United States
Environmental Protection
Agency

Research and Development

Environmental
Research Laboratory
Athens, GA 30605-2700

EPA/600/SR-95/039 March 1995

EPA

Project Summary

Environmental Fate Constants for Additional 27 Organic Chemicals Under Consideration for EPA's Hazardous Waste Identification Projects

Heinz P. Kollig

Under Section 301 of the Resource Conservation and Recovery Act, The U.S. Environmental Protection Agency's (EPA's) Office of Solid Waste is in the process of identifying chemicals to be considered in projects called the hazardous waste identification projects. At this time, there are more than 200 chemical constituents identified in these projects. A previous publication (EPA/600/R-93/132) addressed environmental fate constants and chemical hydrolysis pathways for 189 organic chemicals. This publication addresses an additional 27 organic chemicals. Chemical hydrolysis is addressed. Sorption coefficients are presented. The ionization constant is given when this process affects sorption in the environmental pH range. Additionally, values for water solubility, Henry's law constant, vapor pressure, and diffusivity are reported.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report (see Project Report ordering information at back).

Synopsis of Report

Each chemical is structurally presented and the potential for chemical hydrolysis is addressed. Computed values for water solubility, octanol/water partition coefficient, organic-carbon-normalized sediment/water partition coefficient, Henry's law constant, vapor pressure, and diffusivity are given at 25°C. A short definition is given for each parameter. The organic-carbon-normalized sediment/water partition coefficient is given with consideration of ionization if this process occurs within the environmental pH range.

Table 1. Data for Physical and Chemical Process Parameters

Common Name	Chemical Abstract Service No.	Water Solubility (mg/L)	Sorption Log K_{oc}	Sorption Log_{ow}	Henry's Law Constant (atm-m^3/mol)	Vapor Pressure (torr)	Diffusivity in Air (cm^2/s)	Hydrolysis
1. Anthracene	120-12-7	7.6E-2	4.21	4.53	1.9E-5	6.1E-6	0.055	NHFG
2. Benzenethiol[a] $pk_a = 6.5$	108-98-5	7.6E2	1.32	2.35	4.4E-4	2.4	0.076	NLFG oxidizes
3. Benzo[g,h,i]perylene	191-24-2	1.2E-4	6.28	6.60	1.2E-7	4.0E-11	0.039	NHFG
4. Benzo[k]fluoranthene	207-08-9	9.4E-4	6.0	6.3	5.0E-7	1.4E-9	0.041	NHFG
5. Bromobenzene	108-86-1	4.1E2	2.43	2.75	2.1E-3	4.2	0.073	NLFG[b]
6. n-Butylbenzene	104-51-8	21	3.8	4.1	9.7E-3	1.1	0.060	NHFG
7. sec-Butylbenzene	135-98-8	38	3.6	3.9	9.8E-3	2.1	0.061	NHFG
8. Carbazole	86-74-8	4.0E-1	3.3	3.6	8.6E-7	1.6E-6	0.062	NHFG
9. Crotonaldehyde	4170-30-3	1.3E5	-0.06	0.26	3.1E-5	4.5E1	0.093	
10. Dibenzofuran	132-64-9	4.3	3.8	4.1	1.4E-4	2.7E-3	0.059	NHFG
11. 1,2,3,4,6,7,8-Heptachlorodibenzofuran	67562-39-4	9.5E-7	8.20	8.52	3.7E-5	6.5E-11	0.043	NLFG
12. 1,2,3,4,7,8,9-Heptachlorodibenzofuran	55673-89-7	1.3E-6	8.2	8.5	3.8E-5	9.5E-11	0.043	NLFG
13. 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	35822-46-9	1.9E-7	8.53	8.85	4.1E-5	1.4E-11	0.043	NLFG
14. 1,2,3,4,7,8-Hexachlorodibenzofuran	70648-26-9	7.3E-6	7.54	7.86	4.2E-5	6.3E-10	0.045	NLFG
15. 1,2,3,6,7,8-Hexachlorodibenzofuran	57117-44-9	6.9E-6	7.55	7.87	4.2E-5	5.9E-10	0.045	NLFG
16. 1,2,3,7,8,9-Hexachlorodibenzofuran	72918-21-9	7.3E-6	7.55	7.87	4.3E-5	6.4E-10	0.045	NLFG
17. 2,3,4,6,7,8-Hexachlorodibenzofuran	60851-34-5	7.6E-6	7.54	7.86	4.1E-5	6.3E-10	0.045	NLFG
18. 2-Hexanone	591-78-6	1.8E4	1.0	1.3	8.7E-5	1.2E1	0.072	NHFG
19. Indene	95-13-6	3.9E2	2.5	2.8	5.0E-4	1.3	0.071	NHFG
20. p-Isopropyltoluene	99-87-6	28	3.7	4.0	9.3E-3	1.5	0.060	NHFG
21. 2-Methylchrysene	3351-32-4	8.5E-4	5.82	6.14	1.2E-6	3.1E-9	0.044	NHFG
22. 1-Methylnaphthalene	90-12-0	40	3.52	3.84	2.8E-4	6.6E-2	0.060	NHFG
23. 3-Methylnaphthalene	91-57-6	33	3.54	3.86	3.0E-4	5.8E-2	0.061	NHFG

(continued)

Table 1. (Continued)

Common Name	Chemical Abstract Service No.	Water Solubility (mg/L)	Sorption Log K_{oc}	Sorption Log_{ow}	Henry's Law Constant (atm-m^3/mol)	Vapor Pressure (torr)	Diffusivity in Air (cm^2/s)	Hydrolysis
24. Phenanthrene	85-01-8	1.1	4.25	4.57	2.3E-5	1.0E-4	0.055	NHFG
25. n-Propylbenzene	103-65-1	57	3.35	3.67	9.9E-3	3.6	0.065	NHFG
26. 1,2,4-Trimethylbenzene	95-63-6	70	3.28	3.60	4.9E-3	2.2	0.065	NHFG
27. 1,3,5-Trimethylbenzene	108-67-8	67	3.37	3.69	6.3E-3	2.7	0.065	NHFG

a. Values reported are for neutral species.
b. Bromobenzene was tested in the laboratory for hydrolysis. No disappearance was noted after 29 days at 85°C in 0.1N sodium hydroxide and 0.1N hydrochloric acid.

Heinz P. Kollig (also the EPA Project Officer, see below) is with the Environmental Research Laboratory, Athens, GA 30605-2700.

The complete report, entitled "Environmental Fate Constants for Additional 27 Organic Chemicals Under Consideration for EPA's Hazardous Waste Identification Projects," (Order No. PB95-188074; Cost: $17.50, subject to change) will be available only from

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at

Environmental Research Laboratory
U.S. Environmental Protection Agency
Athens, GA 30605-2700

United States
Environmental Protection Agency
Center for Environmental Research Information
Cincinnati, OH 45268

Official Business
Penalty for Private Use
$300

EPA/600/SR-95/039

BULK RATE
POSTAGE & FEES PAID
EPA
PERMIT No. G-35