

# Chemical Structures of PCBs congeners

Diwen Yang

29 September, 2022

## PCB Chemical properties

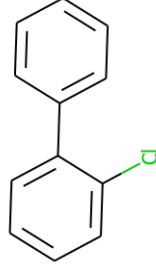
The file `pcbs_annotated.csv` contains information on over 209 pcbs, check it out. Here's a quick glance at it:

```
## # A tibble: 209 x 18
##   pcb      casrn biphe-1 categ-2      cid molec-3 molec-4 canon-5 isome-6 iupac-7
##   <chr>    <chr>  <dbl> <chr>    <dbl> <chr>    <dbl> <chr>    <chr>    <chr>
##  1 2-Chlor~ 2051~    1 Congen~ 249266 C12H9Cl 189. C1=CC= C1=CC= 1-chlo~
##  2 3-Chlor~ 2051~    2 Congen~ 16322 C12H9Cl 189. C1=CC= C1=CC= 1-chlo~
##  3 4-Chlor~ 2051~    3 Congen~ 16323 C12H9Cl 189. C1=CC= C1=CC= 1-chlo~
##  4 2,2'-Di~ 1302~    4 Congen~ 25622 C12H8C~ 223. C1=CC= C1=CC= 1-chlo~
##  5 2,3-Dic~ 1660~    5 Congen~ 27959 C12H8C~ 223. C1=CC= C1=CC= 1,2-di~
##  6 2,3'-Di~ 2556~    6 Congen~ 33100 C12H8C~ 223. C1=CC= C1=CC= 1-chlo~
##  7 2,4-Dic~ 3328~    7 Congen~ 36399 C12H8C~ 223. C1=CC= C1=CC= 2,4-di~
##  8 2,4'-Di~ 3488~    8 Congen~ 36982 C12H8C~ 223. C1=CC= C1=CC= 1-chlo~
##  9 2,5-Dic~ 3488~    9 Congen~ 36980 C12H8C~ 223. C1=CC= C1=CC= 1,4-di~
## 10 2,6-Dic~ 3314~   10 Congen~ 36342 C12H8C~ 223. C1=CC= C1=CC= 1,3-di~
## # ... with 199 more rows, 8 more variables: x_log_p <dbl>, exact_mass <dbl>,
## #   monoisotopic_mass <dbl>, tpsa <dbl>, h_bond_donor_count <dbl>,
## #   h_bond_acceptor_count <dbl>, volume3d <dbl>, fingerprint2d <chr>, and
## #   abbreviated variable names 1: biphenyl, 2: category, 3: molecular_formula,
## #   4: molecular_weight, 5: canonical_smiles, 6: isomeric_smiles, 7: iupac_name
```

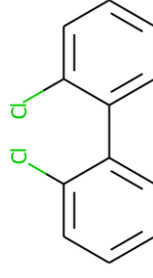
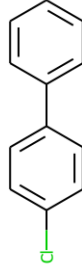
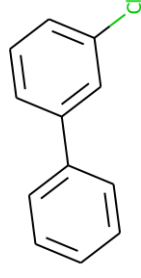
## Making chemically aware table

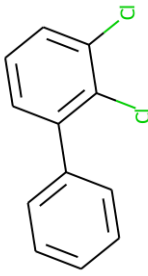
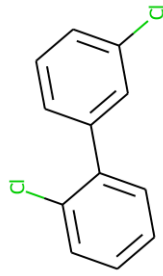
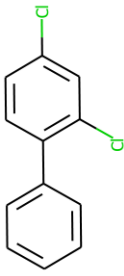
Here's the complete list of available PCBs, and their structures:

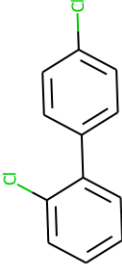
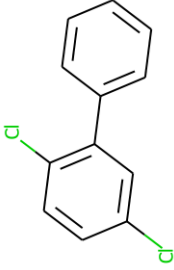
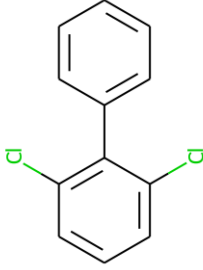
pcb	casrn	molecular_formula	x_log_pstructure
2-Chlorobiphenyl	2051-60-7	C12H9Cl	4.5



