Supporting Information For

Temperature dependence of the rain-gas and snow-gas partition coefficients for nearly a thousand chemicals

Pu-Fei Yang [a,b,c,d], Wan-Li Ma [a,b,c], Hang Xiao [e,f], Kaj M. Hansen [d], Liang Wang [a,b,c], Jing-Jing Sun [g], Li-Yan Liu [a,b,c], Zi-Feng Zhang [a b c], Hong-Liang Jia [g], Yi-Fan Li [a,b,c,h,*]

a. International Joint Research Center for Persistent Toxic Substances (IJRC-PTS), State Key Laboratory of Urban Water Resource and Environment, Harbin Institute of Technology, Harbin, 150090, China

b. International Joint Research Center for Arctic Environment and Ecosystem (IJRC-AEE), Polar Academy, Harbin Institute of Technology (PA-HIT), Harbin, 150090, China

c. Heilongjiang Provincial Key Laboratory of Polar Environment and Ecosystem (HPKL-PEE), Harbin, 150090, China

d. Department of Environmental Science, Aarhus University, Roskilde, Denmark

e. Key Laboratory of Urban Environment and Health, Ningbo Observation and Research Station, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen, 361021, China

f. Zhejiang Key Laboratory of Urban Environmental Processes and Pollution Control, CAS Haixi Industrial Technology Innovation Center in Beilun, Ningbo,

315800, China

g. International Joint Research Centre for Persistent Toxic Substances (IJRC-PTS), College of Environmental Science and Engineering, Dalian Maritime University, Dalian 116026, China.

h. IJRC-PTS-NA, Toronto, ON, M2J 3N8, Canada

Content

Tables

Table S1 Observed logK_{RG} from the published studies

Chemical	CAS	T(℃)	logK_{RG}	Reference
Biphenyl	92-52-4	15	3.9	
PCB-6	25569-80-6	15	4.5	
PCB-6	25569-80-6	15	3.5	
PCB-8	34883-43-7	15	5.1	
PCB-11	2050-67-1	15	2	
PCB-16	38444-78-9	15	3.3	
PCB-17	37680-66-3	15	2.9	
PCB-18	37680-65-2	15	2.9	
PCB-18	37680-65-2	15	4.4	
PCB-18	37680-65-2	15	4.2	
PCB-18	37680-65-2	15	3.1	
PCB-19	38444-73-4	15	2.9	
PCB-26	38444-81-4	15	3.6	
PCB-26	38444-81-4	15	3.5	
PCB-27	38444-76-7	15	3.4	
PCB-28	7012-37-5	15	4.3	
PCB-28	7012-37-5	15	4.6	
PCB-28	7012-37-5	15	4.6	
PCB-28	7012-37-5	15	4.4	
PCB-28	7012-37-5	15	3.1	(Casas et al., 2021)
PCB-31	16606-02-3	15	4.5	
PCB-31	16606-02-3	15	4.3	
PCB-31	16606-02-3	15	3.2	
PCB-32	38444-77-8	15	3.1	
PCB-33	38444-86-9	15	3.2	
PCB-33	38444-86-9	15	5.9	
PCB-33	38444-86-9	15	3.1	
PCB-37	38444-90-5	15	3.3	
PCB-42	36559-22-5	15	3.2	
PCB-44	41464-39-5	15	3.2	
PCB-44	41464-39-5	15	4.3	
PCB-45	70362-45-7	15	3	
PCB-47	2437-79-8	15	3.3	
PCB-48	70362-47-9	15	3.1	
PCB-49	41464-40-8	15	3.2	
PCB-49	41464-40-8	15	4.3	
PCB-49	41464-40-8	15	2.9	
PCB-52	35693-99-3	15	3.6	
PCB-52	35693-99-3	15	4.8	
PCB-52	35693-99-3	15	4.2	

PCB-52	35693-99-3	15	4.2
PCB-52	35693-99-3	15	4.7
PCB-52	35693-99-3	15	2.9
PCB-53	41464-41-9	15	3.1
PCB-60	33025-41-1	15	4.7
PCB-64	52663-58-8	15	3.1
PCB-66	32598-10-0	15	4.1
PCB-66	32598-10-0	15	3.1
PCB-70	32598-11-1	15	4.2
PCB-74	32690-93-0	15	4.1
PCB-74	32690-93-0	15	3.1
PCB-81	70362-50-4	15	3.7
PCB-83	60145-20-2	15	3.2
PCB-87	38380-02-8	15	3.2
PCB-89	73575-57-2	15	3.3
PCB-91	68194-05-8	15	3.9
PCB-91	68194-05-8	15	3.2
PCB-95	38379-99-6	15	4
PCB-95	38379-99-6	15	2.9
PCB-97	41464-51-1	15	3.2
PCB-99	38380-01-7	15	3.8
PCB-99	38380-01-7	15	3.1
PCB-100	39485-83-1	15	3.5
PCB-101	37680-73-2	15	3.5
PCB-101	37680-73-2	15	4.8
PCB-101	37680-73-2	15	4.4
PCB-101	37680-73-2	15	4.9
PCB-101	37680-73-2	15	4.6
PCB-101	37680-73-2	15	4.4
PCB-101	37680-73-2	15	3.1
PCB-118	31508-00-6	15	3.8
PCB-118	31508-00-6	15	4.5
PCB-118	31508-00-6	15	4.5
PCB-119	56558-17-9	15	4.2
PCB-132	38380-05-1	15	4.4
PCB-138	35065-28-2	15	4.3
PCB-138	35065-28-2	15	5.1
PCB-138	35065-28-2	15	4.7
PCB-138	35065-28-2	15	5
PCB-138	35065-28-2	15	4.1
PCB-149	38380-04-0	15	3.9
PCB-153	35065-27-1	15	4.1
PCB-153	35065-27-1	15	5.1
PCB-153	35065-27-1	15	4.6
PCB-153	35065-27-1	15	4.3
PCB-174	38411-25-5	15	4.7

