Annex B

POLLUTANT-RELATED PROPERTIES USED IN VARIOUS POP MODELS

The present Annex contains the information on basic pollutant-related parameters used in modelling of POP behavior in the environment, namely: the Henry's law constant, the subcooled liquid vapor pressure, octanol/water, octanol/air and organic carbon/water partitioning coefficients and degradation rates in various environmental compartments (see Tables B.1-B.6). These data were presented by modelers participating in the POP model intercomparison study carried out under CLRTAP. The information on pollutant-related parameters presented in the form of tables containing the description of a parameter, numerical values of relevant coefficients, comments describing peculiarities of evaluation of a parameter and literature source used for evaluation. For the sake of comparability, the base values and coefficients of temperature dependencies of the considered parameters are given here at the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

In addition, this Annex contains information on "reference" data set of PCB-153 physical-chemical properties and degradation rates used as input data harmonized for all models in the calculations within sensitivity studies of the POP model intercomparison study. Proposed "reference" data set for PCB-153 is presented in Table B.7. For models using "reference" data set as own set of physical-chemical properties, it is proposed to carry out sensitivity studies with the use of alternative data set. The latter (see Table B.8) contains data on physical-chemical properties (including degradation rate constants) mostly taken from CliMoChem and DEHM-POP models.

Table B.1. *The Henry's law constant and the air/water partition coefficient of PCB-153*

Model	Description	Numerical values		Comments	Reference
CAM/POPs	Temperature dependent: $H = H_0 \exp(-a_H (1/T - 1/T_0))$ where T - temperature (^{0}K), H_0 is the value at the reference temperature T_0, and a is a parameter of temperature dependence. Temperature dependent: $K_{aw} = H / (R \cdot T)$	H_0, Pa·m^3/mol	6.09E-01	Coefficient a_H of the exponential equation are recalculated from the coefficient of the following temperature dependence: $H = H_0 \cdot 10^{(-3416\,(1/T - 1/T0))}$ with the help of the following formula: $a_H = \ln(10) \cdot 3416$, It was obtained from the following temperature dependence: $\log(H/H(25^oC)) = \text{slop}\,(1/T - 1/298)$ $H(25^0C)$ - Henry 's law constant at 25^{0}C, Pa·m^3/mol (PCB-153: 2.43)	*Achman et al.,*1993
		a_H	7865.6		
		T_0, ^{0}K	283.15		
G-CIEMS	Temperature dependent: $H = H_0 \exp(-a_H (1/T - 1/T_0))$ where T - temperature (K), H_0 is the value at the reference temperature T_0, and a_H is a parameter of temperature dependence.	H_0, Pa·m^3/mol	4.91E+00	The value a_H can be put directly as input data. When the input data is not given, temperature dependence of vapor pressure is used as surrogate, assuming the temperature-independent water solubility	*Li et al.,* 2003
