Environment Agency

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Verification of bioaccumulation models for use in environmental standards. Part D: compendium of physico-chemical properties

Science Report – SC030197/SR5

The Environment Agency is the leading public body protecting and improving the environment in England and Wales.

It's our job to make sure that air, land and water are looked after by everyone in today's society, so that tomorrow's generations inherit a cleaner, healthier world.

Our work includes tackling flooding and pollution incidents, reducing industry's impacts on the environment, cleaning up rivers, coastal waters and contaminated land, and improving wildlife habitats.

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Science at the Environment Agency

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The work of the Environment Agency's Science Group is a key ingredient in the partnership between research, policy and operations that enables the Environment Agency to protect and restore our environment.

The science programme focuses on five main areas of activity:

- **Setting the agenda**, by identifying where strategic science can inform our evidence-based policies, advisory and regulatory roles;
- **Funding science**, by supporting programmes, projects and people in response to long-term strategic needs, medium-term policy priorities and shorter-term operational requirements;
- **Managing science**, by ensuring that our programmes and projects are fit for purpose and executed according to international scientific standards;
- **Carrying out science**, by undertaking research – either by contracting it out to research organisations and consultancies or by doing it ourselves;
- **Delivering information, advice, tools and techniques**, by making appropriate products available to our policy and operations staff.

Steve Killeen

Head of Science

Executive summary

This report forms Part D of a series of reports on the *Verification of bioaccumulation models for use in environmental standards.* Part D provides a summary of the physico-chemical properties of chemicals used in the verification of models and methods for predicting accumulation in aquatic food chains (Part A), terrestrial food chains (Part B) and human food chains (Part C).

Contents

1 Introduction

This project forms part of a broader programme to support the Environment Agency's work in developing standards for the protection of the environment and human health from chemicals (P6-020/U, *A programme of work on environmental and human health standards for chemicals*).

The Environment Agency must derive standards to protect the environment and human health in order to fulfil its statutory pollution control role. This project is intended to help provide a sound scientific basis for setting such standards and to ensure a transparent and consistent approach to setting standards across different functions within the Environment Agency.

Bioaccumulative substances are of concern to the Environment Agency because they have the potential to biomagnify via the food chain and cause effects on organisms at higher trophic levels. Bioaccumulation is of particular concern when the chemical is toxic as well as persistent or continuously released to the environment.

The Environment Agency currently derives standards to protect the aquatic environment based on acute or chronic aquatic toxicity data divided by an extrapolation factor. This approach does not take into account possible effects on organisms higher in the food chain, nor does it consider routes of exposure other than direct contact with water. For highly lipophilic substances that bioaccumulate, water is unlikely to be the only route of exposure for aquatic organisms and top predators, and exposure via contaminated food or sediment may become important. The Environment Agency needs to consider these additional exposure routes when setting aquatic standards for bioaccumulative and persistent substances.

This project will help the Environment Agency's negotiating position at EU meetings to agree environmental quality standards for pollutants and priority substances listed in Annexes VIII to X to the Water Framework Directive (Directive 2000/60/EC).

When setting soil standards, the Environment Agency must consider indirect exposure routes for organisms at the top of the terrestrial food chain. The method used to derive soil standards will feed into the tiered terrestrial ecological risk assessment (ERA) framework that is being developed by the Environment Agency and the Department for Environment, Food and Rural Affairs (Defra). Once finalised, this framework will be used in Part 2A of the Environmental Protection Act 1990 to assess the impacts of soil contamination on wildlife top predators, and it is also likely to have other uses such as under the Habitats Directive.

In addition to aquatic and terrestrial organisms, bioaccumulation in or uptake through the food chain is also important when considering human exposure to contaminants. Methods for determining human exposure to chemicals from some types of soil contamination are already available in the Contaminated Land Exposure Assessment (CLEA) approach (Environment Agency and Defra, 2002). However, equivalent methods for determining exposure to chemicals from other types of soils, and from other routes such as the aquatic food chain, are not generally available.

This work was commissioned by the Environment Agency to validate models suitable for assessing the potential bioaccumulation of organic chemicals when setting environmental standards. The models selected for verification in this report are based on the results of an initial evaluation of a large number of possible models. The initial evaluation is covered in a separate report (Environment Agency, 2007)

This report (Part D) provides a compendium of the physico-chemical properties of chemicals used for the verification of models for predicting the bioaccumulation of chemicals in the environment. The verification of models for the aquatic environment, the terrestrial environment and the human food chain is considered in Part A, Part B and Part C of this report series respectively.

2 Compendium of physico-chemical properties

The predictive methods used in Parts A to C of this report series rely crucially on certain physico-chemical properties of chemicals. The two most important properties are the $\log_{10}$ of the octanol-water partition coefficient ($\log K_{ow}$) and Henry's law constant (and the associated air-water partition coefficient (K_{aw}) and octanol-air partition coefficient (K_{oa})). These values are difficult to measure for highly lipophilic substances of low water solubility and vapour pressure (as is the case for many chemicals in the various test sets used in this report) and many different values exist in the literature for such properties.

For the analysis carried out in Parts A to C of this series, $\log K_{ow}$ values were generally taken from the original paper outlining the accumulation data or from standard reference books and databases. However, for several of the chemicals, different $\log K_{ow}$ values were associated with the chemical in different data sets. Therefore, in order to make the predictions as consistent as possible across the different methods and data sets, a single preferred value for $\log K_{ow}$ was generally used for the chemical in question. These values are summarised in Table 2.1 for all chemicals considered. No actual validation of $\log K_{ow}$ values was undertaken in this analysis, but rather the preferred values reflected the more commonly quoted values in the literature. A similar problem also occurred for Henry's law constants. Here, values from the EPIWIN v3.12 program (USEPA, 2000) were generally used, with preference given to values in the experimental database within the EPIWIN program rather than predicted ones (in many cases, database values represented values of the Henry's law constant derived from a measured water solubility and vapour pressure).

For the analysis of the Voutsas *et al.* (2002) data set in Section 6.1 of Part A report, the $\log K_{ow}$ values as reported in Voutsas *et al.* (2002) were used in order to compare our predicted bioaccumulation factors with the bioaccumulation factors originally predicted by Voutsas *et al.* (2002). Where $\log K_{ow}$ values used by Voutsas differ from the preferred $\log K_{ow}$ values, this is indicated in Table 2.1.