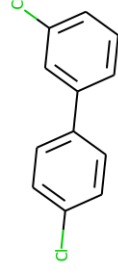
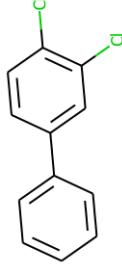
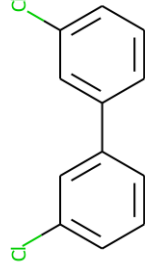
pcb	casrn	molecular_formula	x_log_pstructure
3-Chlorobiphenyl	2051-61-8	C <sub>12</sub> H <sub>9</sub> Cl	4.6
4-Chlorobiphenyl	2051-62-9	C <sub>12</sub> H <sub>9</sub> Cl	4.6
2,2'-Dichlorobiphenyl	13029-08-8	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.0



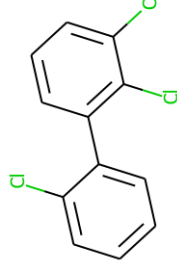
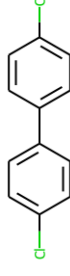
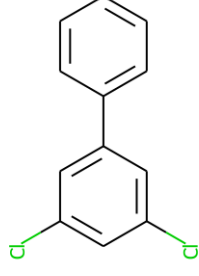
pcb	casrn	molecular_formula	x_log_pstructure
2,3-Dichlorobiphenyl	16605-91-7	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	4.8
			
2,3'-Dichlorobiphenyl	25569-80-6	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.0
			
2,4-Dichlorobiphenyl	33284-50-3	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.3
			

pcb	casrn	molecular_formula	x_log_pstructure
2,4'-Dichlorobiphenyl	34883-43-7	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.1
			
2,5-Dichlorobiphenyl	34883-39-1	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.2
			
2,6-Dichlorobiphenyl	33146-45-1	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.0
			

pcb	casrn	molecular_formula	x_log_pstructure
3,3'-Dichlorobiphenyl	2050-67-1	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.2
3,4-Dichlorobiphenyl	2974-92-7	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.3
3,4'-Dichlorobiphenyl	2974-90-5	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.2



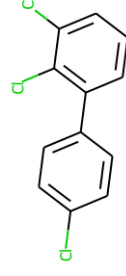
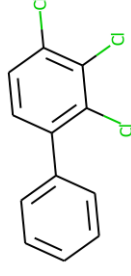
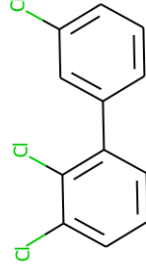
pcb	casrn	molecular_formula	x_log_pstructure
3,5-Dichlorobiphenyl	34883-41-5	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	4.8
4,4'-Dichlorobiphenyl	2050-68-2	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	5.6
2,2',3-Trichlorobiphenyl	38444-78-9	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.3



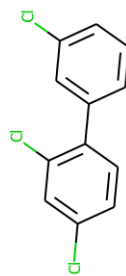
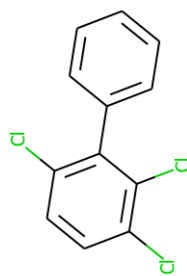
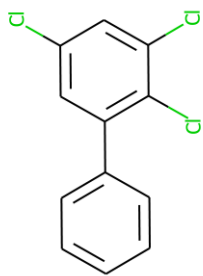
pcb	casrn	molecular_formula	x_log_pstructure
2,2',4-Trichlorobiphenyl	37680-66-3	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.8
∞			
	2,2',5-Trichlorobiphenyl	37680-65-2	5.6
2,2',6-Trichlorobiphenyl	38444-73-4	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.5

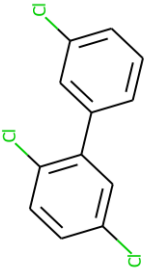
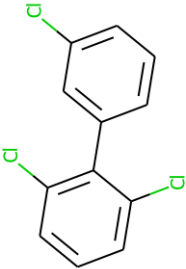
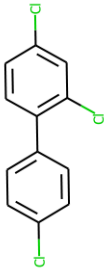


pcb	casrn	molecular_formula	x_log_pstructure
2,3,3'-Trichlorobiphenyl	38444-84-7	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.6
2,3,4-Trichlorobiphenyl	55702-46-0	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.9
2,3,4'-Trichlorobiphenyl	38444-85-8	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.4



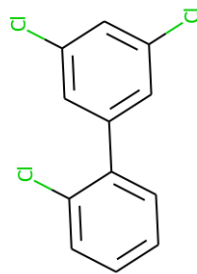
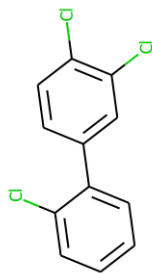
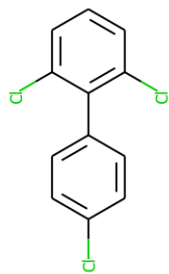
pcb	casrn	molecular_formula	x_log_pstructure
2,3,5-Trichlorobiphenyl	55720-44-0	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.8
2,3,6-Trichlorobiphenyl	55702-45-9	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.7
2,3',4-Trichlorobiphenyl	55712-37-3	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.6