PCB-177	52663-70-4	15	4.3
PCB-180	35065-29-3	15	4.6
PCB-180	35065-29-3	15	5.4
PCB-180	35065-29-3	15	5
PCB-180	35065-29-3	15	4.5
PCB-180	35065-29-3	15	5.1
PCB-180	35065-29-3	15	5.4
PCB-194	35694-08-7	15	5.1
PCB-194	35694-08-7	15	5.6
α-HCH	319-84-6	15	4
α-HCH	319-84-6	15	4.1
α-HCH	319-84-6	15	3.7
α-HCH	319-84-6	15	3.7
γ-HCH	58-89-9	15	4.4
γ-HCH	58-89-9	15	4.5
γ-HCH	58-89-9	15	4.6
γ-HCH	58-89-9	15	5
γ-HCH	58-89-9	15	3.8
γ-HCH	58-89-9	15	4.2
β-HCH	319-85-7	15	4.8
HCB	118-74-1	15	3.4
HCB	118-74-1	15	2.7
HCB	118-74-1	15	3
HCB	118-74-1	15	2.2
DDE	72-55-9	15	3
DDE	72-55-9	15	3.2
DDD	72-54-8	15	4.7
DDT	50-29-3	15	3
DDT	50-29-3	15	3.6
DDT	50-29-3	15	3.5
DDT	50-29-3	15	4.8
DDT	50-29-3	15	3.5
Heptachlor	76-44-8	15	4.1
Heptachlor	76-44-8	15	3.6
Oxychlordane	27304-13-8	15	3.5
α-Chlordane	5103-71-9	15	3.4
α-Chlordane	5103-71-9	15	3.3
γ-Chlordane	5566-34-7	15	3.3
γ-Chlordane	5566-34-7	15	3.4
Trans-nonachlor	39765-80-5	15	3.8
Trans-nonachlor	39765-80-5	15	3
Pentachloroanisole	1825-21-4	15	3.5
Dieldrin	60-57-1	15	3.9
Dieldrin	60-57-1	15	3.8
Endrin	72-20-8	15	4.6
Chlorpyrifos	2921-88-2	15	3.7

Endosulfan I	959-98-8	15	3.4
Endosulfan I	959-98-8	15	3.9
Endosulfan II	33213-65-9	15	5.1
Endosulfan II	33213-65-9	15	5.2
Endosulfansulfate	1031-07-8	15	5.6
Naphthalene	91-20-3	15	6.1
Naphthalene	91-20-3	15	6.6
Acenaphthylene	208-96-8	15	2.7
Acenaphthylene	208-96-8	15	3.9
Acenaphthylene	208-96-8	15	5.6
Acenaphthylene	208-96-8	15	4.5
Acenaphthene	83-32-9	15	3
Acenaphthene	83-32-9	15	3.8
Acenaphthene	83-32-9	15	4.7
Acenaphthene	83-32-9	15	5.2
Fluorene	86-73-7	15	3.2
Fluorene	86-73-7	15	1.8
Fluorene	86-73-7	15	3.1
Fluorene	86-73-7	15	3.4
Fluorene	86-73-7	15	3.5
Fluorene	86-73-7	15	4.4
Fluorene	86-73-7	15	4.5
Fluorene	86-73-7	15	2.9
Dibenzothiophene	132-65-0	15	3.5
Dibenzothiophene	132-65-0	15	4.2
Phenanthrene	85-01-8	15	2.4
Phenanthrene	85-01-8	15	3.5
Phenanthrene	85-01-8	15	3.4
Phenanthrene	85-01-8	15	4.1
Phenanthrene	85-01-8	15	3.4
Phenanthrene	85-01-8	15	3.9
Phenanthrene	85-01-8	15	3.5
Anthracene	120-12-7	15	1.1
Anthracene	120-12-7	15	3.2
Anthracene	120-12-7	15	3.5
Anthracene	120-12-7	15	4.1
Anthracene	120-12-7	15	3.5
Anthracene	120-12-7	15	4.2
Anthracene	120-12-7	15	3.8
Fluoranthene	206-44-0	15	3.8
Fluoranthene	206-44-0	15	3.9
Fluoranthene	206-44-0	15	4.9
Fluoranthene	206-44-0	15	3.8
Fluoranthene	206-44-0	15	3.9
Fluoranthene	206-44-0	15	4.1
Pyrene	129-00-0	15	3.8

Pyrene	129-00-0	15	2.6
Pyrene	129-00-0	15	4
Pyrene	129-00-0	15	4.7
Pyrene	129-00-0	15	4
Pyrene	129-00-0	15	4.3
Benzo[g,h,i]fluoranthene	203-12-3	15	4.8
Benzo[a]anthracene	56-55-3	15	4.1
Benzo[a]anthracene	56-55-3	15	2.7
Benzo[a]anthracene	56-55-3	15	4.7
Benzo[a]anthracene	56-55-3	15	4.9
Benzo[a]anthracene	56-55-3	15	5.2
Benzo[a]anthracene	56-55-3	15	5
Benzo[a]anthracene	56-55-3	15	5.3
Benzo[a]anthracene	56-55-3	15	5.5
Chrysene	218-01-9	15	4.3
Chrysene	218-01-9	15	2.1
Chrysene	218-01-9	15	4.7
Chrysene	218-01-9	15	4.8
Chrysene	218-01-9	15	4.5
Chrysene	218-01-9	15	5.1
Benzo[b]fluoranthene	205-99-2	15	2.7
Benzo[b]fluoranthene	205-99-2	15	5.4
Benzo[b]fluoranthene	205-99-2	15	5.7
Benzo[k]fluoranthene	207-08-9	15	2.4
Benzo[k]fluoranthene	207-08-9	15	5.3
Benzo[k]fluoranthene	207-08-9	15	5.1
Benzo[k]fluoranthene	207-08-9	15	5.7
Benzo[e]pyrene	192-97-2	15	3.8
Benzo[e]pyrene	192-97-2	15	5.9
Benzo[e]pyrene	192-97-2	15	5.3
Benzo[e]pyrene	192-97-2	15	5.2
Benzo[e]pyrene	192-97-2	15	5.6
Benzo[a]pyrene	50-32-8	15	5.3
Benzo[a]pyrene	50-32-8	15	5.5
Benzo[a]pyrene	50-32-8	15	5.7
Perylene	198-55-0	15	4.6
Perylene	198-55-0	15	5.7
Indeno[1,2,3-cd]pyrene	193-39-5	15	5.7
Indeno[1,2,3-cd]pyrene	193-39-5	15	5.5
Indeno[1,2,3-cd]pyrene	193-39-5	15	6.3
Indeno[1,2,3-cd]pyrene	193-39-5	15	5.6
Dibenzo[a,h]anthracene	53-70-3	15	4.8
Dibenzo[a,h]anthracene	53-70-3	15	6.6
Dibenzo[a,h]anthracene	53-70-3	15	5.6
Benzo[g,h,i]perylene	191-24-2	15	7.3
Benzo[g,h,i]perylene	191-24-2	15	5.4