Table 2.1 Summary of physico-chemical properties used in the modelling exercise

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Acenaphthene/ fluorene	83-32-9 (acenaph-thene)	154	93	b	3.9	b	0.29	b	3.92	S & b		18	b	-2.11	6.03
Acetone O-methyl carbamoyloxime									-0.13	R					
Acrylamide	79-06-1	71	85	b	2.2×10^{6}	u	0.90	u	-1.00	u		3.0×10^{-5}	u	-7.90	6.90
Acrylonitrile	107-13-1	53	-84	b	7.4×10^{4}	t	1.3×10^{4}	t	0.25	t		9.6	t	-2.39	2.64
Alachlor	15972-60-8	270	40	b	240	b	2.7×10^{-3}	a	3.52	S & b		8.4×10^{-4}	b	-6.45	9.97
Aldicarb	116-06-3	190	99	b	6.0×10^{3}	b	4.6×10^{-3}	b	1.15	Q		1.5×10^{-4}	b	-7.21	8.36

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Aldoxycarb	1646-88-4	222	141	b	1.0×10^{4}	b	0.012	b	-0.57	R & b		3.4×10^{-4}	b	-6.84	6.27
Aldrin	309-00-2	365	104	d	0.010	g	8.6×10^{-3}	d	6.50	p & b		4.5	b	-2.73	9.23
Aniline	62-53-3	93	-6	b	3.5×10^{4}	s	400	s	0.90	s		0.11	s	-4.35	5.25
Anthracene	120-12-7	178	215	b	0.043	b	3.6×10^{-4}	b	4.46	N	4.54	5.6	b	-2.62	7.08
9,10-Anthra quinone	84-65-1	208	286	b	1.4	b	1.5×10^{-5}	b	2.44	N		2.4×10^{-3}	b	-6.00	8.44
Aroclor 1248	12672-29-6	292	122	a	0.032	a	0.066	b	6.30	S		45	b	-1.73	8.03
Aroclor 1254	11097-69-1	326	135	a	3.4×10^{-3}	b	0.47	b	6.47	Q		29	b	-1.92	8.39
Atratone	1610-17-9	211	117	a	1.8×10^{3}	b	3.9×10^{-4}	b	2.69	S & b		4.5×10^{-5}	b	-7.72	10.41

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Atrazine	1912-24-9	216	173	b	35	b	3.9×10^{-5}	b	2.65	Q		2.4×10^{-4}	b	-7.00	9.65
Benfluralin	1861-40-1	335	66	b	0.10	b	8.7×10^{-3}	b	5.29	S & b		29	b	-1.91	7.20
Benomyl	17804-35-2	290	140	b	3.8	b	4.9×10^{-7}	b	3.11	Q		5.0×10^{-7}	b	-9.68	12.79
Benzaldehyde O-methylcarbamoyl oxime									1.49	R					
Benzene	71-43-2	78	6	b	1.8×10^{3}	r	1.0×10^{5}	r	2.13	r		433	r	-0.74	2.87
Benzene, C10-13 alkyl derivates	67774-74-7	243	<-70	e	0.041	e	1.3	e	9.12	e		95	e	-1.40	10.52
Benzo[a] anthracene	56-55-3	228	84	b	9.4×10^{-3}	b	2.8×10^{-5}	b	5.82	N	5.61	1.2	b	-3.29	9.11

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
1,2-Benzoanthraquinone	2498-66-0	258	170	b	0.030	a	5.2×10^{-6}	a	3.45	N		4.6×10^{-3}	a	-5.71	9.16
Benzo[a]pyrene	50-32-8	252	177	b	1.6×10^{-3}	b	7.3×10^{-7}	b	6.13	b	6.35	0.046	b	-4.71	10.84
Benzo[b] fluoranthene	205-99-2	252	168	b	1.5×10^{-3}	b	6.7×10^{-5}	b	6.29	N	5.98	0.067	b	-4.55	10.84
Benzo[k] fluoranthene	207-08-9	252	217	b	8.0×10^{-4}	b	1.3×10^{-7}	b	6.59	N	6.04	0.059	b	-4.60	11.19
Benzo[b+k] fluoranthene	see above								6.12	T					
Benzo[ghi] perylene	191-24-2	276	278	b	2.6×10^{-4}	b	1.3×10^{-8}	b	7.00	N		0.034	b	-4.85	11.85
Benzoylprop-ethyl	22212-55-1	366	180	a	20	b	1.4×10^{-6}	a	4.57	Q		1.2×10^{-4}	e	-7.31	11.88

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Bisphenol-A	80-05-7	228	153	b	300	q	5.3×10^{-6}	q	3.40	q		4.0×10^{-6}	q	-8.77	12.17
Bromacil	314-40-9	261	158	b	815	b	4.1×10^{-5}	b	2.11	S & b		1.1×10^{-5}	b	-8.35	10.46
4-(4-Bromo phenoxy)phenyl urea	85879-22-7	307	178	a	19	a	7.1×10^{-6}	a	3.70	R & b		2.8×10^{-4}	a	-6.92	10.62
4-Bromophenyl urea	1967-25-5	215	226	b	5.0×10^{3}	b	0.015	a	1.98	R & b		4.3×10^{-3}	a	-5.74	7.72
Carbazole	86-74-8	167	246	b	1.8	b	1.0×10^{-4}	b	2.94	N		2.8×10^{-3}	a	-5.93	8.87
Carbofuran	1563-66-2	221	151	b	320	b	6.5×10^{-4}	b	2.32	S & b		3.1×10^{-4}	b	-6.88	9.20
Chlordane (unspecified isomers)	57-74-9	410	104	f	0.056	b p	1.3×10^{-3}	f	6.00	Q		4.9	b	-2.68	8.68
Chlordane (*trans* isomer)	5103-74-2	410	104	f	0.056	b p	1.3×10^{-3}	f	6.16	p		4.9	b	-2.68	8.84

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Chlordane (*cis*-isomer)	5103-71-9	410	104	f	0.056	b p	1.3×10^{-3}	f	6.16	p		4.9	b	-2.68	8.84
Chlordane (*gamma*-isomer)	5566-34-7	as above	as above		as above		as above		6.00	J		4.9	b	-2.68	8.68
4-Chloro benzaldehyde O-methylcarbamoyl oxime									2.27	R					
4-Chloro-2-methylphenol	1570-64-5	143	51	b	2.3×10^{3}	v	27	v	3.09	v		0.11	v	-4.33	7.42
3-Chlorophenol	108-43-0	129	33	b	2.6×10^{4}	b	17	b	2.50	P & b		0.035	b	-4.83	7.33
4-Chlorophenyl urea	140-38-5	171	102	a	1.6×10^{3}	a	0.022	a	1.80	R & b		2.1×10^{-3}	a	-6.05	7.85
Chloropropylate	5836-10-2	339	73	b	10	b	2.4×10^{-5}	b	4.49	Q		8.1×10^{-4}	b	-6.46	10.95

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Chlorpyrifos	2921-88-2	351	42	b	1.1	b	2.7×10^{-3}	b	4.97	Q		0.30	b	-3.90	8.87
Chrysene	218-01-9	228	258	b	3.5×10^{-3}	b	8.3×10^{-7}	b	5.81	b	5.61	0.53	b	-3.65	9.46
Clopidol	2971-90-6	192	320	b	10	b	1.6×10^{-4}	b	2.90	Q		$1.0\text{x}10^{-4}$	a	-7.36	10.26
Coumaphos	56-72-4	363	93	b	1.5	b	1.3×10^{-5}	b	4.13	Q & b		3.1×10^{-3}	b	-5.88	10.01
Cyanazine	21725-46-2	241	168	b	170	b	1.8×10^{-5}	b	2.02	Q		3.0×10^{-7}	b	-9.90	11.92
Cyclohexane	110-82-7	84	7	b	58	o	1.0×10^{4}	o	3.44	o		1.5×10^{4}	o	0.80	2.64
Cyhexatin (Tricyclohexyltin hydroxide)	13121-70-5	385	196	b	8.2×10^{-3}	a	2.7×10^{-7}	a	5.39	Q		0.013	a	-5.26	10.65
DDD (*p,p'*-isomer (dichlorodiphenyl dichloroethane)	72-54-8	320	110	b	0.090	b	1.8×10^{-4}	b	6.02	b		0.67	b	-3.55	9.57