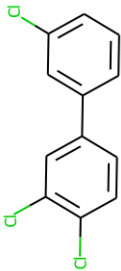
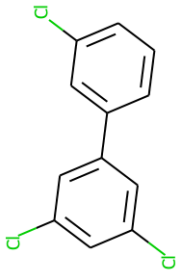
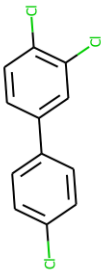


pcb	casrn	molecular_formula	x_log_pstructure
2,3',5-Trichlorobiphenyl	38444-81-4	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.8
			
2,3',6-Trichlorobiphenyl	38444-76-7	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.7
			
2,4,4'-Trichlorobiphenyl	7012-37-5	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.6
			

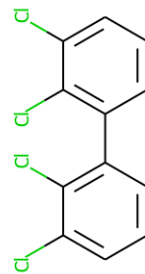
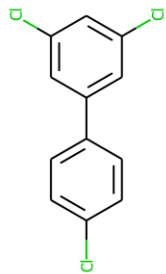
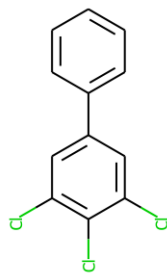
pcb	casrn	molecular_formula	x_log_pstructure
2,4,5-Trichlorobiphenyl	15862-07-4	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.9
			
2,4,6-Trichlorobiphenyl	35693-92-6	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.7
			
2,4',5-Trichlorobiphenyl	16606-02-3	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.8
			

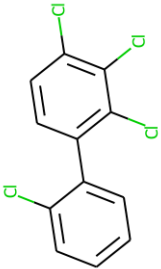
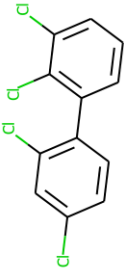
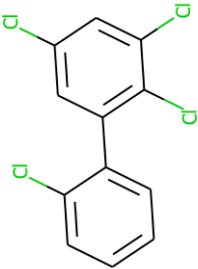
pcb	casrn	molecular_formula	x_log_pstructure
2,4',6'-Trichlorobiphenyl	38444-77-8	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.7
2,3',4'-Trichlorobiphenyl	38444-86-9	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.9
2,3',5'-Trichlorobiphenyl	37680-68-5	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.6



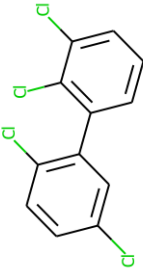
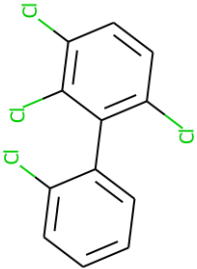
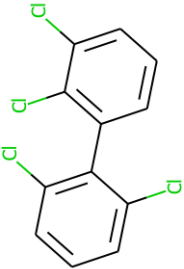
pcb	casrn	molecular_formula	x_log_pstructure
3,3',4-Trichlorobiphenyl	37680-69-6	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.9
			
3,3',5-Trichlorobiphenyl	38444-87-0	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.8
			
3,4,4'-Trichlorobiphenyl	38444-90-5	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.9
			

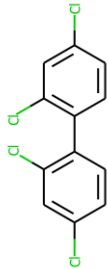
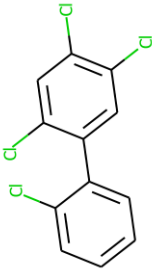
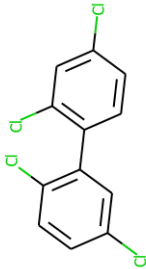
pcb	casrn	molecular_formula	x_log_pstructure
3,4,5-Trichlorobiphenyl	53555-66-1	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	6.0
3,4',5-Trichlorobiphenyl	38444-88-1	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub>	5.4
2,2',3,3'-Tetrachlorobiphenyl	38444-93-8	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.2

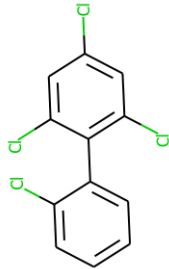
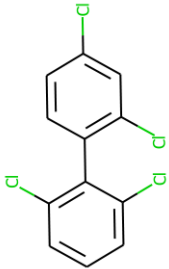
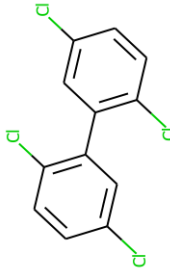