		a_H	7851.7		
		T_0, ^{0}K	283.15		
SimpleBox	Temperature dependent: $H = H_0 \exp(-a_H (1/T - 1/T_0))$ where T - temperature (K), H_0 is the value at the reference temperature T_0, and a_H is a parameter of temperature dependence.	H_0, Pa·m^3/mol	4.91E+00		*Li et al.,* 2003
		a_H	7851.7		
		T_0, ^{0}K	283.15		
EVN-BETR and UK-MODEL	Temperature independent:	H, Pa·m^3/mol	19.8	Calculated as H = Vapour Pressure (Pa) / Water Solubility (mol/m^3) at 25^{o}C	*Li et al.,* 2003
	Temperature dependent: $K_{aw} = K^0_{aw} \exp(-a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K), K^0_{aw} is the value at the reference temperature T_0, and a_{Kaw} is a parameter of temperature dependence.	K_{aw}, dimen-sionless	2.08E-03	At 10^{o}C, calculated as $K_{aw}(T_0) = 10^{\log Kaw} \cdot a$, $a = \exp[(\Delta H_{vap} / R) \cdot (1 / T_0 - 1 / T)]$. ΔH_{vap} = 62.8 KJ/mol: Enthalpy of vaporisation (from water to air) here: $a_{Kaw} = \Delta H_{vap} / R$	
		a_{Kaw}	7553.5		
		T_0, ^{0}K	283.15		
CliMoChem	Temperature dependent: $K_{aw} = K^0_{aw} \exp(-a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K), K^0_{aw} is the value at the reference temperature T_0, and a_{Kaw} is a parameter of temperature dependence.	K^0_{aw}, dimen-sionless	2.01E-03	$K_{aw}(T) = K_{aw}(T_{ref}) \exp(dH_{Kaw}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{aw}(T_{ref})$=Henry 's law constant at T_{ref} (dimensionless): PCB 153: 9.18E-3 dH_{Kaw} = phase transfer enthalpy (J/mol): PCB 153: 71000 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
		a_{Kaw}	8540		
		T_0, ^{0}K	283.15		
DEHM-POP	Temperature dependent: $K_{aw} = K^0_{aw} \exp(-a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K), K^0_{AW} is the value at the reference temperature T_0, and a_{Kaw} is a parameter of temperature dependence.	K^0_{aw}, dimen-sionless	2.01E-03	$K_{aw}(283.15) = K^0_{aw}(298.15)\exp(-a_{Kaw}(1/T\text{-}1/T_0)$, where $K^0_{aw}(298.15)$ = 9.18E-3 for PCB 153	*Beyer at al.,* 2002
		a_{Kaw}	8536		
		T_0, ^{0}K	283.15		
MSCE-POP	Temperature dependent: $H = H_0 \exp(-a_H (1/T - 1/T_0))$ where T - temperature (K), H_0 is the value at the reference temperature T_0, and a_H is a parameter of temperature dependence. Temperature dependent: $K_{aw} = H / (R \cdot T)$	H_0, Pa·m^3/mol	3.781	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log H = -A/T(K) + B$ with the help of the following formulas: $a_H = \ln(10) \cdot A$, $H_0 = 10^{(-A/T0 + B)}$; where $A = \Delta H_W / 2.303R$; $B = \log H_{298} + \Delta H_W / 2.303R(298)$. H_{298} is Henry's law constant (Pa·m^3/mol) at 25^{0}C (for PCB-153: 16.48); ΔH_W is the enthalpy of volatilization from water, kJ/mol (for PCB-153: 69.4)	*Burkhard et al*., 1985; *Dunnivant et al.,* 1992
		a_H, K	8347		
		T_0, K	283.15		