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
DDD (*p,p*-isomer)		as above	as above		as above		as above		6.91	J		as above		as above	as above
DDE (*p,p'*-isomer) (Dichlorodiphenyl dichloroethylene)	72-55-9	318	89	b	0.040	b	8.0×10^{-4}	b	6.51	J & b		4.2	b	-2.75	9.26
DDE (*p,p*-isomer)		as above	as above		as above		as above		6.96	J		as above		as above	as above
DDT- all isomers (Dichlorodiphenyl trichloroethane)	50-29-3	355	108	g	3.4×10^{-3}	g	2.5×10^{-5}	g	6.19	g	6.90	0.84	b	-3.45	9.64
DEHP (bis(2-ethylhexyl) phthalate)	117-81-7	391	-55	b	3.0×10^{-3}	n	0.034	n	7.50	n		4.4	n	-2.73	10.23
Diazinon	333-41-5	304	<25	b	40	b	0.012	b	3.31	Q		0.011	b	-5.32	8.63
Dibenz[a,h] anthracene	53-70-3	278	270	b	1.0×10^{-3}	b	1.9×10^{-9}	a	6.50	U		1.6×10^{-4}	b	-7.18	13.68

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Dibenzo[a] anthracene[1]									6.61	N					
Dibenzothiophene	132-65-0	184	97	b	1.5	b	0.027	b	3.46	N		3.4	b	-2.84	6.30
Dibutyl phthalate	84-74-2	278	-35	b	10	m	9.7×10^{-3}	m	4.57	m		0.27	m	-3.94	8.51
Dicamba	1918-00-9	221	115	b	8.3×10^{3}	b	4.5×10^{-3}	b	3.01	Q		2.2×10^{-4}	b	-7.03	10.04
Dichlobenil	1194-65-6	172	145	b	21	b	0.13	b	2.74	b		1.0	b	-3.36	6.10
3,4-Dichloroaniline	95-76-1	162	72	b	580	x	0.18	x	2.70	x		0.050	x	-4.68	7.38
3,4-Dichloro benzaldehyde O-methylcarbamoyl oxime									2.89	R					

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
2,6-Dichlorobenzamide	2008-58-4	190	199	b	2.7×10^{3}	b	6.3×10^{-4}	a	0.77	b		1.1×10^{-5}	a	-8.33	9.10
1,2-Dichloro benzene	95-50-1	147	-17	b	80	b	196	b	3.43	J		195	b	-1.09	4.52
1,3-Dichloro benzene	541-73-1	147	-25	b	125	b	287	b	3.53	J		266	b	-0.95	4.48
1,4-Dichloro benzene	106-46-7	147	53	c	83	c	170	c	3.40	c	3.44	244	b	-0.99	4.39
2,7-Dichloro dibenzo-*p*-dioxin (DiCDD)	33857-26-0	253	209	b	3.8×10^{-3}	b	1.2×10^{-4}	b	5.75	b		6.0	b	-2.60	8.35
2,4-Dichloro phenol	120-83-2	163	45	b	4.5×10^{3}	b	15	b	3.06	b		0.20	b	-4.06	7.12
3,4-Dichloro phenol	95-77-2	163	68	b	9.3×10^{3}	b	0.49	a	3.20	P		0.22	a	-4.03	7.23
2,4-Dichloro phenoxyacetic acid (2,4-D)	94-75-7	221	141	b	677	b	8.4	b	2.81	Q		3.6×10^{-3}	b	-5.82	8.63

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
3-(3,4-Dichloro phenoxy)benzalde hyde O-methyl carbamoyloxime									4.60	R					
3,4-Dichloro phenylurea	2327-02-8	205	122	a	395	a	4.3×10^{-3}	a	2.64	R		4.0×10^{-3}	a	-5.78	8.42
3,6-Dichloro picolinic acid	1702-17-6	192	151	b	7.9×10^{3}	b	1.6×10^{-3}	b	1.75	Q		3.1×10^{-4}	b	-6.89	8.64
DIDP (Diisodecyl phthalate)	26761-40-0	447	-46	b	2.0×10^{-4}	l	5.1×10^{-5}	l	8.80	l		114	l	-1.32	10.12
Dieldrin	60-57-1	381	176	g	0.10	g	2.4×10^{-5}	g	5.40	p & b		1.0	b	-3.37	8.77
Diflubenzuron	35367-38-5	311	239	b	0.080	b	1.2×10^{-7}	b	3.82	Q		4.7×10^{-4}	b	-6.71	10.53
1,4-Dioxane	123-91-1	88	12	b	1.0×10^{6}	a	5.1×10^{3}	b	-0.27	O		0.49	b	-3.69	3.42

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Diuron	330-54-1	233	158	b	42	b	$9.2x10^{-6}$	b	2.68	S & b		5.1×10^{-5}	b	-7.67	10.35
Edetic acid	60-00-4	292	245	b	400	k	5.0×10^{-10}	a	-5.01	k		6.4×10^{-13}	a	-15.57	10.56
Endosulfan	115-29-7	407	106	b	0.33	b	8.0×10^{-5}	b	3.83	b		6.6	b	-2.56	6.39
Endrin	72-20-8	381	200	g	0.23	j	2.7×10^{-5}	g	5.60	g		1.0	b	-3.37	8.97
Ethirimol	23947-60-6	209	160	b	150	b	2.7×10^{-4}	b	4.39	S		3.7×10^{-4}	b	-6.80	11.19
Ethofumesate	26225-79-6	286	71	b	50	b	6.5×10^{-4}	b	3.27	Q		3.7×10^{-3}	b	-5.80	9.07
Famphur (phosphoric acid, *o*-4-(dimethyl amino)sulfonyl phenyl *o,o*-dimethyl ester)	52-85-7	325	53	b	229	a	3.6×10^{-4}	a	2.28	Q		1.1×10^{-3}	a	-6.34	8.62

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Fenoprop (silvex)	93-72-1	270	182	b	71	b	3.4×10^{-4}	a	3.86	Q		$3.5x10^{-3}$	a	-5.82	9.68
Fenthion	55-38-9	278	8	b	7.5	b	1.4×10^{-3}	b	3.16	Q		0.15	b	-4.20	7.36
Fenvalerate	51630-58-1	420	60	b	0.020	b	2.0×10^{-7}	b	6.20	Q & b		$3.5x10^{-3}$	b	-5.83	12.03
Flamprop-isopropyl	52756-22-6	364	73	b	12	b	8.5×10^{-5}	b	4.41	Q		2.6×10^{-3}	b	-5.96	10.37
Fluchloralin	33245-39-5	356	42	b	0.90	b	$2.8x10^{-3}$	b	4.79	Q		1.1	b	-3.33	8.12
Fluoranthene	206-44-0	202	108	b	0.26	b	1.2×10^{-3}	b	5.20	U	5.22	0.90	b	-3.42	8.62
4-Fluorophenyl urea	659-30-3	154	83	a	6.2×10^{3}	a	0.15	a	1.04	R & b		2.4×10^{-3}	a	-6.00	7.04
Haloxyfop	69806-34-4	362	108	b	43	b	$5.3x10^{-5}$	a	4.63	S		$1.1x10^{-3}$	a	-6.32	10.95