Benzo[g,h,i]perylene	191-24-2	15	7
Benzo[g,h,i]perylene	191-24-2	15	5.7
Benzo[g,h,i]perylene	191-24-2	15	5.7
Coronene	191-07-1	15	5.4
Dibenzofuran	132-64-9	15	3
9-Fluorenone	486-25-9	15	4
9,10-Anthracenedione	84-65-1	15	4.4
BDE-28	41318-75-6	15	3.5
BDE-47	5436-43-1	15	5.2
BDE-47	5436-43-1	15	3.4
BDE-47	5436-43-1	15	4.4
BDE-47	5436-43-1	15	4.7
BDE-99	60348-60-9	15	5
BDE-99	60348-60-9	15	4.2
BDE-99	60348-60-9	15	4.3
BDE-100	189084-64-8	15	4.6
BDE-153	68631-49-2	15	6.1
BDE-153	68631-49-2	15	5.3
BDE-154	207122-15-4	15	6
BDE-154	207122-15-4	15	5.5
BDE-183	207122-16-5	15	5.9
BDE-183	207122-16-5	15	5.3
BDE-209	1163-19-5	15	6
BDE-209	1163-19-5	15	6.1
BDE-209	1163-19-5	15	6.8
BDE-209	1163-19-5	15	5.4

The logK_{RG} values have been well summarized by Casas et al.(2021). In this study we set an average temperature value as 15℃, around which most studies are conducted.

Table S2 Observed logK_{SG} from the published studies

Chemical	CAS	T(℃)	logK_{SG}	Volume	Reference
Cyclopentanone	120-92-3	0.0	1.58	Snow	(Xu and Vogel, 2021)
Cyclopentanone	120-92-3	-2.0	0.67	Snow	
Cyclopentanone	120-92-3	-7.0	0.74	Snow	
Cyclopentanone	120-92-3	-13.0	1.03	Snow	
Cyclopentanone	120-92-3	-20.0	1.35	Snow	
Cyclopentanone	120-92-3	0.2	1.43	Snow	
Cyclopentanone	120-92-3	-2.3	0.93	Snow	
Cyclopentanone	120-92-3	-7.3	0.88	Snow	
Cyclopentanone	120-92-3	-13.8	1.16	Snow	
Cyclopentanone	120-92-3	-20.0	1.63	Snow	
D4	107-51-7	0.0	0.43	Snow	
D4	107-51-7	-2.0	0.65	Snow	
D4	107-51-7	-7.0	0.81	Snow	
D4	107-51-7	-13.0	1.08	Snow	
D4	107-51-7	-20.0	1.17	Snow	
D5	110-86-1	0.2	1.16	Snow	
D5	110-86-1	-2.3	1.22	Snow	
D5	110-86-1	-7.3	1.35	Snow	
D5	110-86-1	-13.8	1.62	Snow	
D5	110-86-1	-20.0	1.59	Snow	
8:2 FTOH	678-39-7	0.0	3.54	Water	(Wang et al., 2015)
6:2 FTOH	647-42-7	0.0	4.60	Water	
10:2 FTOH	865-86-1	0.0	3.82	Water	
12:2 FTOH	39239-77-5	0.0	3.66	Water	
EtFOSA	4151-50-2	0.0	4.51	Water	
MeFOSE	24448-09-7	0.0	6.38	Water	
EtFOSE	1691-99-2	0.0	5.30	Water	
6:2 FTA	17527-29-6	0.0	4.54	Water	
8:2 FTA	27905-45-9	0.0	3.88	Water	
TCEP	115-96-8	0.0	4.75	Water	(Li et al., 2017)
TDCP	13674-87-8	0.0	4.90	Water	
TnBP	126-73-8	0.0	5.46	Water	
TPeP	2528-38-3	0.0	4.48	Water	
TPhP	115-86-6	0.0	4.74	Water	
Act	208-96-8	0.7	4.27	Water	(Casal et al., 2018)
Act	208-96-8	0.7	4.88	Water	
Act	208-96-8	1.3	4.63	Water	
Flu	86-73-7	0.7	3.44	Water	
Flu	86-73-7	0.7	4.09	Water	
Flu	86-73-7	1.3	4.15	Water	
Phe	85-01-8	0.7	3.73	Water	
Phe	85-01-8	0.7	4.37	Water	
Phe	85-01-8	1.3	4.62	Water	
Ant	120-12-7	0.7	3.76	Water	
Ant	120-12-7	0.7	4.26	Water	
Ant	120-12-7	1.3	4.17	Water	
DBT	132-65-0	0.7	4.45	Water	
DBT	132-65-0	0.7	4.04	Water	