Table B.2. *The octanol/air partition coefficient of PCB-153*

Model	Description	Numerical values		Comments	Reference
CAM/POPs	Temperature dependent: $K_{oa} = 10^{(a/T + b)}$ where: T - temperature; P - liquid vapour pressure p_{0L} (Pa)	a	-529-19.25 log$P$	These values are calculated with the help of temperature dependencies of p_{0L}	*Harner et al.,* 1996; 1998
		b	8.2995-0.95 log$P$		
SimpleBox	Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	2.05E+10		*Li et al.,* 2003
		a_{Koa}	11294.2		
		T_0, K	283.15		
G-CIEMS	Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	2.05E+10	K_{oa} is used as optional only when the input value is given.	*Li et al.,* 2003
		a_{Koa}	11294.2		
		T_0, K	283.15		
EVN-BETR and UK-MODEL	Temperature dependent: $K_{oa} = K_{ow} / K_{aw}$	K^0_{oa} (T_0), dimensionless	6.97E+09	At 10°C, calculated as $K_{oa} = K_{ow} / K_{aw}$	
		T_0, K	283.15		
DEHM-POP	Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	2.74E+10	$K_{oa}(283.15) = K^0_{oa}(298.15) \exp(a_{Koa}(1/T - 1/T_0)$, where K^0_{oa} (298.15) = 4.14E+9, 1.16E+8, 1.68E+10 for PCB 153, 28 and 180 respectively $a_{Koa} = dHK_{oa}/R$ $dH\ K_{oa}$ = phase transfer enthalpy (J/mol) PCB 153: -88400 R = universal gas constant (8.3145 J/mol K)	*Beyer et al.,* 2002
		a_{Koa}	10636.8		
		T_0, K	283.15		
MSCE-POP	Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	3.64E+10	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_{oa} = 4695/T(\mathrm{K}) - 6.02$ with the help of the following formulas: $a_p = \ln(10) \cdot 4695$, $K^0_{oa}(T_0) = 10^{(4695/T0 - 6.02)}$	*Harner and Bidleman,* 1996
		a_{Koa}	10811		
		T_0, K	283.15		