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Heptachlor	76-44-8	373	95	g	0.056	f	0.040	g	6.10	p & b		30	b	-1.90	8.00
Heptachlor epoxide	1024-57-3	398	160	b	0.20	b	2.6×10^{-3}	b	5.40	Q		2.1	b	-3.05	8.45
1,2,3,4,6,7,8-Heptachloro dibenzo-*p*-dioxin (HpCDD)	35822-46-9	425	264	b	2.4×10^{-6}	b	7.5×10^{-8}	b	8.20	b		18	b	-2.13	10.33
1,2,3,4,6,7,9-Heptachloro dibenzo-*p*-dioxin (HpCDD)	58200-70-7	425	182	a	4.2×10^{-5}	a	3.5×10^{-6}	a	8.85	a		325	a	-0.86	9.71
1,2,3,4,6,7,8-Heptachloro dibenzofuran (HpCDF)	67562-39-4	409	184	a	1.4×10^{-6}	b	2.7×10^{-6}	a	7.92	b		31	a	-1.89	9.81
1,2,3,4,7,8,9-Heptachloro dibenzofuran (HpCDF)	55673-89-7	409	184	a	1.4×10^{-6}	b	2.7×10^{-6}	a	7.92	b		31	a	-1.89	9.81
Hexachloro benzene	118-74-1	285	228	c	5.0×10^{-3}	c	0.24	c	5.50	c		172	b	-1.14	6.64

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Hexachloro benzene	see above								5.73	J					
Hexachloro butadiene	87-68-3	261	-21	c	3.2	c	20	c	4.70	c	4.78 4.84 5.60	1.0×10^{3}	b	-0.36	5.06
Hexachloro cyclohexane (β-HCH)	608-73-1	291	112	g	17	g	$1.3\text{x}10^{-3}$	f	3.70	V		0.52	b	-3.66	7.36
Hexachloro cyclohexane (α-HCH)		as above	as above	as above	as above		as above	as above	3.80	J	as above	as above		as above	as above
1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin (HxCDD)	39227-28-6	391	273	b	4.4×10^{-6}	b	5.1×10^{-9}	b	7.80	b		0.40	b	-3.77	11.57
1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin (HxCDD)	57653-85-7	391	285	b	1.9×10^{-4}	a	4.8×10^{-9}	b	7.98	M		8.5	a	-2.44	10.42
1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin (HxCDD)	19408-74-3	391	285	b	1.9×10^{-4}	a	4.8×10^{-9}	b	8.21	a		8.5	a	-2.44	10.65
1,2,3,4,7,8-Hexachlorodibenzofuran	70648-26-9	375	171	a	3.5×10^{-4}	a	1.5×10^{-5}	a	7.92	a		95	a	-1.40	9.32

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
(HxCDF)															
1,2,3,6,7,8-Hexachloro dibenzofuran (HxCDF)	57117-44-9	375	171	a	3.5×10^{-4}	a	1.5×10^{-5}	a	7.92	a		95		-1.40	9.32
1,2,3,7,8,9-Hexachloro dibenzofuran (HxCDF)	72918-21-9	375	173	a	1.6×10^{-3}	a	1.0×10^{-5}	a	7.58	a		34	a	-1.85	9.43
2,3,4,6,7,8-Hexchloro dibenzofuran (HxCDF)	60851-34-5	375	171	a	3.5×10^{-4}	a	1.5×10^{-5}	a	7.92	a		95	a	-1.40	9.32
Hexachloroethane	67-72-1	237	187	b	50	b	28	b	4.14	J		394	b	-0.78	4.92
Indeno[1,2,3-cd]pyrene	193-39-5	276	164	b	1.9×10^{-4}	b	1.7×10^{-8}	a	6.58	U		0.035	b	-4.83	11.41
Indeno[cd]pyrene[1]									5.69	N					
Isodrin	456-73-6	365	240	b	0.017	b	8.0×10^{-4}	p	6.50	p & b		4.5	b	-2.73	9.23

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Isoproturon	34123-59-6	206	158	b	65	b	3.3×10^{-6}	b	2.87	b		1.1×10^{-5}	b	-8.32	11.19
Kerb (pronamide)	23950-58-5	256	155	b	15	b	5.8×10^{-5}	b	3.18	Q		9.9×10^{-4}	b	-6.38	9.56
Lindane (gamma-Hexachlorocyclohexane or γ-HCH)	58-89-9	291	112	g	17	g	1.3×10^{-3}	f	3.70	V		0.52	b	-3.66	7.36
Linuron	330-55-2	249	93	b	75	b	1.9×10^{-4}	b	3.20	b		6.3×10^{-4}	b	-6.57	9.77
Malathion	121-75-5	330	3	b	143	b	4.5×10^{-4}	b	2.89	Q		5.0×10^{-4}	b	-6.68	9.57
Medium-chain chlorinated paraffins	85535-85-9	488	0	h	0.027	h	2.7×10^{-4}	h	7.00	h		4.9	h	-2.69	9.69
Methoxychlor	72-43-5	346	98	g	0.040	g	5.6×10^{-3}	a	5.08	p & b		0.021	b	-5.06	10.14
									4.40[2]					-5.06	9.46[3]
4,4'-Methylene dianiline	101-77-9	198	93	b	1.3×10^{3}	w	2.9×10^{-6}	w	1.59	w		4.4×10^{-7}	w	-9.73	11.32

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
3-Methylphenyl urea	63-99-0	150	94	a	2.1×10^{3}	a	0.043	a	-0.12	R		1.1×10^{-3}	a	-6.35	6.23
3-(Methylthio) phenylurea	85879-21-6	182	119	a	954	a	3.1×10^{-3}	a	1.57	R		2.3×10^{-4}	a	-7.01	8.58
Metolachlor	51218-45-2	284	-40	b	530	b	$4.2\text{x}10^{-3}$	b	3.13	S & b		9.1×10^{-4}	b	-6.41	9.54
Mirex	2385-85-5	546	485	i	0.20	g	4.0×10^{-5}	i	5.28	p & S		82	b	-1.46	6.74
Musk ketone	81-14-1	294	160	a	0.46	y	$4.0\text{x}10^{-5}$	y	4.30	y		0.026	y	-4.96	9.26
Musk xylene	81-15-2	297	110	b	0.15	z	3.0×10^{-5}	z	4.90	z		0.060	z	-4.60	9.50
Naphthalene	91-20-3	128	80	b	30	A	11	A	3.70	A		45	b	-1.72	5.42
Naphthol	1321-67-1	144	95	b	866	b	0.037	b	2.84	Q		5.8×10^{-3}	b	-5.61	8.45

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Nitrobenzene	98-95-3	123	6	b	2.1×10^{3}	b	33	b	1.85	S & b		2.4	b	-2.99	4.84
Nonachlor - *trans* isomer	39765-80-5	444	148	a	1.4×10^{-3}	a	1.3×10^{-4}	b	6.35	J & b		21	a	-2.05	8.40
Nonylphenol	25154-52-3	220	42	b	6.0	B	0.30	B	4.45	B		11	B	-2.33	6.78
Octachloro dibenzo-*p*-dioxin (OCDD)	3268-87-9	460	330	b	4.0×10^{-7}	b	1.1×10^{-10}	b	8.20	b		0.68	b	-3.54	11.74
Octachloro dibenzofuran (OCDF)	39001-02-0	444	258	b	1.2×10^{-6}	b	5.0×10^{-10}	b	8.60	b		9.3	a	-2.41	11.01
Octachlorostyrene	29082-74-4	380	120	a	4.6×10^{-3}	a	1.8×10^{-3}	a	6.29	J		384	a	-0.79	7.08
O-Ethyl O-*p*-nitrophenyl phosphono thionate	2104-64-5	323	36	b	3.1	b	$1.3\text{x}10^{-4}$	b	4.78	R & b		0.045	b	-4.72	9.50
Oxadiazon	19666-30-9	345	90	b	0.70	b	1.5×10^{-5}	b	4.09	Q		$7.4\text{x}10^{-3}$	b	-5.51	9.60