DBT	132-65-0	1.3	5.03	Water	
Flt	206-44-0	0.7	3.86	Water	
Flt	206-44-0	0.7	4.91	Water	
Flt	206-44-0	1.3	4.86	Water	
Pyr	129-00-0	0.7	4.13	Water	
Pyr	129-00-0	0.7	5.16	Water	
Pyr	129-00-0	1.3	5.64	Water	
B[a]ant	56-55-3	0.7	3.32	Water	
B[a]ant	56-55-3	0.7	4.20	Water	
B[a]ant	56-55-3	1.3	3.70	Water	
Cry	218-01-9	0.7	4.48	Water	
Cry	218-01-9	0.7	4.74	Water	
Cry	218-01-9	1.3	5.42	Water	
B[b]f	205-99-2	0.7	2.21	Water	
B[b]f	205-99-2	0.7	2.95	Water	
B[b]f	205-99-2	1.3	2.87	Water	
HCB	118-74-1	0.7	2.83	Water	
HCB	118-74-1	0.7	3.25	Water	
HCB	118-74-1	1.2	2.96	Water	
β-HCH	319-85-7	1.2	3.6	Water	
γ-HCH	58-89-9	1.2	3.26	Water	
δ-HCH	319-86-8	0.7	3.51	Water	
PCB18	37680-65-2	0.7	2.68	Water	
PCB18	37680-65-2	0.7	3.3	Water	
PCB17	37680-66-3	0.7	3.01	Water	
PCB17	37680-66-3	0.7	3.23	Water	
PCB17	37680-66-3	1.2	4.14	Water	
PCB52	35693-99-3	0.7	3.64	Water	
PCB52	35693-99-3	0.7	4.44	Water	
PCB52	35693-99-3	1.2	3.13	Water	
PCB49	41464-40-8	0.7	3.33	Water	
PCB49	41464-40-8	0.7	3.88	Water	
PCB49	41464-40-8	1.2	3.65	Water	(Casal et al., 2019)
PCB44	41464-39-5	0.7	3.59	Water	
PCB44	41464-39-5	0.7	4.01	Water	
PCB44	41464-39-5	1.2	3.47	Water	
PCB74	32690-93-0	0.7	2.75	Water	
PCB74	32690-93-0	1.2	2.85	Water	
PCB70	32598-11-1	0.7	3.32	Water	
PCB70	32598-11-1	0.7	3.44	Water	
PCB70	32598-11-1	1.2	2.64	Water	
PCB95	38379-99-6	0.7	3.16	Water	
PCB95	38379-99-6	1.2	3.47	Water	
PCB87	38380-02-8	0.7	3.24	Water	
PCB87	38380-02-8	0.7	3.51	Water	
PCB87	38380-02-8	1.2	3.6	Water	
PCB110	38380-03-9	0.7	4.09	Water	
PCB110	38380-03-9	0.7	3.92	Water	
PCB110	38380-03-9	1.2	4.23	Water	

PCB151	52663-63-5	0.7	2.45	Water
PCB151	52663-63-5	0.7	2.75	Water
PCB151	52663-63-5	1.2	2.63	Water
PCB149	38380-04-0	0.7	3.7	Water
PCB149	38380-04-0	0.7	3.42	Water
PCB149	38380-04-0	1.2	2.99	Water
PCB118	31508-00-6	0.7	3.21	Water
PCB118	31508-00-6	0.7	3.9	Water
PCB118	31508-00-6	1.2	3.62	Water
PCB153	35065-27-1	0.7	3.61	Water
PCB153	35065-27-1	0.7	3.82	Water
PCB153	35065-27-1	1.2	3.81	Water
PCB132	38380-05-1	0.7	2.57	Water
PCB132	38380-05-1	0.7	2.94	Water
PCB132	38380-05-1	1.2	2.65	Water
PCB105	32598-14-4	1.2	3.46	Water
PCB138	35065-28-2	0.7	4.06	Water
PCB138	35065-28-2	0.7	4.42	Water
PCB138	35065-28-2	1.2	3.96	Water
PCB187	52663-68-0	0.7	2.95	Water
PCB187	52663-68-0	0.7	3.48	Water
PCB187	52663-68-0	1.2	2.79	Water
PCB128	38380-07-3	0.7	3.25	Water
PCB128	38380-07-3	0.7	3.82	Water
PCB128	38380-07-3	1.2	3.83	Water
PCB177	52663-70-4	0.7	1.27	Water
PCB177	52663-70-4	0.7	2.8	Water
PCB177	52663-70-4	1.2	2.35	Water
PCB171	52663-71-5	0.7	2.67	Water
PCB171	52663-71-5	0.7	3.54	Water
PCB171	52663-71-5	1.2	3.48	Water
PCB180	35065-29-3	0.7	2.2	Water
PCB180	35065-29-3	0.7	3.16	Water
PCB180	35065-29-3	1.2	2.87	Water
PCB191	74472-50-7	0.7	3.42	Water
PCB170	35065-30-6	0.7	2.96	Water
PCB170	35065-30-6	1.2	3.13	Water

The logK_{SG} values are calculated from some published studies. Xu and Vogel (2021) provide snow/air concentration ratios for some chemicals and collected in this study. Wang et al. (2015) and Li et al.(2017) observe concentration of snow and air separately. In this study, we calculate logK_{SG} based on the definition of partition coefficients. In Casal et al.'s studies, the observed snow concentration and the air equilibrated in-situ with soil/snow concentrations (Casal et al., 2019, 2018). This study selects air equilibrated concentrations on snow and calculates logK_{SG} based on the definition. The

"Volume" column represents if the logK_{SG} is based on the volume of snow or the equivalent meltwater.