Table B.3. *The subcooled liquid vapour pressure of PCB-153*

Model	Description	Numerical values		Comments	Reference
CAM/ POPs	Temperature dependent: $p_{0L} = p^0_{ol} \exp (- a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{0L} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{0L}, Pa	9.69E-05	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $p_{0L} = 10^{(m/T + b)}$; $a_p = \ln(10) \cdot m$; $p^0_{0L} = 10^{(m/T0 + b)}$ where T - temperature (^{0}K); m = -4775: parameter of temperature dependence, and b = 12.85: parameter depended on molecular weight. It was obtained from the following original equation: $\log(p_{0L}) = -Q / (2.303\ RT) + b$ where: T - temperature; R - Universal Gas Constant Q - the heat of vaporisation (KJ/mol)	*Harner et al*., 1996; *Falconer et al*., 1995
		a_p	10995		
		T_0, K	283.15		
SimpleBox	Temperature dependent: $p_{0L} = p^0_{0L} \exp (- a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{0L} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{0L}, Pa	8.82E-05		*Li et al*., 2003
		a_p	10846.6		
		T_0, K	283.15		
G-CIEMS	Temperature dependent: $p_{0L} = p^0_{ol} \exp (- a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{0L} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{0L}, Pa	8.82E-05	In case of K_{oa} value is assigned in input data, temperature dependence of vapor pressure is not used in calculation.	*Li et al*., 2003
		a_p	10846.6		
		T_0, K	283.15		
EVN-BETR and UK-MODEL	Temperature independent:	P_0, Pa	6.60E-04	T = 25^{o}C	*Li et al.,* 2003
MSCE-POP	Temperature dependent: $p_{0L} = p^0_{0L} \exp (- a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{0L} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{0L}, Pa	9.69E-05	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log p_{0L}$ (Pa) = -4775/T(K) + 12.85 with the help of the following formulas: $a_p = \ln(10) \cdot 4775$, $p^0_{0L} = 10^{(-4775/T0 + 12.85)}$	*Falconer and Bidleman,* 1994
		a_p	10995		
		T_0, K	283.15		

Table B.4. *The octanol/water partition coefficient of PCB-153*

Model	Description	Numerical values		Comments	Reference
CAM/ POPs	Temperature dependent: $K_{ow} = K_{oa} \cdot H/RT$ where T - temperature (^{0}K); R - Universal Gas Constant; H - Henry's law constant; K_{oa} - Octanol/air partition coefficient (dimensionless)	-	-	These values are calculated with the help of temperature dependencies of H and K_{oa}	This study
SimpleBox	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence.	K^0_{ow} (T_0), dimensionless	1.45E+07		*Li et al.,* 2003
		a_{Kow}	3740.7		
		T_0, K	283.15		
G-CIEMS	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence.	K^0_{ow} (T_0), dimensionless	1.45E+07		*Li et al.,* 2003
		a_{Kow}	3740.7		
		T_0, K	283.15		
EVN-BETR and UK-MODEL	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence.	K^0_{ow}, dimensionless	1.45E+07	For 10°C, calculated as $K_{ow}(T_0) = 10^{\log Kow} \cdot a$, $a = \exp[(\Delta H_{sol} / R) \cdot (1 / T_0 - 1/T)]$. ΔH_{sol} = -31.1 KJ/mol: Enthalpy of solution (from octanol to water) here: $a_{Kow} = \Delta H_{sol} / R$	*Li et al.,* 2003
		a_{Kow}	3740.5		
		T_0, K	283.15		
CliMoChem	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence (-dH/R)	K^0_{ow}, dimensionless	8.17E+06	$K_{ow}(T) = K_{ow}(T_{ref})\exp((dHK_{ow}/R)(1/T_{ref} - 1/T))$ dimensionless T = temperature (283.15K); T_{ref} = reference temperature (298.15 K) $K_{ow}(T_{ref})$ = Octanol/water partition coefficient at T_{ref} PCB 153: 5.62E+6; dHK_{ow} = phase transfer enthalpy (J/mol) PCB 153: -17500 R = universal gas constant (8.3145 J/mol K)	*Beyer et al.,* 2002
		a_{Kow}	2104.8		
		T_0, K	283.15		
DEHM-POP	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is *a* parameter of temperature dependence (-dH/R)	K^0_{ow}, dimensionless	8.17E+06	$K_{ow}(283.15)=K^0_{ow}(298.15)\exp(aK_{ow}(1/T - 1/T_0)$, where $K^0_{ow}(298.15)$ = 5.62E+6 for PCB 153 $a_{Kow} = dHk_{ow}/R$ dHK_{ow} = phase transfer enthalpy (J/mol) PCB 153: -17500 R = universal gas constant (8.3145 J/mol K)	*Beyer et al.,* 2002
		a_{Kow}	2102.4		
		T_0, K	283.15		
MSCE-POP	Temperature independent	K_{ow}, dimensionless	7.94E+6	log K_{ow} = 6.9	*Mackay et al*., 1992

