) Ellgehausen, H.; D'Hondt, C.; Fuerer, R. Reversed-phase chromatography as a general method for determining octan-1-ol/water partition coefficients. *Pestic. Sci.* **1981**, *12*, 219−227.

(89) Biggar, J. W.; Riggs, R. L. Apparent solubility of organochlorine insecticides in water at various temperatures. *Hilgardia* **1974**, 42.

(90) Biggar, J. W.; Dutt, G. R.; Riggs, R. L. Predicting and measuring the solubility of p,p′-DDT in water. *Bull. Environ. Contam. Toxicol.* **1967**, *2*, 90−100.

(91) Babers, F. H. The solubility of DDT in water determined radiometrically. *J. Am. Chem. Soc.* **1955**, *77*, 4666.

(92) Robeck, G. G.; Dostal, K. A.; Cohen, J. M.; Kreissl, J. Effectiveness of water treatment processes in pesticide removal. *J.—Am. Water Works Assn.* **1965**, 181−199.

(93) Gerstl, Z.; Mingelgrin, U. Sorption of organic substances by soils and sediments. *J. Environ. Sci. Health B* **1984**, *19*, 297−312.

(94) Swann, R. L.; Laskowski, D. A.; McCall, P. J.; Kuy, K. V.; Dishburger, H. J. A rapid method for the estimation of the environmental parameters octanol/water partition coefficient, soil sorption constant, water-to-air ratio, and water solubility. *Residue Rev.* **1983**, *85*, 17−28.

(95) Fendinger, N. J.; Glotfelty, D. E.; Freeman, H. P. Comparison of Two Experimental Techniques for Determining Air/Water Henry's Law Constants. *Environ. Sci. Technol.* **1989**, *23*, 1528−1531.

(96) Rapaport, R. A.; Eisenreich, S. J. Chromatographic Determination of Octanol−Water Coefficients K_{OW}'s for 58 Polychlorinated Biphenyl Congeners. *Environ. Sci. Technol.* **1984**, *18*, 163−170.

(97) Finizio, A.; Vighi, M.; Sandroni, D. Determination of n-octanol/water partition coefficient K_{OW} of pesticide. Critical review and comparison of methods. *Chemosphere* **1997**, *34*, 131−161.

(98) Sarna, L. P.; Hodge, P. E.; Webster, G. R. B. Octanol-water partition coefficients of chlorinated dioxins and dibenzofurans by reversed-phase HPLC using several C18 columns. *Chemosphere* **1984**, *13*, 975−983.

(99) Westcott, J. W.; Simon, C. G.; Bidleman, T. F. Determination of Polychlorinated Biphenyl Vapor Pressures by Semimicro Gas Saturation Method. *Environ. Sci. Technol.* **1981**, *15*, 1375−1378.

(100) Westcott, J. W.; Bidleman, T. F. Determination of polychlorinated biphenyl vapor pressures by capillary gas chromatography. *J. Chromatogr.* **1981**, *210*, 331−336.

(101) Chiou, C. T.; Freed, V. H.; Schmedding, D. W.; Kohnert, R. L. Partition Coefficient and Bioaccumulation of Selected Organic Chemicals. *Environ. Sci. Technol.* **1977**, *11*, 475−477.

(102) Bidleman, T. F.; Billings, W. N.; Foreman, W. T. Vapor−Particle Partitioning of Semivolatile Organic Compounds: Estimates from Field Collections. *Environ. Sci. Technol.* **1986**, *20*, 1038−1043.

(103) Sanborn, J. R.; Metcalf, R. L.; Bruce, W. N.; Lu, P.-Y. The fate of chlorane and toxaphene in a terrestrial-aquatic model ecosystem. *Environ. Entomol.* **1976**, *5*, 533−538.

(104) Johnson-Logan, L. R.; Broshears, R. E.; Klaine, S. J. Partition Behavior and the Mobility of Chlordane in Groundwater. *Environ. Sci. Technol.* **1992**, *26*, 2234−2239.

(105) Simpson, C. D.; Wilcock, R. J.; Smith, T. J.; Wilkins, A. L.; Langdon, A. G. Determination of octanol−water partition coefficients for the major components of technical chlordane. *Bull. Environ. Contam. Toxicol.* **1995**, *55*, 149−153.

(106) Park, K. S.; Bruce, W. N. The determination of the water solubility of aldrin, dieldrin, heptachlor, and heptachlor epoxide. *J. Econ. Entomol.* **1968**, *61*, 770−774.

(107) Noegrohati, S.; Hammers, W. E. Regression models for octanol−water partition coefficients, and for bioconcentration in fish. *Toxicol. Environ. Chem.* **1992**, *34*, 155−173.

(108) Grayson, B. T.; Forbraey, L. A. Determination of the vapour pressure of pesticides. *Pestic. Sci.* **1982**, *13*, 269−278.

(109) Porter, P. In *Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives*; Zweig, G.; Ed.; Academic Press: New York, 1964; Vol. 2, pp 143−163.

(110) Richardson, L. T.; Miller, D. M. Fungitoxicity of chlorinated hydrocarbon insecticides in relation to water solubility and vapor pressure. *Can. J. Botany* **1960**, *38*, 163−168.

(111) Briggs, G. G. Theoretical and Experimental Relationships between Soil Adsorption, Octanol−Water Partition Coefficients, Water Solubilities, Bioconcentration Factors, and the Parachor. *J. Agric. Food. Chem.* **1981**, *29*, 1055−1059.

(112) Spencer, W. F.; Cliath, M. M. Vapor Density of Dieldrin. *Environ. Sci. Technol.* **1969**, *3*, 670−674.

(113) Eye, J. D. Aqueous transport of dieldrin residues in soils. *J.—Water Pollut. Control Fed.* **1968**, *40*, R316−R332.

(114) Bowman, B. T.; Sans, W. W. Effect of temperature on the water solubility of insecticides. *J. Environ. Sci. Health B* **1985**, *20*, 625−631.

(115) Slater, R. M.; Spedding, D. J. Transport of dieldrin between air and water. *Arch. Environ. Contam. Toxicol.* **1981**, *10*, 25−33.

(116) Bowman, B. T.; Sans, W. W. Further water solubility determinations of insecticidal compounds. *J. Environ. Sci. Health B* **1983**, *18*, 221−227.

(117) Fernandez-Gutierrez, A.; Martinez-Vidal, J. L.; Arrebola-Liebanas, F. J.; Gonzalez-Casado, A.; Vilchez, J. L. Determination of endosulfan and some pyrethroids in waters by micro liquid-liquid extraction and GC-MS. *Fresenius' J. Anal. Chem.* **1998**, *360*, 568−572.

(118) Rice, C. P.; Chernyak, S. M.; Hapeman, C. J.; Bilboulian, S. Air-water distribution of the endosulfan isomers. *J. Environ. Qual.* **1997**, *26*, 1101−1106.

(119) Hermens, J. L. M.; Leeuwangh, P. Joint toxicity of mixture of 8 and 24 chemicals to the guppy (poecilia reticulata). *Ecotoxicol. Environ. Saf.* **1982**, *6*, 302−310.

(120) Cole, J. G.; Mackay, D. Correlating environmental partitioning properties of organic compounds: the three solubility approach. *Environ. Toxicol. Chem.* **2000**, *19*, 265−270.

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