

**Comparison of Environmental Fate Predictions from the PBT Profiler with Data found in the Literature**  
**Dr. Heather Burleigh-Flayer, PPG Industries**  
**May 2000**

Chemical CAS RN	Distribution (%)				Half-Life in Air [Days]	Half-Life in Water [Days]	Half-Life in Soil [Days]	Half-Life in Sediment [Days]	Overall		Fish CHV (mg/l)
	Air	Water	Soil	Sediment					Persistence [Days]	BCF	
Monochlorobenzene 108-90-7	- <sup>2</sup>	-	-	-	7	71	229	708	12	32	-
	26 <sup>1</sup> - <sup>3</sup>	31 -	43 -	0 -	14	15 -	15 -	60 -	8.63 -	31 -	2.98 -
	- <sup>4</sup>	-	-	-	11	68-150	22-150	-	-	12-447	-
1,2-Dichlorobenzene 95-50-1	-	-	-	-	23	71	229	708	41	130	-
	12 94	19 2	69 4	1 0.1	25 -	38 -	38 -	150 -	19 -	87 150	1.08 0.8-2
	-	-	-	-	24	28-180	180-240	-	-	36-562	-
1,3-Dichlorobenzene 541-73-1	-	-	-	-	23	71	229	708	41	140	-
	12 -	19 -	69 -	1 -	15 -	38 -	38 -	150 -	19 -	104 -	1.08 -
	-	-	-	-	14	28-180	180	-	-	39-740	-
1,4-Dichlorobenzene 106-46-7	-	-	-	-	23	71	229	708	41	120	-
	13 91	19 0.3	67 6	1 0.1	33 -	38 -	38 -	150 -	18 -	89 120	1.08 0.8
	-	-	-	-	31	28-180	180-240	-	-	12-2512	-
1,2,3-Trichlorobenzene 87-61-6	-	-	-	-	23	71	229	708	72	630	-
	6 -	12 -	79 -	3 -	38 -	60 -	60 -	240 -	33 -	262 301	0.36 -
	-	-	-	-	-	1788	-	-	-	52-2630	-
1,2,4-Trichlorobenzene 120-82-1	-	-	-	-	23	71	229	708	72	630	-
	6 82	12 1	79 16	2 0.4	19 -	60 -	60 -	240 -	33 -	249 301	0.36 0.05 - 0.7
	-	-	-	-	19	1.5-180	28-180	-	-	5-4074	-
Hexachlorobenzene 118-74-1	-	-	-	-	708	2292	2292	2292	1037	16000	-
	1 -	3 -	56 -	40 -	40 -	180 -	180 -	720 -	129 -	5153 -	0.012 -
	-	-	-	-	-	-	-	-	-	-	-

<sup>1</sup>PBT Profiler Estimate

<sup>2</sup>MacLeod, M. and Mackay, D., An Assessment of the Environmental Fate and Exposure of Benzene and the Chlorobenzenes in Canada, *Chemosphere*, vol. 38, p. 1777 - 1796, 1999.

(Tables 1 - Half-Lives, Table 4 - BCF, and Table 5 - Persistence)

<sup>3</sup>Memorandum to the Chlorobenzene Producers Association, Highlights of Meeting with EPA on "Persistent Bioaccumulator" Testing Program, Prepared by Randall Stone, May 10, 1996.

Modeled distribution data is from Mackay, D., Shiu, W., and Ma, K., *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals*. Vol. 1., Lewis Publishers, Ann Arbor, Michigan, 1991. BCF values are based on the geometric mean from studies determined to be of high quality.

<sup>4</sup>Staples, C., A Compilation of Fate Data for a Series of Chlorinated Benzene Compounds, Prep. for Chlorobenzene Producers Assoc., Apr. 29, 1996. Half-Lives were calculated.