Table B.5. *The organic carbon/water partition coefficient of PCBs, dm^3/kg*

Model	Description	Numerical values		Comments	Reference
CAM/POPs	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41	K_{oc} is calculated from K_{ow}, where K_{ow} is the temperature dependent octanol-water partitioning coefficient	*Karickhoff,* 1981 *Mackay,* 1991 *Schnoor,* 1996
		b	1		
SimpleBox	Regression relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41	K_{oc} is calculated from K_{ow}, where K_{ow} is the temperature dependent octanol-water partition coefficient	*Karikhoff,* 1981
		b	1		
G-CIEMS	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	1.26		
		b	0.81		
EVN-BETR and UK-MODEL	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41		*Karikhoff*, 1981
		b	1		
CliMoChem	Regresion relation: $K_{oc} = regc\ \ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.35	K_{oc} is calculated from K_{ow}, where K_{ow} is the temperature dependent octanol-water partition coefficient	*Seth et al.,* 1999
		b	1		
DEHM-POP	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41		*Mackay,* 1999
		b	1		
MSCE-POP	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41		*Karikhoff,* 1981
		b	1		

Table B.6. *Degradation rate constants (or half-lives) of PCB-153 in the environmental media*

Model	Description	Numerical values		Comments	Reference
CAM/ POPs	Degradation in atmosphere: Temperature dependent: $k_{air} = k^0_{air} \exp(-a_{kair}(1/T - 1/T_0))$ where T - temperature (K), k^0_{air} is the value at the reference temperature T_0, and a_{kair} is a parameter of temperature dependence	k^0_{air} (T_0), cm^3/(molec·s)	2.11E-13	Coefficients of the exponential equation are recalculated from the following temperature dependence: $K_{OH} = K_{OH}^0 \exp(a(1/T_0 - 1/T)$ where K_{OH}^0 = 2.7E-13 is the value at the reference temperature T_0 (298 K), a = 1400 is parameter of temperature dependence.	This study
		a_{kair}	1400		
		T_0, *K*	283.15		
CliMoChem	Degradation in atmosphere: Temperature dependent: $k_{air} = k^0_{air} \exp(-a_{kair}(1/T - 1/T_0))$ where T - temperature (K), k^0_{air} is the value at the reference temperature T_0, and a_{kair} is a parameter of temperature dependence	k^0_{air} (T_0), cm^3/(molec·s)	1.18E-13	$k_{air}(T) = k_{air}(T_{ref}) \exp((-E_{aair}/R)(1/T - 1/T_0))$ T = temperature (283.15 K), T_0 = reference temperature (298.15 K) $k_{air}(T_0)$ = degradation rate constant at T_0 (cm^3/d), PCB 153: 1.42E-8; E_{aai} = activation energy (J/mol), PCB 153: 15400; R = universal gas constant (8.3145 J/mol K) k^0_{air} =degradation rate constant at 283.15 (cm^3/d), PCB 153: 1.02E-08 $a_{kair} = E_a/R$	*Beyer et al.*, 2002
		a_{kair}	1852.2		
		T_0, *K*	283.15		
	Degradation in soil: Temperature dependent: $k_{soil} = k^0_{soil} \exp(-a_{ksoil}(1/T - 1/T_0))$ where T - temperature (K), k^0_{soil} is the value at the reference temperature T_0, and a_{ksoil} is a parameter of temperature dependence	k^0_{soil} (T_0), 1/*s*	6.16E-10	$k_{soil}(T) = k_{soil}(T_{ref}) \exp((-E_{asoil}/R)(1/T - 1/T_0))$ T = temperature (283.15 K), T_0 = reference temperature (298.15 K) $k_{soil}(T_0)$ = degradation rate constant at T_0 (1/*d*), PCB 153: 1.01E-4; E_{asoil} = activation energy (J/mol) PCB 153: 30000 R = universal gas constant (8.3145 J/mol K) k^0_{soil} = degradation rate constant at 283.15 (1/*d*), PCB 153: 5.32E-05 $a_{ksoil} = E_{asoil}/R$	
		a_{ksoil}	3608.2		
		T_0, *K*	283.15		