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Oxamyl	23135-22-0	219	101	b	2.8×10^{5}	b	0.031	b	-0.47	R		2.4×10^{-5}	b	-7.99	7.52
Oxychlordane	27304-13-8	424	144	b	0.014	a	$9.3\text{x}10^{-4}$	a	5.48	a		8.8	a	-2.43	7.91
PBDE 47	5436-43-1	486	162	a	0.054	a	$9.3\text{x}10^{-6}$	b	6.80	W		11	a	-2.35	9.15
PBDE 66		486	162	a	0.054	a	3.2×10^{-5}	a	6.80	W		11	a	-2.35	9.15
PBDE 85	182346-21-0	565	183	a	0.011	a	9.6×10^{-7}	a	7.30	W		23	a	-2.01	9.31
PBDE 99	60348-60-9	565	183	a	0.011	a	4.1×10^{-6}	b	7.40	W		23	a	-2.01	9.41
PBDE 100		565	183	a	0.011	a	$3.3\text{x}10^{-6}$	a	7.30	W		23	a	-2.01	9.31
PBDE 153		644	197	a	$2.1\text{x}10^{-3}$	a	3.8×10^{-7}	a	7.90	W		59	a	-1.60	9.50

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PBDE 154		644	197	a	2.1×10^{-3}	a	3.8×10^{-7}	a	7.80	W		59	a	-1.60	9.40
PBDE 196		801	226	a	7.4×10^{-5}	a	4.9×10^{-9}	a	8.80	W		355	a	-0.82	9.62
PBDE 206		880	240	a	1.4×10^{-5}	a	5.4×10^{-10}	a	8.90	W		840	a	-0.45	9.35
PBDE 207		880	240	a	1.4×10^{-5}	a	5.4×10^{-10}	a	9.00	W		840	a	-0.45	9.45
PBDE 209	1163-19-5	959	255	a	2.6×10^{-6}	a	6.2×10^{-10}	a	9.50	W		2.1×10^{4}	a	0.95	8.55
PCB 4	13029-08-8	223	62	b	1.9	b	0.37	b	4.97	b		23	b	-2.01	6.98
PCB 8	34883-43-7	223	81	a	1.2	b	0.28	b	5.10	c	5.07	23	b	-2.01	7.11
PCB 16	38444-78-9	258	101	b	0.29	b	5.3×10^{-3}	a	5.16	J		20	b	-2.07	7.23

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 17	37680-66-3	258	101	a	0.83	b	5.3×10^{-3}	a	5.25	J		5.3	a	-2.65	7.90
PCB 18	37680-65-2	258	101	a	0.40	b	0.14	b	5.60	c	5.24	25	b	-1.97	7.57
PCB 22	38444-85-8	258	101	a	0.14	b	5.3×10^{-3}	a	5.72	X	5.58	14	b	-2.22	7.94
PCB 24/27	55702-45-9 (PCB 24)	258	101	a	0.080	b	5.3×10^{-3}	a	5.40	J		22	b	-2.03	7.43
PCB 28	7012-37-5	258	57	c	0.16	c	0.026	c	5.80	b		20	b	-2.07	7.87
PCB 28/31		as above	as above		as above		as above		as above	J	5.60 5.67	as above		as above	as above
PCB 31	16606-02-3	258	101	a	0.14	b	0.053	b	5.67	J		19	b	-2.09	7.76
PCB 32	38444-77-8	258	101	a	0.16	b	5.3×10^{-3}	a	5.40	J		20	b	-2.07	7.47

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 33	38444-86-9	258	101	a	0.13	b	0.14	b	5.80	c	5.60	16	b	-2.16	7.96
PCB 37	38444-90-5	258	101	a	0.072	b	5.3×10^{-3}	a	5.90	b		10	b	-2.37	8.27
PCB 40	38444-93-8	292	122	a	0.016	b	9.8×10^{-3}	b	5.60	c		10	b	-2.37	7.97
PCB 40	as above								5.66	J					
PCB 42	36559-22-5	292	122	a	0.061	b	1.1×10^{-3}	a	5.60	J		14	b	-2.22	7.82
PCB 44	41464-39-5	292	122	a	0.10	b	1.1×10^{-3}	a	6.00	J	5.75	14	b	-2.22	8.22
PCB 47	2437-79-8	292	122	a	0.28	b	0.012	b	5.90	c		19	b	-2.09	7.99
PCB 47/48		as above	as above		as above		as above		as above	J	5.82	as above		as above	as above

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 49	41464-40-8	292	122	a	0.078	b	1.1×10^{-3}	b	6.10	J	5.85	21	b	-2.05	8.15
PCB 50/60/81	62796-65-0 (PCB 50)	292	122	a	0.070	b	1.1×10^{-3}	a	6.03	J		6.2	a	-2.58	8.61
PCB 52	35693-99-3	292	87	c	0.030	c	2.0×10^{-3}	c	6.10	c	5.84	20	b	-2.07	8.17
PCB 53	41464-41-9	292	122	a	0.048	b	3.0×10^{-3}	b	5.50	c	5.62	18	b	-2.11	7.61
PCB 60	33025-41-1	292	122	a	0.039	b	1.1×10^{-3}	a	6.31	c	5.90	23	a	-2.02	8.33
PCB 64	52663-58-8	292	122	a	0.032	a	1.1×10^{-3}	a	6.10	J	5.95	14	b	-2.22	8.32
PCB 66	32598-10-0	292	122	a	0.037	b	6.2×10^{-3}	b	5.80	c	6.20	12	b	-2.29	8.09
PCB 66/95		as above	as above		as above		as above				5.80	as above		as above	as above

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 70	32598-11-1	292	122	a	0.036	b	5.4×10^{-3}	b	6.28	X	5.90	10	b	-2.37	8.65
PCB 70/66		as above	as above		as above		as above		as above		6.17	as above		as above	as above
PCB 74	32690-93-0	292	122	a	5.0×10^{-3}	b	1.1×10^{-3}	a	6.20	J	6.10	10	b	-2.37	8.57
PCB 77	32598-13-3	292	122	a	5.7×10^{-4}	b	2.2×10^{-3}	b	6.36	J		11	a	-2.33	8.69
PCB 81	70362-50-4	292	122	a	0.032	a	1.1×10^{-3}	a	6.36	J		6.2	a	-2.58	8.94
PCB 82	52663-62-4	326	135	a	0.029	b	3.0×10^{-4}	a	6.20	J		19	a	-2.09	8.29
PCB 84	52663-60-2 84	326	135	a	0.054	b	3.0×10^{-4}	a	6.60	X		10	a	-2.36	8.96
PCB 84/92		as above	as above		as above		as above		as above		6.04	as above		as above	as above