Table S3 ΔU_{OW} and ΔS_{OW} values from published experimental studies

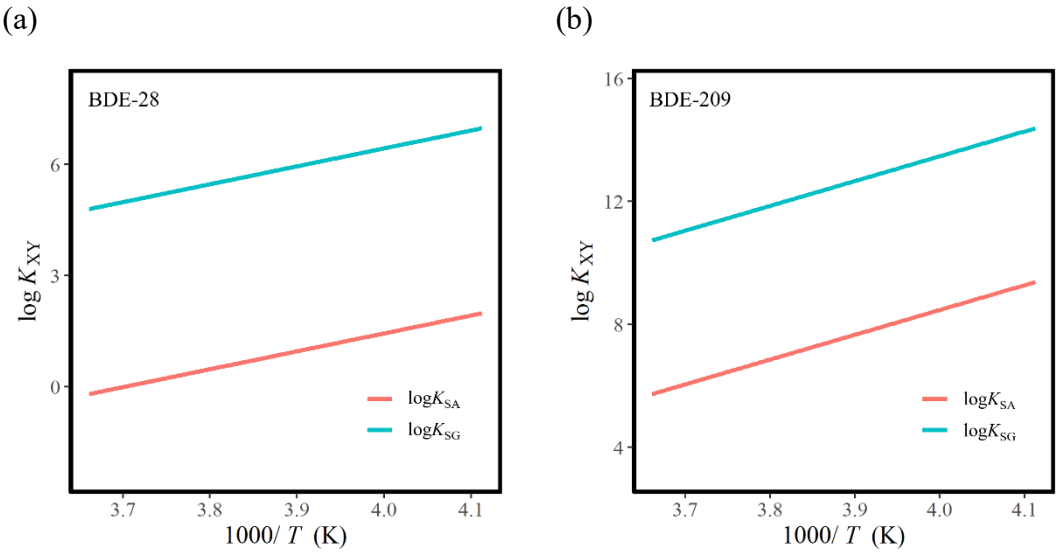
CAS	Chemical	ΔU_{OW} kJ/mol	ΔS_{OW} J/mol K	Reference
82419-36-1	Ofloxacin	23.28	70.79	(Zhang and Wang, 2010)
70458-96-7	Norfloxacin	18.35	89.60	(Zhang and Wang, 2010)
98079-51-7	Lomefloxacin	19.76	44.41	(Zhang and Wang, 2010)
85721-33-1	Ciprofloxacin	26.44	68.51	(Zhang and Wang, 2010)
70458-92-3	Pefloxacin	46.31	139.6	(Zhang and Wang, 2010)
51940-44-4	Pipemidic acid	20.33	44.59	(Zhang and Wang, 2010)
57-68-1	Sulfamethazine	-20.00	-62.00	(Zhang et al., 2007)
122-11-2	Sulfadimethoxine	-41.83	-124.9	(Zhang et al., 2007)
651-06-9	Sulfameter	-28.00	-89.00	(Zhang et al., 2007)
1220-83-3	Sulfamonomethoxine	-42.03	-137.4	(Zhang et al., 2007)
723-46-6	Sulfamethoxazole	-62.45	-192.7	(Zhang et al., 2007)
59-40-5	Sulfaquinoxaline	-34.98	-106.9	(Zhang et al., 2007)
102-65-8	Sulfaclozine	-41.25	-133.5	(Zhang et al., 2007)
121-34-6	3-Methoxy-4-hydroxybenzoic acid	-20.20	-40.64	(Noubigh et al., 2010)
121-33-5	Vanillin	-17.35	-35.20	(Noubigh et al., 2010)
99-50-3	3,4-Dihydroxybenzoic acid	-12.42	-27.41	(Noubigh et al., 2010)
100-15-2	N-Methyl-4-nitroaniline	-15.06	-10.44	(Boddu et al., 2008)
71-43-2	Benzene	7.06	67.35	(David and Moldoveanu, 2019a)
108-88-3	Toluene	5.95	72.99	(David and Moldoveanu, 2019a)
100-41-4	Ethylbenzene	6.38	82.93	(David and Moldoveanu, 2019a)
103-65-1	n-Propylbenzene	5.14	98.17	(David and Moldoveanu, 2019a)

Table S4 ΔU_{OW} and A_{OW} values from published experimental studies

CAS	Chemical	ΔU_{OW}	A_{OW}	Reference
613-12-7	2-Methylanthracene	-22.1	1.093	(Lei et al., 2000)
217-59-4	Triphenylene	-21.8	1.313	(Lei et al., 2000)
56-55-3	Pyrene	-23.3	1.238	(Lei et al., 2000)
205-99-2	Benz[b]fluoranthene	-25.4	1.371	(Lei et al., 2000)
90-13-1	1-Chloronaphthalene	-18.0	0.841	(Lei et al., 2000)
91-58-7	2-chloronaphthalene	-17.7	0.821	(Lei et al., 2000)
2050-69-3	1,2-PCN	-20.3	1.064	(Lei et al., 2000)
1825-31-6	1,4-PCN	-20.1	1.269	(Lei et al., 2000)
20020-02-4	1,2,3,4-PCN	-25.8	1.832	(Lei et al., 2000)
150224-24-1	1,2,3,5,8-PCN	-27.4	2.035	(Lei et al., 2000)
67922-26-3	1,2,3,4,6-PCN	-27.7	2.166	(Lei et al., 2000)
103426-94-4	1,2,3,5,7,8-PCN	-29.4	2.413	(Lei et al., 2000)
103426-96-6	1,2,3,4,6,7-PCN	-29.8	2.489	(Lei et al., 2000)
58863-14-2	1,2,3,4,5,6,7-PCN	-31.8	2.638	(Lei et al., 2000)
2234-13-1	1,2,3,4,5,6,7,8-PCN	-31.8	2.998	(Lei et al., 2000)
95-50-1	1,2-Dichlorobenzene	-17.8	0.1831	(Bahadur et al., 1997)
106-46-7	1,4-Dichlorobenzene	-17.1	0.2338	(Bahadur et al., 1997)
108-70-3	1,3,5-Trichlorobenzene	-18.2	1.1228	(Bahadur et al., 1997)
634-66-2	1,2,3,4-Tetrachlorobenzene	-21.1	0.6978	(Bahadur et al., 1997)
634-90-2	1,2,3,5-Tetrachlorobenzene	-20.2	1.0159	(Bahadur et al., 1997)
608-93-5	Pentachlorobenzene	-22.8	0.9255	(Bahadur et al., 1997)
118-74-1	Hexachlorobenzene	-24.4	1.1806	(Bahadur et al., 1997)