	Degradation in water: Temperature dependent: $k_{water} = k^0_{water} \exp(-a_{kwater}(1/T - 1/T_0)$ where T - temperature (K), k0water is the value at the reference temperature T_0, and a_{kwater} is a parameter of temperature dependence	k^0_{water} (T_0), 1/*s*	8.47E-10	$k_{water}(T) = k_{water}(T_{ref}) \exp((-E_{awater}/R)(1/T - 1/T_0))$ T = temperature (283.15 K), T_0 = reference temperature (298.15 K) $k_{water}(T_0)$ = degradation rate constant at T_0 (1/*d*), PCB 153: 1.39E-4; E_{awater}=activation energy (J/mol), PCB 153: 30000 R = universal gas constant (8.3145 J/mol K) k^0_{water} =degradation rate constant at 283.15 (1/*d*), PCB 153: 7.32E-05; $a_{kwater} = E_{awater}/R$	
		a_{kwater}	3608.2		
		T_0, *K*	283.15		

Model	Description	Numerical values		Comments	Reference
	Degradation in vegetation*: Temperature dependent: $k_{veg} = k^0_{veg}\exp(-a_{kveg}(1/T - 1/T_0))$ where T - temperature (K), k^0_{veg} is the value at the reference temperature T_0, and a_{ksed} is a parameter of temperature dependence	k^0_{veg} (T_0), 1/s	1.14E-07	$k_{veg}(T) = k_{veg}(T_{ref})\exp((-E_{aveg}/R)(1/T - 1/T_0))$ T = temperature (283.15 K), T_0 = reference temperature (298.15 K) $k_{veg}(T_0)$ = degradation rate constant at T_0 (1/*d*), PCB 153: 1.37E-2; E_{aveg} = activation energy (J/mol), PCB 153: 15400 R = universal gas constant (8.3145 J/mol K) $k_{veg}(T_0)$ = degradation rate constant at T_0(1/*d*), PCB 153: 9.86E-03; $a_{kveg} = E_{aveg}/R$	
		a_{kveg}	1852.2		
		T_0, *K*	283.15		
MSCE-POP	Degradation in atmosphere: Temperature dependent: $k_{air} = k^0_{air}\exp(-a_{kair}(1/T - 1/T_0))$ where T - temperature (K), k^0_{air} is the value at the reference temperature T_0, and a_{kair} is a parameter of temperature dependence	k^0_{air} (T_0), cm^3/(molec·s)	1.18E-13	Coefficients of the exponential equation are recalculated from the following temperature dependence: $k_{air} = A \cdot exp(-E_a/RT)$ with the help of the following formulas: $a_{kair}=E_a/R$, $k^0_{air} = A \cdot exp(-Ea/RT_0)$, where A = 8.12 E-11 is the pre-exponential multiplier value, cm^3/(molec· s); E_A = 15380 is the activation energy of interaction with OH-radical in air, J/mol	*Beyer and Matthies,* 2001
		a_{kair}	1849.8		
		T_0, *K*	283.15		
	Degradation in soil: Temperature independent	k_{soil}, 1/s	1.17E-09	Degradation rate constant in soil is conversed from half-life values (PCB-153: 165000 hours): k_d = 0.693/ $t_{1/2}$, where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	*Sinkkonen and Paasivirta,* 2000
	Degradation in water: Temperature independent	k_{water}, 1/s	1.6E-09	Degradation rate constant in water is conversed from half-life values (PCB-153: 120000 hours): k_d = 0.693/ $t_{1/2}$, where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	
SimpleBox	Degradation in atmosphere: Temperature independent	k_{air}, 1/s	3.50E-08	PCB-153: 5500 hours	*Mackay et al.,*1992
	Degradation in soil: Temperature independent	k_{soil},1/s	3.50E-09	PCB-153: 55000 hours	
	Degradation in water: Temperature independent	k_{water},1/s	3.50E-09	PCB-153: 55000 hours	
G-CIEMS	Degradation in atmosphere: Temperature independent	k_{air},1/s	3.50E-08	PCB-153: 5500 hours	*Mackay et al.,* 1992
	Degradation in soil: Temperature independent	k_{soil},1/s	3.50E-09	PCB-153: 55000 hours	
	Degradation in water: Temperature independent	k_{water},1/s	3.50E-09	PCB-153: 55000 hours	
EVN-BETR and UK-MODEL	Degradation in atmosphere: Temperature independent	k_{air},1/s	3.50E-08	PCB-153: 5500 hours	*Mackay et al.,*1992
	Degradation in soil: Temperature independent	k_{soil},1/s	3.50E-09	PCB-153: 55000 hours	
	Degradation in water: Temperature independent	k_{water},1/s	3.50E-09	PCB-153: 55000 hours	
	Degradation in sediment: Temperature independent	k_{sed},1/s	3.50E-09	PCB-153: 55000 hours	
	Degradation in vegetation: Temperature independent	k_{veg},1/s	1.13E-08	PCB-153 half-life in vegetation: 17000 hours	