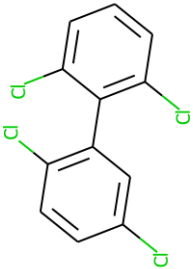
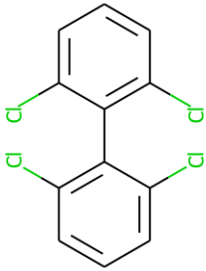
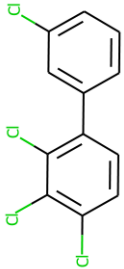
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4-Tetrachlorobiphenyl	52663-59-9	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.1
			
2,2',3,4'-Tetrachlorobiphenyl	36559-22-5	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.0
			
2,2',3,5-Tetrachlorobiphenyl	70362-46-8	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	5.8
			

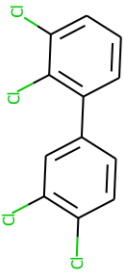
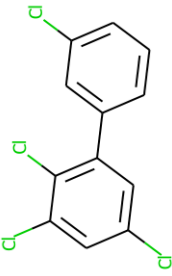
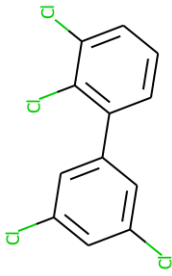


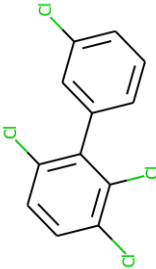
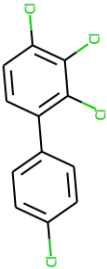
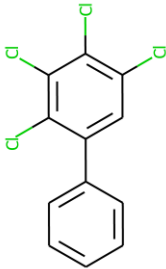
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,5'-Tetrachlorobiphenyl	41464-39-5	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	5.8
			
2,2',3,6'-Tetrachlorobiphenyl	70362-45-7	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	5.4
			
2,2',3,6'-Tetrachlorobiphenyl	41464-47-5	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	5.4
			

pcb	casrn	molecular_formula	x_log_pstructure
2,2',4,4'-Tetrachlorobiphenyl	2437-79-8	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.3
			
2,2',4,5-Tetrachlorobiphenyl	70362-47-9	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.6
			
2,2',4,5'-Tetrachlorobiphenyl	41464-40-8	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.4
			

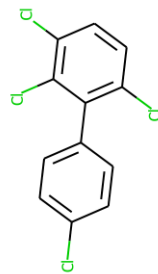
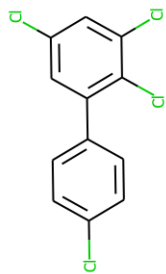
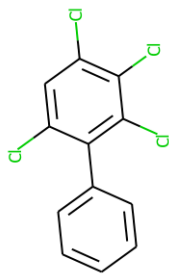
pcb	casrn	molecular_formula	x_log_pstructure
2,2',4,6-Tetrachlorobiphenyl	62796-65-0	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.1
			
2,2',4,6'-Tetrachlorobiphenyl	68194-04-7	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.1
			
2,2',5,5'-Tetrachlorobiphenyl	35693-99-3	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.1
			

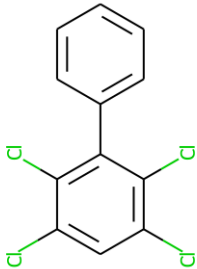
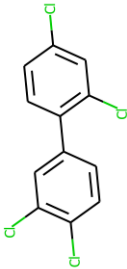
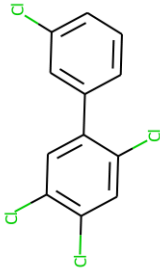
pcb	casrn	molecular_formula	x_log_pstructure
			
2,2',5,6'-Tetrachlorobiphenyl	41464-41-9	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	5.6
			
2,2',6,6'-Tetrachlorobiphenyl	15968-05-5	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	5.9
			
2,3,3',4-Tetrachlorobiphenyl	74338-24-2	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.2

pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',4'-Tetrachlorobiphenyl	41464-43-1	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.0
			
2,3,3',5'-Tetrachlorobiphenyl	70424-67-8	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.2
			
2,3,3',5'-Tetrachlorobiphenyl	41464-49-7	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.2
			