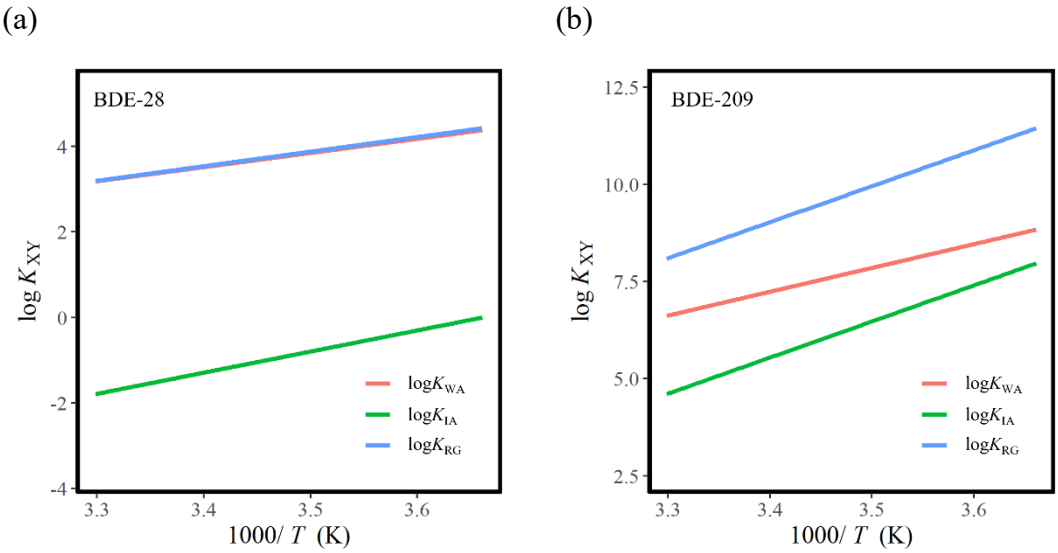
Figures

Figure S1 Temperature dependence of logK_{SG} and logK_{SA} for BDE-28 and BDE-209



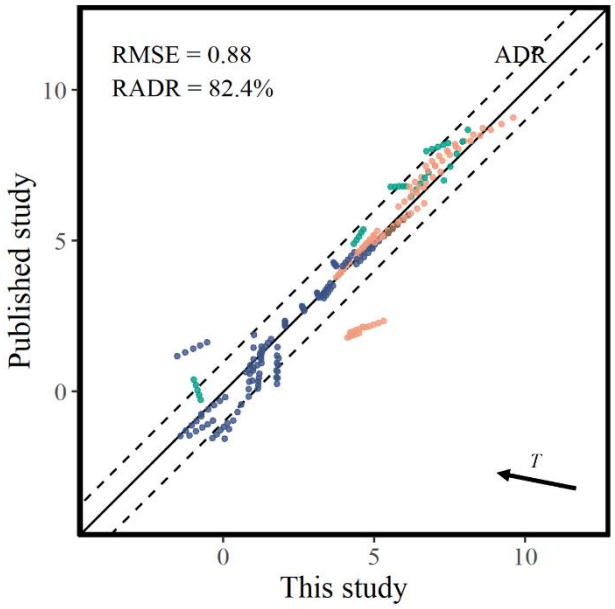
Variation of logK_{SG} and logK_{SA} of (A) BDE-28 and (B) BDE-209 as functions of 1/T (from -30°C to 0°C). The green lines are logK_{SG}, and the red lines are logK_{SA}.

Figure S2 Temperature dependence of logK_{RG}, logK_{WA} and logK_{IA} for BDE-28 and BDE-209



Variation of logK_{RG}, logK_{IA}, and logK_{WA} of (A) BDE-28 and (B) BDE-209 as functions of 1/T (from 0°C to 30°C). The green lines are logK_{SG}, and the red lines are logK_{SA}.

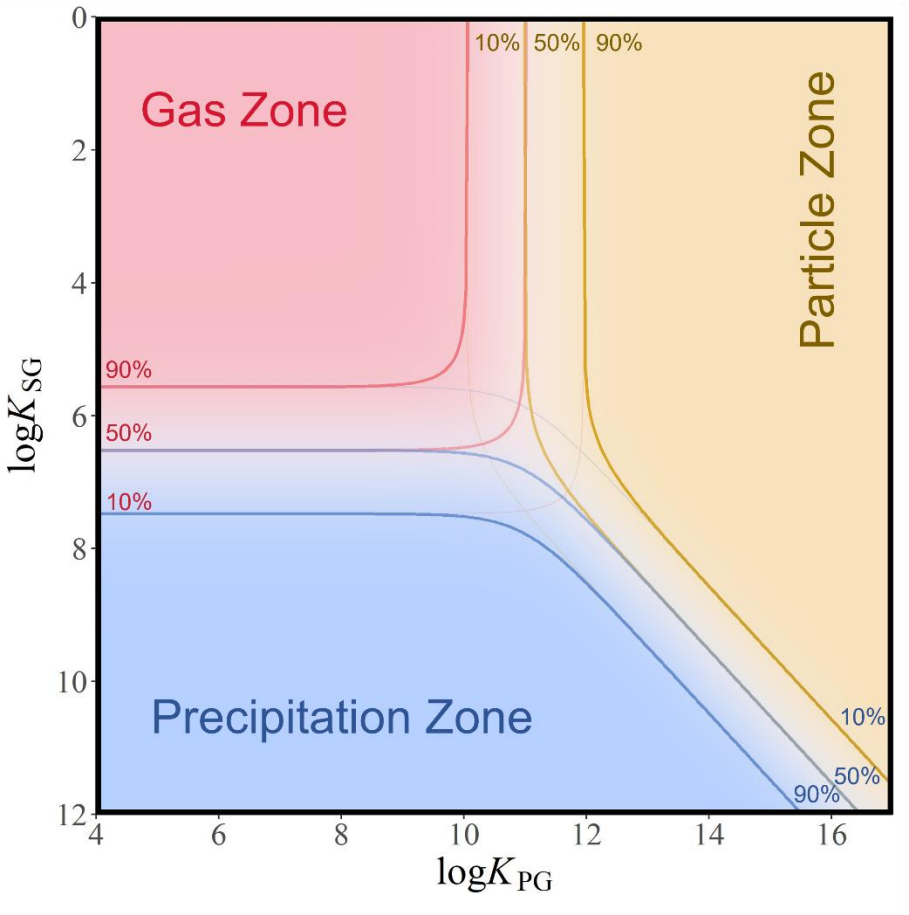
Figure S3 Temperature-dependent evaluation for logK_{OW}



Temperature-dependent evaluation of logK_{OW}. The experimental data are cited from published studies (Bahadur et al., 1997; David and Moldoveanu, 2019b; Jin et al., 2022; Lei et al., 2000; Noubigh et al., 2010; Viamajala et al., 2007; Xu and Kropscott, 2014; Zhang et al., 2007; Zhang and Wang, 2010). The black arrow shows the temperature is increasing from the right to the left.