* - because of insufficient data on degradation rate constants in vegetation, the values are taken from atmospheric degradation [*Möller*, 2002] and multiplied with an average OH-radical concentration of 970000 1/cm^3 [*Beyer et al*., 2002].

Table B.7*. "Reference data set" of physical-chemical properties and degradation rates of PCB-153**

Description	Numerical values		Comments	Ref.
Air/water Henry's law constant, H, Pa·m^3/mol				
Temperature dependent: $H = H_0 \exp (- a_H (1/T - 1/T_0))$ where T - temperature (K), H_0 is value at the reference temperature T_0, and a_H is a parameter of temperature dependence.	H_0 (T_0), Pa·m^3/mol	4.91E+00	Coefficients are recalculated from the following temperature dependence: $\log H = \log H(25^0C) - (\Delta U_{aw} + R \cdot 298.15)/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_{aw} - internal energy of phase transfer, kJ/mol (for PCB-153: 62.8). $H(25^0C)$ - Henry 's law constant at 25^{0}C, Pa·m^3/mol (PCB-153: 19.8).	*Li et al.*, 2003
	a_H	7851.7		
Air/water partition coefficient, K_{aw}, dimensionless				
Temperature dependent: $K_{aw} = K^0_{aw} \exp (- a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K), K^0_{AW} is the value at the reference temperature T_0, and a_{Kaw} is a parameter of temperature dependence.	K^0_{AW} (T_0), dimensionless	2.09E-03	Coefficients are recalculated from the following temperature dependence: $\log K_{aw} = \log K_{aw}(25^0C) - \Delta U_{aw}/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_{aw} - internal energy of phase transfer, kJ/mol (for PCB-153: 62.8). $K_{aw}(25^0C)$ - dimensionless air/water partition coefficient at 25^{0}C, estimated from: $K_{aw}(25^0C) = H(25^0C)/(R \cdot 298.15)$	*Li et al.*, 2003
	a_{Kaw}	7553.5		
Subcooled liquid vapour pressure, p_{0L}, Pa				
Temperature dependent: $p_{0L} = p^0_{0L} \exp (- a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{0L} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{0L} (T_0), Pa	8.82E-05	Coefficients are recalculated from the following temperature dependence: $\log p_{0L} = \log p_{0L}(25^0C) - (\Delta U_a + R \cdot 298.15)/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_a - internal energy of phase transfer, kJ/mol (for PCB-153: 87.7). p_{0L} (25^{0}C) - vapour pressure at 25^{0}C, *Pa* (for PCB-153: 6.06E-4)	*Li et al.*, 2003
	a_p	10846.6		
Octanol/water partition coefficient, K_{ow}, dimensionless				
Temperature dependent: $K_{ow} = K^0_{ow} \exp (a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{OW} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence.	K^0_{ow} (T_0), dimensionless	1.45E+07	Coefficients are recalculated from the following temperature dependence: $\log K_{ow} = \log K_{ow}(25^0C) - \Delta U_{OW}/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_{ow} - internal energy of phase transfer, kJ/mol (for PCB-153:-31.1). K_{ow}(25^{o}C) - octanol/water partition coefficient at 25^{0}C, dimensionless (for PCB-153: 7.44E+6)	*Li et al.*, 2003
	a_{Kow}	3740.7		
Octanol/air partition coefficient, K_{oa}, dimensionless				
Temperature dependent: $K_{oa} = K^0_{oa} \exp (a_{Koa} (1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	2.05E+10	Coefficients are recalculated from the following temperature dependence: $\log K_{oa} = \log K_{oa}(25^0C) - \Delta U_{oa}/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_{oa} - internal energy of phase transfer, kJ/mol (for PCB-153: -93.9). $K_{oa}(25^0C)$ - octanol/air partition coefficient at 25^{0}C, dimensionless (for PCB-153: 2.76E+9);	*Li et al.*, 2003
	a_{Koa}	11294.2		
Organic carbon/water partition coefficient, K_{oc}, dimensionless				
Regression relation: $K_{oc} = regc\ K_{ow}^{\ b}$ where *regc* and *b* are regression coefficients	*regc*	0.41	K_{oc} is calculated from K_{ow}, where K_{ow} is the temperature dependent octanol-water partitioning coefficient	*Karik-hoff*, 1981
	b	1		
Water solubility, S_{WL}, mol/m^3				
Temperature independent	S_{WL} (T), mol/m^3	1.80E-05	Values are calculated for T = 283.15 with the help of the following temperature dependence: $\log S_{WL} = \log S_{WL}(25^0C) - \Delta U_W/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: R - Universal Gas Constant; ΔU_W - internal energy of phase transfer, kJ/mol (for PCB-153: 25.0). S_{WL}(25^{0}C) - water solubility, mol/m^3 at 25^{0}C (PCB-153: 3.07E-5);	*Li et al.*, 2003
Degradation rate constants, k_d, 1/s				
Degradation in atmosphere: Temperature independent	k_{air}, 1/s	3.50E-08	Degradation rate constant in the air is conversed from half-life values, h (PCB-153: 5500): $k_d = 0.693/ t_{1/2}$ where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	*Mackay et al*, 1992
Degradation in soil: Temperature independent	k_{soil}, 1/s	3.50E-09	Degradation rate constant in soil is conversed from half-life values (PCB-153: 55000): $k_d = 0.693/ t_{1/2}$ where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	
Degradation in water: Temperature independent	k_{water},1/s	3.50E-09	Degradation rate constant in water is conversed from half-life values (PCB-153: 55000): $k_d = 0.693/ t_{1/2}$ where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	
Degradation in sediment: Temperature independent	k_{sed}, 1/s	3.50E-09	Degradation rate constant in sediment is conversed from half-life values (PCB-153: 55000): $k_d = 0.693/ t_{1/2}$ where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here at the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

Table B.8*. "Alternative" data set of physical-chemical properties and degradation rates of PCB-153**