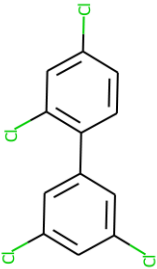
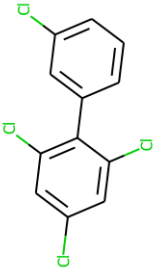
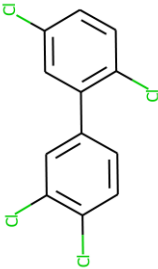
pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',6-Tetrachlorobiphenyl	74472-33-6	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.3
			
2,3,4,4'-Tetrachlorobiphenyl	33025-41-1	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.5
			
2,3,4,5-Tetrachlorobiphenyl	33284-53-6	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.4
			

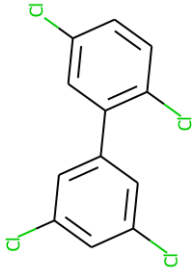
pcb	casrn	molecular_formula	x_log_pstructure
2,3,4,6-Tetrachlorobiphenyl	54230-22-7	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	5.8
2,3,4',5-Tetrachlorobiphenyl	74472-34-7	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.2
2,3,4',6-Tetrachlorobiphenyl	52663-58-8	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.3



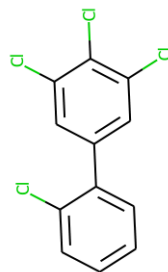
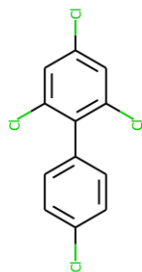
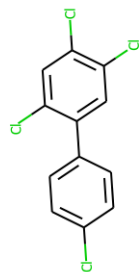
pcb	casrn	molecular_formula	x_log_pstructure
2,3,5,6-Tetrachlorobiphenyl	33284-54-7	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	5.9
			
2,3',4,4'-Tetrachlorobiphenyl	32598-10-0	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.3
			
2,3',4,5-Tetrachlorobiphenyl	73575-53-8	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.5
			

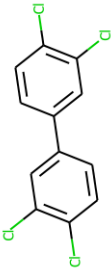
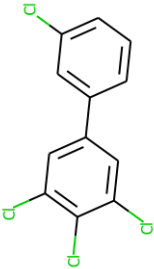
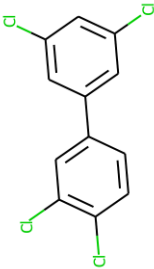


pcb	casrn	molecular_formula	x_log_pstructure
			
2,3',4,5'-Tetrachlorobiphenyl	73575-52-7	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.6
			
2,3',4,6-Tetrachlorobiphenyl	60233-24-1	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.3
			
2,3',4',5-Tetrachlorobiphenyl	32598-11-1	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.2

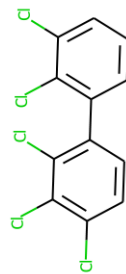
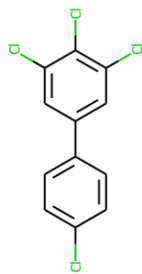
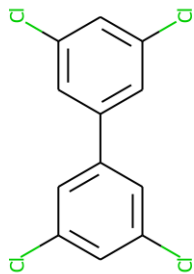
pcb	casrn	molecular_formula	x_log_pstructure
	41464-46-4	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.5
	41464-42-0	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.4
	74338-23-1	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.1

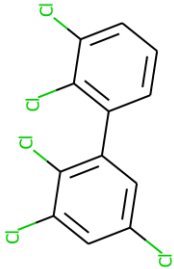
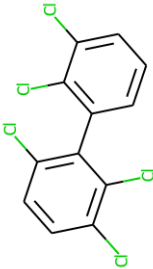
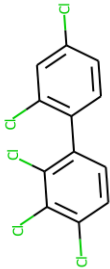
pcb	casrn	molecular_formula	x_log_pstructure
2,4,4',5-Tetrachlorobiphenyl	32690-93-0	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.7
2,4,4',6-Tetrachlorobiphenyl	32598-12-2	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.3
2,3',4',5'-Tetrachlorobiphenyl	70362-48-0	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.5

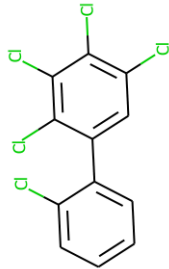
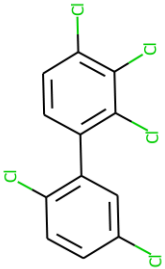
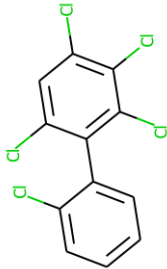