The logK_{OW}'s data points also showing a good match between the results from the present study and the published experimental data. The *RMSE* is 0.88 and 82.4% of data points fall in the ADR.

Figure S4 Schematic diagrams of chemical space map.



Texts

Text S1 Calculation of K_{PG}

$$K_{\mathrm{PG}} = 10^{-2.91} f_{\mathrm{OM,Particle}} K_{\mathrm{OA}} \rho_{\mathrm{P}} \quad (\mathrm{S1})$$

where, $f_{\mathrm{OM,Particle}}$ is the fraction of organic matter in particle, 0.2 is assumed; ρ_{P} is the density of particles (1500 kg m^{-3}).

Text S2 Derivation of temperature dependence of partition coefficients

Partition coefficient K_{XY} can be calculated as

$$\ln K_{XY} = \ln \frac{C_X}{C_Y} \quad (S2)$$

where C_X and C_Y are concentrations of the targeted chemical in phase X and Y, respectively, and K_{XY} is the partition coefficient between phase X and Y.

Then concentration of the targeted chemical is defined as the quotient of chemical mole fraction in media (x, dimensionless) and molar volume (V, m^3/mol).

$$C = \frac{x}{V} \quad (S3)$$

Eq. S2 can be written as

$$\ln K_{XY} = \ln \left(\frac{x_X / V_X}{x_Y / V_Y} \right) = \ln \left(\frac{x_X}{x_Y} \right) - \ln \left(\frac{V_X}{V_Y} \right) \quad (S4)$$

where x_X and x_Y are mole fractions of solute in phase X and Y, respectively; and V_X and V_Y are respectively the molar volumes in phase X and phase Y. According to definition,

$$\ln K'_{XY} = \ln \left(\frac{x_X}{x_Y} \right) \quad (S5)$$

based on Eq. S2, S5 and Eq. 3 in the main text, we have,

$$\frac{d \ln K_{XY}}{dT} = \frac{\Delta H_{XY}}{RT^2} - \frac{d \ln V_X}{dT} + \frac{d \ln V_Y}{dT} \quad (S6)$$

K_{AW}. X represents air and Y represents water.

According to the ideal gas equation ($PV = RT$) and assuming the molar volume of water won't change by temperature. Eq. S6 can be written as,

$$\frac{d ln K_{AW}}{dT} = \frac{\Delta H_{AW} - RT}{RT^2} \quad (S7)$$

According to the first law of thermodynamics,

$$\frac{d ln K_{AW}}{dT} = \frac{\Delta U_{AW}}{RT^2} \quad (S8)$$

K_{OA}. X represents octanol and Y represents air.

Similarly,

$$\frac{d\ln K_{OA}}{dT} = \frac{\Delta H_{OA} + RT}{RT^2} \quad (S9)$$

According to the first law of thermodynamics (note that ΔH_{OA} in Eq. S9 is negative),

$$\frac{d\ln K_{OA}}{dT} = \frac{\Delta U_{OA}}{RT^2} \quad (S10)$$

***K*OW. X represents octanol and Y represents water.**

Assuming that the molar volume of both octanol and water won't change with temperature, and no work would be done on gas during this process,

$$\frac{d\ln K_{OW}}{dT} = \frac{\Delta H_{OW}}{RT^2} \approx \frac{\Delta U_{OW}}{RT^2} \quad (S11)$$

Text S3 Derivation of temperature dependence of adsorption coefficients

Similarly, the *K*' value in Eq. 3 from the main text can also be converted to adsorption coefficient *K* as

$$\ln K_{\mathrm{XY}} = \ln\left(\frac{x_{\mathrm{X}}/A_{\mathrm{X}}}{x_{\mathrm{Y}}/V_{\mathrm{Y}}}\right) = \ln K'_{\mathrm{XY}} - \ln\left(\frac{A_{\mathrm{X}}}{V_{\mathrm{Y}}}\right) \quad (\mathrm{S12})$$

where, K_{XY} is the adsorption coefficient between media X and Y; A_{X} is molar area on adsorbate of X.

Thus, we have

$$\frac{d\ln K_{\mathrm{XY}}}{dT} = \frac{\Delta H_{\mathrm{XY}}}{RT^2} - \frac{d\ln A_{\mathrm{X}}}{dT} + \frac{d\ln V_{\mathrm{Y}}}{dT} \quad (\mathrm{S13})$$

K_{IA} or K_{SA}. X represents water or snow(ice) surface and Y represents water.

According to the ideal gas equation ($PV = RT$) and assuming the molar area of water, snow or ice do not change by temperature, we have

$$\frac{d\ln K_{\mathrm{IA}}}{dT} = \frac{\Delta H_{\mathrm{IA}} + RT}{RT^2} \; or \; \frac{d\ln K_{\mathrm{SA}}}{dT} = \frac{\Delta H_{\mathrm{SA}} + RT}{RT^2} \quad (\mathrm{S14})$$

According to the first law of thermodynamics (both ΔH_{IA} and ΔH_{SA} are negative), we can obtain the result as:

$$\frac{d\ln K_{\mathrm{IA}}}{dT} = \frac{\Delta U_{\mathrm{IA}}}{RT^2} \; or \; \frac{d\ln K_{\mathrm{SA}}}{dT} = \frac{\Delta U_{\mathrm{SA}}}{RT^2} \quad (\mathrm{S15})$$

Text S4 Equations for K_{OW} calculation and evaluation

Specific equations for K_{OW} calculation

$$\log K_{OW0}(298.15\text{K}) = 2.41V + 0.43L - 1.41S - 0.18A - 3.45B + 0.34 \quad (S16)$$

$$\Delta H_{OW} = 18.9V - 8.3L + 5.3S - 20.1A + 34.3B + 1.7 \quad (S17)$$

$$\Delta U_{OW} = \Delta H_{OW} \quad (S18)$$

Apart from these, other calculation processes are the same as other P&A coefficients.