Description	Numerical values		Comments	Ref.
Air/water partition coefficient, K_{aw}, dimensionless				
Temperature dependent: $K_{aw} = K^0_{aw} \exp(-a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K); K^0_{aw} is the value at the reference temperature T_0; a_{Kaw} is a parameter of temperature dependence.	$K^0_{aw}(T_0)$, dimensionless	2.01E-03	$K_{aw}(T) = K_{aw}(T_{ref}) \exp(dHK_{aw}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{aw}(T_{ref})$ = Henry 's law constant at T_{ref} (dimensionless) PCB 153: $9.18 \cdot 10^{-3}$; dHK_{aw} = phase transfer enthalpy (J/mol) PCB 153: 71000 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{Kaw}	8536		
Subcooled liquid vapour pressure, p_{0L}, Pa				
Temperature dependent: $p_{0L} = p^0_{0L} \exp(-a_p(1/T - 1/T_0))$ where T - temperature (K); p^0_{0L} is the value at the reference temperature T_0; a_p is a parameter of temperature dependence.	$p^0_{0L}(T_0)$,	6.89E-05	Not used in DEHM-POP and CliMoChem models $p_{0L}(T) = p_{0L}(T_{ref}) \exp(dHp_{0L}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $p_{0L}(T_{ref})$ = Subcooled liquid vapour pressure at T_{ref} (Pa) PCB 153: $4.62 \cdot 10^{-4}$; dHp_{0L} = phase transfer enthalpy (J/mol) PCB 153: 89030 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_p	10707.8		
Octanol/water partition coefficient, K_{ow}, dimensionless				
Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K); K^0_{ow} is the value at the reference temperature T_0; a_{Kow} is a parameter of temperature dependence.	$K^0_{ow}(T_0)$, dimensionless	8.17E+06	$K_{ow}(T) = K_{ow}(T_{ref}) \exp((dHK_{ow}/R)(1/T_{ref} - 1/T))$ dimensionless T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{ow}(T_{ref})$ = octanol/water partitioning coefficient at T_{ref} PCB 153: $5.62 \cdot 10^6$ dHK_{ow} = phase transfer enthalpy (J/mol) PCB 153: -17500 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{Kow}	2102.4		
Octanol/air partition coefficient, K_{oa}, dimensionless				
Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T – temperature, K; K^0_{oa} is the value at the reference temperature T_0; a_{Koa} is a parameter of temperature dependence.	$K^0_{oa}(T_0)$, dimensionless	2.74E+10	Not used in CliMoChem model $K_{oa}(T) = K_{oa}(T_{ref}) \exp((dHK_{oa}/R)(1/T_{ref} - 1/T))$ dimensionless T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{oa}(T_{ref})$ = octanol/water partitioning coefficient at T_{ref} PCB 153: $4.14 \cdot 10^9$ dHK_{oa} = phase transfer enthalpy (J/mol) PCB 153: -88440 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{Koa}	10636.8		
Organic carbon/water partition coefficient, K_{oc}, dimensionless				
Regression relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.35	K_{oc} is calculated from K_{ow}, where K_{ow} is the temperature dependent octanol-water partition coefficient	*Seth et al.,* 1999
	b	1		
Water solubility, S_{WL}, mol/m^3				
Temperature independent	$S_{WL}(T)$, mol/m^3	1.38E-05	Not used in DEHM-POP and CliMoChem models. Values are calculated for T = 283.15 with the help of the following temperature dependence: $S_{WL}(T) = S_{WL}(T_{ref}) \exp(dHS_{WL}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K); $S_{WL}(T_{ref})$ = water solubility at T_{ref} (mol/m^3) PCB 153: $2.03 \cdot 10^{-5}$ dHS_{WL} = phase transfer enthalpy (J/mol) PCB 153: 18060 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
Degradation rate constants, k_d, 1/s				
Degradation in atmosphere: Temperature independent	$k_{air}(T)$, 1/s	9.78E-08	The rate constants of the second order degradation process in air used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe. Then multiplying the second order rate constants by mean annual OH-radical concentration in the surface layer of 2 km depth at the latitude of 450N (0.8·106 molec/cm^3) [*Yu Lu and Khall,* 1991], the first order degradation rate constants were calculated.	*This study*
Degradation in soil: Temperature independent	$k_{soil}(T)$, 1/s	7.29E-10	The rate constants of the first order degradation process in soil used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*

Description	Numerical values		Comments	Ref.
Degradation in water: Temperature independent	$k_{water}(T)$, 1/s	8.27E-10	The rate constants of the first order degradation process in water used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*
Degradation in vegetation: Temperature independent	$K_{veg}(T)$, 1/s	1.18E-07	The rate constants of the first order degradation process in vegetation used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here for the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".