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 85	65510-45-4	326	135	a	7.8×10^{-3}	b	3.0×10^{-4}	a	6.30	J		6.7	b	-2.55	8.85
PCB 87	38380-02-8	326	135	a	0.029	b	2.3×10^{-3}	b	6.50	c & J	6.29	7.5	b	-2.50	9.00
PCB 87/97		as above	as above	as above	as above		as above		as above		6.29	as above		as above	as above
PCB 91	68194-05-8	326	135	a	0.022	b	3.0×10^{-4}	a	6.13	J		10	a	-2.36	8.49
PCB 92	52663-61-3	326	135	a	4.9×10^{-3}	b	3.0×10^{-4}	a	6.35	J		7.1	a	-2.52	8.87
PCB 95	38379-99-6	326	135	a	0.021	b	3.0×10^{-4}	a	5.80	c	6.13	12	b	-2.29	8.09
PCB 95/66		as above	as above		as above		as above		as above			as above		as above	as above
PCB 97	41464-51-1	326	135	a	0.028	b	3.0×10^{-4}	a	6.77	X	6.60	7.5	b	-2.50	9.27

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 99	38380-01-7	326	135	a	3.7×10^{-3}	b	2.9×10^{-3}	b	6.60	c	6.39	7.9	b	-2.48	9.08
PCB 99/113		as above	as above		as above		as above		as above			as above		as above	as above
PCB 101	37680-73-2	326	77	c	0.010	c	3.5×10^{-3}	c	6.40	c	6.38	9.1	b	-2.41	8.81
PCB 101/90		as above	as above		as above		as above		as above			as above		as above	as above
PCB 105	32598-14-4	326	135	a	3.4×10^{-3}	b	8.7×10^{-4}	b	6.00	c	6.40 6.65	29	b	-1.92	7.92
PCB 107/108/144/135	70424-68-9 (PCB 107)	326	135	a	7.3×10^{-3}	a	3.0×10^{-4}	a	6.94	X		10	a	-2.36	9.30
PCB 110	38380-03-9	326	135	a	7.3×10^{-3}	b	3.0×10^{-4}	a	6.30	c	6.48 6.50	19	a	-2.09	8.39
PCB 111	39635-32-0	395	164	a	7.5×10^{-4}	b	1.7×10^{-5}	a	6.92	X		24	a	-1.99	8.91

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 114	65510-44-3	326	135	a	0.016	b	7.3×10^{-4}	a	6.95	X		19	a	-2.09	9.04
PCB 118	31508-00-6	326	135	a	0.013	b	1.2×10^{-3}	b	6.40	J		29	b	-1.91	8.31
PCB 118	see above								6.74	J					
PCB 123/147	65510-44-3 (PCB 123)	326	135	a	7.3×10^{-3}	a	3.0×10^{-4}	a	6.93	X		19	a	-2.09	9.02
PCB 126	57465-28-8	326	135	a	7.3×10^{-3}	a	3.0×10^{-4}	a	6.95	X	6.89	10	a	-2.36	9.31
PCB 128	38380-07-3	361	146	a	3.5×10^{-4}	b	3.4×10^{-4}	b	6.74	J		1.3	b	-3.25	9.99
PCB 132	38380-05-1	361	146	a	8.1×10^{-3}	b	7.7×10^{-5}	a	7.24	X	6.58	4.5	b	-2.73	9.97
PCB 132/105		as above	as above		as above		as above		as above			as above		as above	as above

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 136	38411-22-2	361	146	a	$4.5x10^{-3}$	b	$7.7x10^{-5}$	a	6.22	J		8.9	b	-2.42	8.64
PCB 138	35065-28-2	361	79	c	1.5×10^{-3}	c	$5.0x10^{-4}$	c	6.70	c	6.83 7.00	2.1	b	-3.05	9.75
PCB 138/163/164		as above	as above		as above		as above		as above			as above		as above	as above
PCB 141	52712-04-6	361	146	a	7.6×10^{-3}	b	7.7×10^{-5}	a	7.33	X	6.82	2.3	b	-3.01	10.34
PCB 146	51908-16-8	361	146	a	9.5×10^{-4}	b	7.7×10^{-5}	a	7.36	X	6.89 6.90	2.5	b	-2.97	10.33
PCB 148	74472-41-6	361	146	a	1.6×10^{-3}	a	7.7×10^{-5}	a	7.29	X		17	a	-2.14	9.43
PCB 149	38380-04-0	361	146	a	4.2×10^{-3}	b	1.1×10^{-3}	b	7.21	X	6.67 6.80	140	b	-1.23	8.44
PCB 151	52663-63-5	361	146	a	0.014	b	3.1×10^{-4}	b	7.16	X	6.64 6.90	6.0	b	-2.60	9.76

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 153	35065-27-1	361	103	c	1.0×10^{-3}	c	7.0×10^{-4}	c	6.90	c	6.92	2.3	b	-3.01	9.91
PCB 156	38380-08-4	361	146	a	5.3×10^{-3}	b	2.1×10^{-4}	a	7.60	b	7.18	14	b	-2.21	9.81
PCB 157	69782-90-7	361	146	a	1.6×10^{-3}	a	7.7×10^{-5}	a	7.44	X		16	a	-2.16	9.60
PCB 158	74472-42-7	361	107	b	8.1×10^{-3}	b	2.1×10^{-4}	a	7.37	X		45	a	-1.72	9.09
PCB 167	52663-72-6	361	146	b	2.2×10^{-3}	b	7.7×10^{-5}	a	7.68	K		16	a	-2.16	9.84
PCB 169	32774-16-6	361	146	a	5.1×10^{-4}	b	7.7×10^{-5}	a	7.50	X	7.42	11	a	-2.33	9.83
PCB 170	35065-30-6	395	164	a	3.5×10^{-3}	b	8.4×10^{-5}	a	7.08	c	7.27	0.91	b	-3.41	10.49
PCB 170/190		as above	as above		as above		as above		as above		7.30	as above		as above	as above

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 174	38411-25-5	395	164	a	1.0×10^{-3}	b	1.7×10^{-5}	a	7.77	X	7.00	1.4	b	-3.22	10.99
PCB 177	52663-70-4	395	164	a	1.5×10^{-3}	b	1.7×10^{-5}	a	7.79	X		24	a	-1.99	9.78
PCB 179	52663-64-6	395	164	a	4.5×10^{-3}	b	1.7×10^{-5}	a	7.45	Y		2.4	b	-2.99	10.44
PCB 180	35065-29-3	395	109	c	3.1×10^{-4}	c	1.3×10^{-4}	c	7.20	c	7.36 7.40	1.0	b	-3.37	10.57
PCB 182/187	60145-23-5 (PCB 182)	395	164	a	8.3×10^{-4}	b	1.7×10^{-5}	a	7.17	c	7.20	24	a	-1.99	9.16
PCB 183	52663-69-1	395	164	a	4.9×10^{-3}	b	1.3×10^{-4}	a	7.00	J		14	a	-2.23	9.23
PCB 184	74472-48-3	395	164	a	$3.7x10^{-4}$	a	5.4×10^{-3}	b	7.80	J		34	b	-1.84	9.64
PCB 187/182	52663-68-0 (PCB 187)	395	164	a	4.5×10^{-3}	b	1.7×10^{-5}	a	7.19	J		14	a	-2.23	9.42