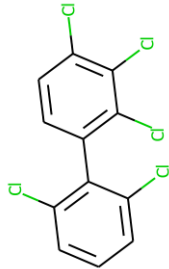
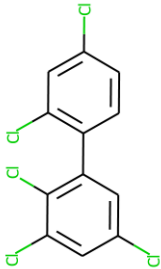
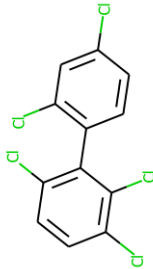
pcb	casrn	molecular_formula	x_log_pstructure
3,3',4,4'-Tetrachlorobiphenyl	32598-13-3	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.6
			
3,3',4,5-Tetrachlorobiphenyl	70362-49-1	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.1
			
3,3',4,5'-Tetrachlorobiphenyl	41464-48-6	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.5
			

pcb	casrn	molecular_formula	x_log_pstructure
3,3',5,5'-Tetrachlorobiphenyl	33284-52-5	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.1
3,4,4',5-Tetrachlorobiphenyl	70362-50-4	C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub>	6.6
2,2',3,3',4-Pentachlorobiphenyl	52663-62-4	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.7

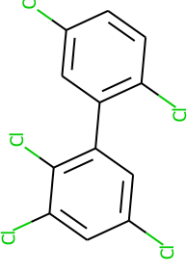
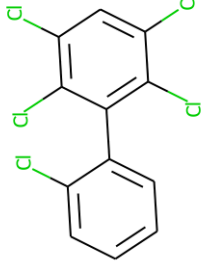
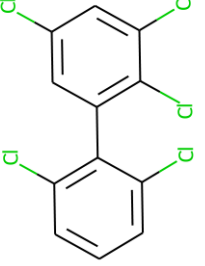


pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',5-Pentachlorobiphenyl	60145-20-2	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.8
			
2,2',3,3',6-Pentachlorobiphenyl	52663-60-2	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.0
			
2,2',3,4,4'-Pentachlorobiphenyl	65510-45-4	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.6
			

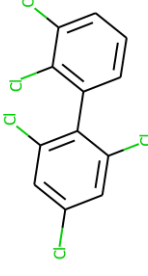
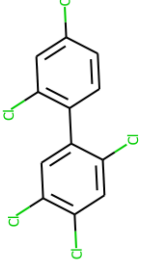
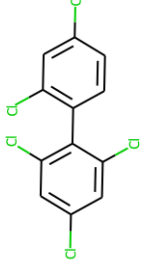
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,5-Pentachlorobiphenyl	55312-69-1	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.7
			
2,2',3,4,5'-Pentachlorobiphenyl	38380-02-8	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.4
			
2,2',3,4,6-Pentachlorobiphenyl	55215-17-3	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.3
			

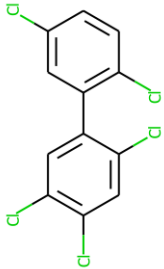
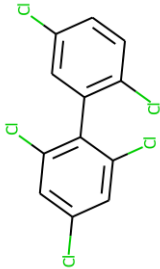
pcb	casrn	molecular_formula	x_log_pstructure
			
2,2',3,4,6'-Pentachlorobiphenyl	73575-57-2	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.3
			
2,2',3,4',5-Pentachlorobiphenyl	68194-07-0	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.8
			
2,2',3,4',6-Pentachlorobiphenyl	68194-05-8	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.3

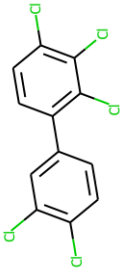


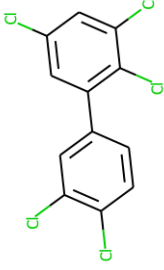
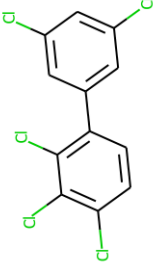
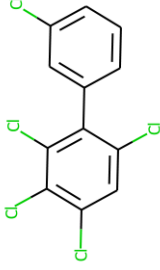
pcb	casrn	molecular_formula	x_log_pstructure
	52663-61-3	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	7.0
	73575-56-1	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.2
	73575-55-0	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.2

pcb	casrn	molecular_formula	x_log_pstructure
			
2,2',3,5',6-Pentachlorobiphenyl	38379-99-6	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.5
			
2,2',3,6,6'-Pentachlorobiphenyl	73575-54-9	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.1
			
2,2',3,4',5'-Pentachlorobiphenyl	41464-51-1	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.7