Some specific equations for K_{OW} calculation

There are two other more widely used equations derived from Clausius–Clapeyron Equations to estimate logK_{OW}'s dependence on temperature (Lei et al., 2000; Zhang et al., 2007), given by

$$\log K_{OW} = -\frac{\Delta U_{OW}}{\ln(10)RT} + \frac{\Delta S_{OW}}{\ln(10)R} \quad (S19)$$

$$\log K_{OW} = -\frac{\Delta U_{OW}}{\ln(10)RT} + A_{OW} \quad (S20)$$

Besides published A_{OW} and B_{OW} values, dozens of experimental records based on these two equations are collected (Table S3-4, SI).

Reference

Bahadur, N.P., Shiu, W.-Y., Boocock, D.G.B., Mackay, D., 1997. Temperature Dependence of Octanol−Water Partition Coefficient for Selected Chlorobenzenes. J. Chem. Eng. Data 42, 685–688. https://doi.org/10.1021/je970020p

Boddu, V.M., Abburi, K., Maloney, S.W., Damavarapu, R., 2008. Physicochemical properties of an insensitive munitions compound, N-methyl-4-nitroaniline (MNA). Journal of Hazardous Materials 155, 288–294. https://doi.org/10.1016/j.jhazmat.2007.11.074

Casal, P., Cabrerizo, A., Vila-Costa, M., Pizarro, M., Jiménez, B., Dachs, J., 2018. Pivotal Role of Snow Deposition and Melting Driving Fluxes of Polycyclic Aromatic Hydrocarbons at Coastal Livingston Island (Antarctica). Environ. Sci. Technol. 52, 12327–12337. https://doi.org/10.1021/acs.est.8b03640

Casal, P., Casas, G., Vila-Costa, M., Cabrerizo, A., Pizarro, M., Jiménez, B., Dachs, J., 2019. Snow Amplification of Persistent Organic Pollutants at Coastal Antarctica. Environ. Sci. Technol. 53, 8872–8882. https://doi.org/10.1021/acs.est.9b03006

Casas, G., Martinez-Varela, A., Vila-Costa, M., Jiménez, B., Dachs, J., 2021. Rain Amplification of Persistent Organic Pollutants. Environ. Sci. Technol. 55, 12961–12972. https://doi.org/10.1021/acs.est.1c03295

David, V., Moldoveanu, S.C., 2019a. Variation with temperature of octanol/water partition coefficient for the homologous series from benzene to propylbenzene. SEPARATION SCIENCE PLUS 2, 457–464. https://doi.org/10.1002/sscp.201900033

David, V., Moldoveanu, S.C., 2019b. Variation with temperature of octanol/water partition coefficient for the homologous series from benzene to propylbenzene. SEPARATION SCIENCE PLUS 2, 457–464. https://doi.org/10.1002/sscp.201900033

Jin, H.-J., Zhang, C.-Y., Chai, X.-S., 2022. Determination of methanol partition coefficient in octanol/water system by a three-phase ratio variation headspace gas chromatographic method. Journal of Chromatography A 1665, 462825. https://doi.org/10.1016/j.chroma.2022.462825

Lei, Y.D., Wania, F., Shiu, W.Y., Boocock, D.G.B., 2000. HPLC-Based Method for Estimating the Temperature Dependence of n-Octanol−Water Partition Coefficients. J. Chem. Eng. Data 45, 738–742. https://doi.org/10.1021/je9902488

Li, J., Xie, Z., Mi, W., Lai, S., Tian, C., Emeis, K.-C., Ebinghaus, R., 2017. Organophosphate Esters in Air, Snow, and Seawater in the North Atlantic and the Arctic. Environ. Sci. Technol. 51, 6887–6896. https://doi.org/10.1021/acs.est.7b01289

Noubigh, A., Mgaidi, A., Abderrabba, M., 2010. Temperature Effect on the Distribution of Some Phenolic Compounds: An Experimental Measurement of 1-Octanol/Water Partition Coefficients. J. Chem. Eng. Data 55, 488–491.

https://doi.org/10.1021/je900271h

Viamajala, S., Peyton, B.M., Richards, L.A., Petersen, J.N., 2007. Solubilization, solution equilibria, and biodegradation of PAH's under thermophilic conditions. Chemosphere 66, 1094–1106. https://doi.org/10.1016/j.chemosphere.2006.06.059

Wang, Z., Xie, Z., Mi, W., Möller, A., Wolschke, H., Ebinghaus, R., 2015. Neutral Poly/Per-Fluoroalkyl Substances in Air from the Atlantic to the Southern Ocean and in Antarctic Snow. Environ. Sci. Technol. 49, 7770–7775. https://doi.org/10.1021/acs.est.5b00920

Xu, S., Kropscott, B., 2014. Evaluation of the three-phase equilibrium method for measuring temperature dependence of internally consistent partition coefficients (KOW, KOA, and KAW) for volatile methylsiloxanes and trimethylsilanol. Environmental Toxicology and Chemistry 33, 2702–2710. https://doi.org/10.1002/etc.2754

Xu, S., Vogel, A., 2021. Measuring snow scavenging of two airborne cyclic volatile methylsiloxanes under controlled conditions. Chemosphere 285, 131291. https://doi.org/10.1016/j.chemosphere.2021.131291

Zhang, C., Wang, Y., 2010. Determination and Correlation of 1-Octanol/Water Partition Coefficients for Six Quinolones from 293.15 K to 323.15 K. Chemical Research in Chinese Universities 26, 636–639.

Zhang, C., Wang, Y., Wang, F., 2007. Determination and Temperature Dependence of n-Octanol/Water Partition Coefficients for Seven Sulfonamides from (298.15 to 333.15) K. Bulletin of the Korean Chemical Society 28, 1183–1186. https://doi.org/10.5012/bkcs.2007.28.7.1183