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 189	39635-31-9	395	164	a	7.5×10^{-4}	b	1.7×10^{-5}	a	8.00	X		14	a	-2.23	10.23
PCB 191	74472-50-7	395	164	a	3.1×10^{-4}	b	1.7×10^{-5}	a	7.93	X		14	a	-2.23	10.16
PCB 192/172	74472-51-8 (PCB 192)	395	164	a	3.1×10^{-4}	b	1.7×10^{-5}	a	7.94	X		24	a	-1.99	9.93
PCB 193	69782-91-8	395	164	a	3.1×10^{-4}	b	1.7×10^{-5}	a	7.92	X		14	a	-2.23	10.15
PCB 194	35694-08-7	430	181	a	2.7×10^{-4}	b	3.8×10^{-6}	a	7.40	c	7.80	1.0	b	-3.37	10.77
PCB 195	52663-78-2	430	181	a	2.2×10^{-4}	b	3.8×10^{-6}	a	7.56	J		1.1	a	-3.33	10.89
PCB 199	52663-75-9	430	181	a	2.2×10^{-4}	b	3.8×10^{-6}	a	7.20	J		1.0	a	-3.37	10.57
PCB 201	40186-71-8	430	181	a	2.7×10^{-4}	b	3.8×10^{-6}	a	8.35	X	7.50	1.7	b	-3.14	11.49

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
PCB 202	2136-99-4	430	181	a	1.5×10^{-4}	b	5.2×10^{-4}	b	7.73	b		1.8	b	-3.11	10.84
PCB 203/196	52663-76-0 (PCB 203)	430	181	a	1.4×10^{-4}	b	3.8×10^{-6}	a	7.65	J		34	a	-1.85	9.50
PCB 209	2051-24-3	499	306	b	7.4×10^{-6}	b	1.4×10^{-5}	b	8.18	J		952	b	-0.40	8.58
ΣPCBs – ICES[4]		292			0.030		2.0×10^{-3}		6.50	Z					
Pentachloroaniline	527-20-8	265	235	b	19	a	4.7×10^{-4}	b	4.82	b		0.084	a	-4.45	9.27
Pentachloro benzene	608-93-5	250	86	b	0.83	b	0.13	b	5.18	K	5.11	71	b	-1.52	6.70
Pentachloro butadiene (E-isomer)	55880-77-8	226	-21	a	16	a	103	a	4.54	J		2.9×10^{3}	a	0.09	4.45
Pentachloro butadiene (Z-isomer)		as above	as above	as above	as above		as above		4.54	J		as above		as above	as above

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
1,2,3,7,8-Pentachloro dibenxo-*p*-dioxin (PeCDD)	40321-76-4	356	240	b	8.5×10^{-4}	a	5.8×10^{-8}	b	6.64	b		2.2	a	-3.02	9.66
1,2,3,7,8-Pentachloro dibenzofuran (PeCDF)	57117-41-6	340	156	a	2.4×10^{-4}	b	4.6×10^{-5}	a	6.92	b		18	a	-2.12	9.04
2,3,4,7,8-Pentachloro dibenzofuran (PeCDF)	57117-31-4	340	156	a	2.4×10^{-4}	b	4.6×10^{-5}	a	6.92	b		18	a	-2.12	9.04
Pentachloro nitrobenzene	82-68-8	295	144	b	0.44	b	6.7×10^{-3}	b	4.18	Q		4.5	b	-2.72	6.90
Pentachloro phenol	87-86-5	266	174	b	14	b	0.015	b	5.24	S		2.5×10^{-3}	b	-5.98	11.22
Pentachloro toluene	877-11-2	264	225	b	0.47	a	1.8×10^{-3}	a	6.20	J		78	b	-1.48	7.68
Phenanthrene	85-01-8	178	99	b	1.2	b	0.016	b	4.57	U		4.3	b	-2.74	7.31
Phenol	108-95-2	94	41	b	8.4×10^{4}	G	20	G	1.47	G		0.022	G	-5.03	6.50

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
3-Phenoxy benzaldehyde O-methylcarbamoyl oxime									3.12	R					
4-Phenoxyphenyl urea	78508-44-8	228	150	a	83	a	8.1×10^{-5}	a	2.80	R & b		1.5×10^{-4}	a	-7.21	10.01
Phenylurea	64-10-8	136	147	b	6.3×10^{3}	a	0.38	a	0.80	R		3.0×10^{-3}	a	-5.89	6.69
Phorate	298-02-2	260	<-15	b	50	b	0.085	b	4.70	Q		0.44	b	-3.73	8.43
Phosphamidon	297-99-4	300	-45	b	1.0×10^{6}	b	2.2×10^{-3}	b	1.34	Q		5.1×10^{-4}	a	-6.67	8.01
Photomirex	39801-14-4	511	144	a	1.3×10^{-4}	a	8.9×10^{-4}	a	7.14	J		474	a	-0.70	7.84
Piperazine	110-85-0	86	106	b	1.5×10^{5}	H	39	H	-1.25	H		0.022	H	-5.03	3.78

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Polybrominated diphenyl (hexabrominated congener)	36355-01-8	628	72	b	0.011	b	6.9×10^{-6}	b	9.10	a		0.43	b	-3.74	12.84
Polybrominated biphenyl (unspecified congeners)		as above	as above		as above		as above		9.35	Q		as above		-3.74	13.09
Pyrene	129-00-0	202	151	b	0.14	b	6.0×10^{-4}	b	5.18	S		1.2	b	-3.29	8.47
Ronnel	299-84-3	322	41	b	1.0	b	0.010	b	4.88	Q & b		3.2	b	-2.86	7.74
Simazine	122-34-9	202	226	b	6.2	b	2.9×10^{-6}	b	2.18	S & b		9.5×10^{-5} {202}[5]	b	-7.39 {-1.07}[5]	7.39{3.25}[5]
Sulfotep	3689-24-5	322	<25	b	30	b	0.014	b	3.99	b		0.24	b	-3.99	7.98
Sodium pentachloro phenate	See penta chloro phenol								5.24						

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Telodrin	297-78-9	412	121	b	0.16	a	3.9×10^{-4}	b	5.20	Y		1.8	a	-3.13	8.33
tert-Butyl methyl ether	1634-04-4	88	-109	b	4.2×10^{4}	C	270	C	1.06	C		44	C	-1.73	2.79
3,3',4,4'-Tetrachloro azobenzene	14047-09-7	320	129	a	0.019	a	4.0×10^{-4}	a	6.46	S		19	a	-2.09	8.55
Tetrachloro benzene (unknown isomers or mixture of isomers)	12408-10-5	216	55	b	5.1	b	11	b	4.60	b		77	b	-1.49	6.09
1,2,3,4-Tetra chlorobenzene	634-66-2	216	48	b	5.9	b	5.2	b	4.64	K	4.59 4.60	77	b	-1.49	6.13
1,2,3,5-Tetra chlorobenzene	634-90-2	216	55	b	5.1	b	11	b	4.68	L	4.62 4.56	160	b	-1.17	5.85
1,2,4,5-Tetra chlorobenzene	94-94-3	216	140	c	1.3	c	9.6	c	4.50	c	4.64	101	b	-1.37	5.87