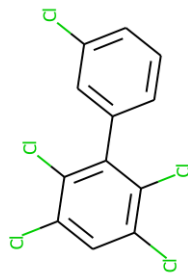
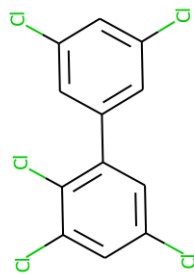
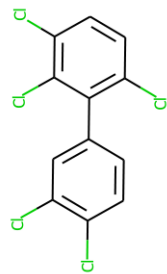
pcb	casrn	molecular_formula	x_log_pstructure
	60233-25-2	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.3
	38380-01-7	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	7.2
	39485-83-1	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.3

pcb	casrn	molecular_formula	x_log_pstructure
	37680-73-2	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.5
	68194-06-9	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.3
	60145-21-3	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.2

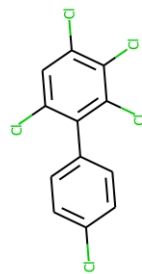
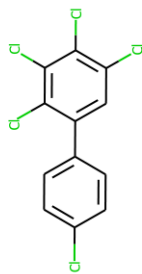
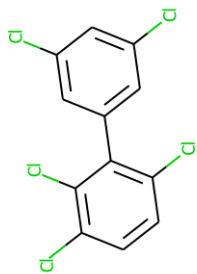
pcb	casrn	molecular_formula	x_log_pstructure
	56558-16-8	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	5.8
	32598-14-4	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.6
	70424-69-0	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.9

pcb	casrn	molecular_formula	x_log_pstructure
	70424-68-9	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.9
	70362-41-3	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	7.0
	74472-35-8	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.6

pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',4',6-Pentachlorobiphenyl	38380-03-9	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.6
2,3,3',5,5'-Pentachlorobiphenyl	39635-32-0	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.8
2,3,3',5,6-Pentachlorobiphenyl	74472-36-9	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.7

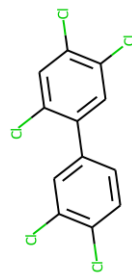
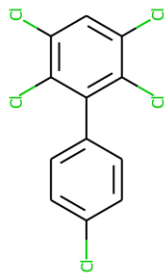
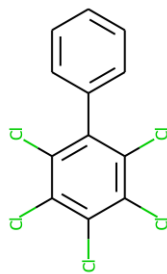


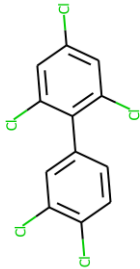
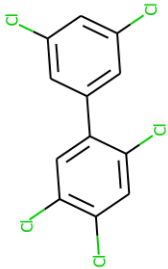
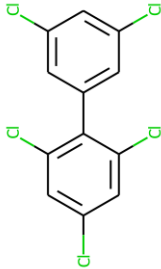
pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',5',6-Pentachlorobiphenyl	68194-10-5	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.6
2,3,4,4',5-Pentachlorobiphenyl	74472-37-0	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	7.0
2,3,4,4',6-Pentachlorobiphenyl	74472-38-1	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.6



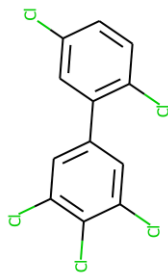
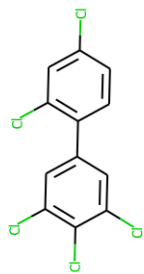
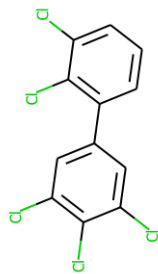


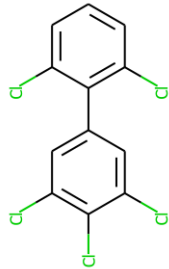
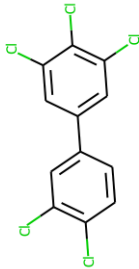
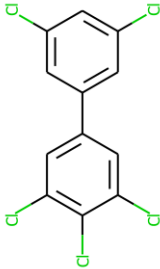
pcb	casrn	molecular_formula	x_log_pstructure
2,3,4,5,6-Pentachlorobiphenyl	18259-05-7	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.7
2,3,4',5,6-Pentachlorobiphenyl	68194-11-6	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.5
2,3',4,4',5-Pentachlorobiphenyl	31508-00-6	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	7.1