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
1,1,4,4-Tetra chlorobutadiene	36038-53-6	192	-37	a	53	a	333	a	4.29	J		2.0×10^{3}	a	-0.06	4.35
Z-1,1,2,4-Tetra chlorobutadiene		192	-37	a	53	a	333	a	4.23	J		2.0×10^{3}	a	-0.06	4.29
1,2,3,4-Tetra chlorodibenzo-*p*-dioxin (TCDD)	30746-58-8	322	188	b	6.3×10^{-4}	b	6.4×10^{-6}	b	6.60	b		2.0	b	-3.07	9.67
2,3,7,8-Tetra chlorodibenzo-*p*-dioxin (TCDD)	1746-01-6	322	305	b	2.0×10^{-4}	b	2.0×10^{-7}	b	6.80	b		5.1	b	-2.67	9.47
2,3,7,8-Tetra chlorodibenzo furan (TCDF)	51207-31-9	306	139	a	6.9×10^{-4}	b	2.0×10^{-4}	a	6.53	b		27	a	-1.95	8.48
Tetrachloro ethylene	127-18-4	166	-22	b	149	D	1.9×10^{3}	D	2.53	D		2.1×10^{3}	D	-0.05	2.58
2,3,4,5-Tetra chlorophenol	4901-51-3	232	117	b	193	a	0.022	a	4.50	P		0.17	a	-4.13	8.63
Thionazin	297-97-2	248	-2	b	1.1×10^{3}	b	0.40	b	1.86	a		0.087	b	-4.43	6.29

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
Toluene	108-88-3	92	-95	b	515	E	3.0×10^{3}	E	2.65	E		537	E	-0.64	3.29
Toxaphene	8001-35-2	414	77	b	0.55	b	8.9×10^{-4}	b	5.50	Q		0.61	b	-3.59	9.09
Trichlopyr	55335-06-3	256	149	b	440	b	1.7×10^{-4}	b	2.09	Q		9.8×10^{-5}	b	-7.38	9.47
Trichlorobenzene (unknown isomers or mixture of isomers)	12002-48-1	181	64	b	30	b	61	b	4.19	b		192	b	-1.09	5.28
1,2,3-Trichloro benzene	87-61-6	181	54	b	18	b	28	b	4.10	L	4.05 4.09 4.14	127	b	-1.27	5.37
1,2,4-Trichloro benzene	120-82-1	181	18	c	40	c	61	c	4.10	m	4.02	144	b	-1.22	5.32
1,3,5-Trichloro benzene	108-70-3	181	64	b	30	b	61	b	4.20	L	4.19	192	b	-1.09	5.29
Trichloroethylene	79-01-6	132	-85	b	1.1×10^{3}	F	8.6×10^{3}	F	2.29	F		1.0×10^{3}		-0.36	2.65

Chemical[3]	CAS number	Molecular weight (g mole^{-1})	Melting point		Solubility at ~25°C		Vapour pressure Pa at ~25°C		Log K_{ow}[6]			Henry's law constant (H) at ~25°C		Log K_{aw}[7] at ~13°C	Log K_{oa}[8]
			Value (°C)	Source	Value (mg l^{-1})	Source	Value (Pa)	Source	Preferred value	Source	Alternate value from Voutsas *et al.* (2002)	Value (Pa m^{-3} mol^{-1})	Source		
2,4,5-Trichloro phenol	95-954	197	69	b	1.2×10^{3}	b	1.0	b	3.90	P		0.16	b	-4.16	8.06
2,4,5-Trichloro phenoxy acetic acid (2,4,5-T)	93-76-5	255	153	b	278	b	5.0×10^{-3}	b	3.36	Q		2.9×10^{-3}	a	-5.91	9.27
3,5,6-Trichloro pyridinol	6515-38-4	198	82	a	125	a	0.14	a	2.27	Q		0.34	a	-3.85	6.12
2,3,6-Trichloro toluene	2077-46-5	195	34	a	8.4	a	9.8	a	4.80	J		152	b	-1.19	5.99
2,4,5-Trichloro toluene	6639-30-1	195	82	b	8.4	a	2.6	a	4.80	J		152	b	-1.19	5.99
Trifluralin	1582-09-8	335	49	b	0.18	b	6.1×10^{-3}	b	5.33	Q		10	b	-2.36	7.69

Sources: a) Value estimated using the EPIWIN v3.12 software (USEPA, 2000).
b) Value from the experimental database within the EPIWIN v3.12 software (USEPA, 2000).
c) Value from MacKay *et al.* (1992).
d) Value from Richardson and Gangolli (1992-1994).
e) Value from ECB (1999).
f) Value from Worth (1979).
g) Value from Verschueren (1983).
h) Value from ECB (2005a).
i) Value from WHO (1984).
j) Value from WHO (1992).
k) Value from ECB (2004a).
l) Value from ECB (2003a).
m) Value from ECB (2004b).
n) Value from ECB (2001a).
o) Value from ECB (2004c).
p) Value from HSDB (2006).
q) Value from ECB (2003b).
r) Value from ECB (2005b).
s) Value from ECB (2004d).
t) Value from ECB (2004e).
u) Value from ECB (2002a).
v) Value from ECB (2002b).
w) Value from ECB (2001b).
x) Value from ECB (2001c).
y) Value from ECB (2005c).
z) Value from ECB (2005d).
A) Value from ECB (2003c).
B) Value from ECB (2002c).
C) Value from ECB (2002d).
D) Value from ECB (2005e).
E) Value from ECB (2003d).
F) Value from ECB (2004f).
G) Value from ECB (2006a).
H) Value from ECB (2005f).
J) Value for Voutsas *et al.* (2002).
K) Value from Belfroid *et al.* (1994 and 1995).
L) Value from Beyer (1996).
M) Value from Defra (2003).
N) Value from Matscheko *et al.* (2002).
O) Value from ECB (2002e).
P) Value from van Gestel and Ma (1988).
Q) Value from Travis and Arms (1988).
R) Value from Briggs *et al.* (1982).
S) Value from Polder *et al.* (1995).
T) Mean value for benzo[b]fluoranthene and benzo[k]fluoranthene from ECB (2006b).
U) Value from ECB (2006b).
V) Value from WHO (1991).
W) Estimated value from Ellinger *et al.* (2003).
X) Estimated value from Oberg, 2001.
Y) Value from Jager (2003) and van der Wal *et al.* (2004).
Z) Average of the six main components of the ΣPCB – ICES (see note 4 below).

Notes:

1) The identity of the actual isomer in the study was not clear and so the log K_{ow} value from that paper was used.
2) Value from Travis and Arms (1988) used in the analysis of the Travis and Arms (1988) data set in Part C of this report series.
3) The specific polybrominated diphenyl ethers (PBDEs) and polychlorinated biphenyls (PCBs) have been identified here using the IUPAC numbering system.
4) ΣPCB – ICES = Total PCBs as defined by the International Council for the Exploration of the Sea (ICES). These are the congeners PCB 28, PCB 52, PCB 101, PCB 118, PCB 138, PCB 153 and PCB 180. PCB 118 was not included in the total in the Mersey data set discussed in Part A of this report series.
5) Incorrect values. For some calculations carried out in Part C of this series, the incorrect values given in { } for log K_{aw} and log K_{oa} were inadvertently used in some of the calculations. This will have affected somewhat the level of accumulation predicted in the models for this substance, but will have little impact on the overall conclusions from the verification exercise.
6) Log K_{ow} = $\log_{10}$ of the octanol-water partition coefficient (K_{ow}).
7) Log K_{aw} = $\log_{10}$ of the air-water partition coefficient (K_{aw} or dimensionless Henry's law constant). Estimated from the Henry's law constant for a temperature of 285 K (13°C).
8) Log K_{oa} = $\log_{10}$ the octanol-air partition coefficient (K_{oa}). Estimated from log K_{oa} = log K_{ow} – log K_{aw}

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