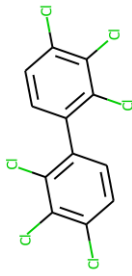
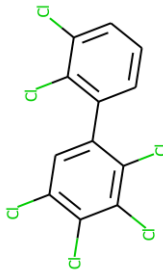
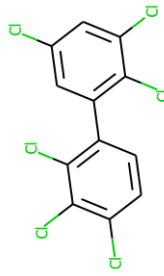


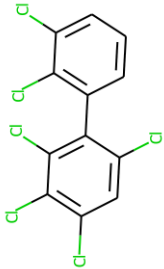
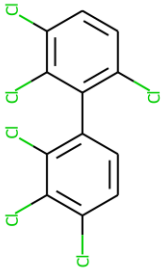
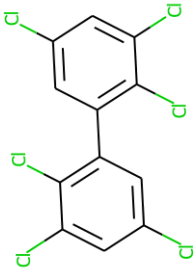
pcb	casrn	molecular_formula	x_log_pstructure
			
2,3',4,4',6-Pentachlorobiphenyl	56558-17-9	C12H5Cl5	6.6
			
2,3',4,5,5'-Pentachlorobiphenyl	68194-12-7	C12H5Cl5	6.9
			
2,3',4,5',6-Pentachlorobiphenyl	56558-18-0	C12H5Cl5	6.5

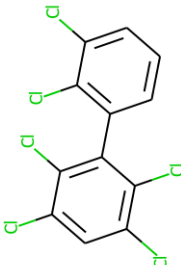
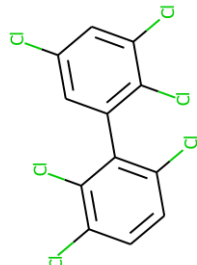
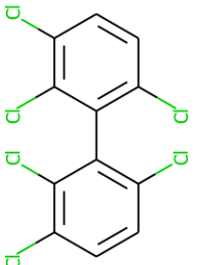
pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',4',5',5'-Pentachlorobiphenyl	76842-07-4	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	7.0
2,3',4',4',5',5'-Pentachlorobiphenyl	65510-44-3	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.9
2,3',4',5',5',5'-Pentachlorobiphenyl	70424-70-3	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.9

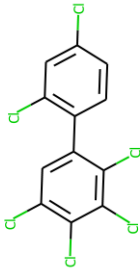
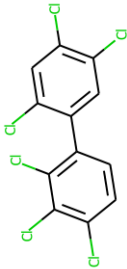
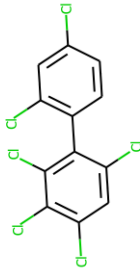


pcb	casrn	molecular_formula	x_log_pstructure
2,3',4',5',6-Pentachlorobiphenyl	74472-39-2	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.5
			
3,3',4,4',5-Pentachlorobiphenyl	57465-28-8	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	7.3
			
3,3',4,5,5'-Pentachlorobiphenyl	39635-33-1	C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub>	6.8
			

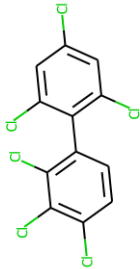
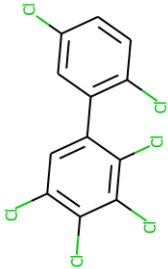
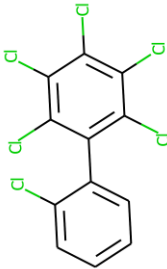
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,4'-Hexachlorobiphenyl	38380-07-3	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.3
			
2,2',3,3',4,5'-Hexachlorobiphenyl	55215-18-4	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.3
			
2,2',3,3',4,5'-Hexachlorobiphenyl	52663-66-8	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.4
			

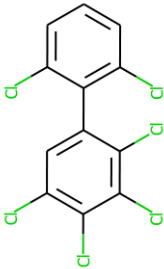
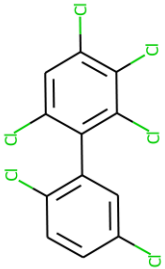
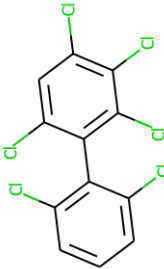
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,6-Hexachlorobiphenyl	61798-70-7	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.8
			
2,2',3,3',4,6'-Hexachlorobiphenyl	38380-05-1	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.0
			
2,2',3,3',5,5'-Hexachlorobiphenyl	35694-04-3	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.1
			

pcb	casrn	molecular_formula	x_log_pstructure
			
2,2',3,3',5,6-Hexachlorobiphenyl	52704-70-8	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.8
			
2,2',3,3',5,6'-Hexachlorobiphenyl	52744-13-5	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.1
			
2,2',3,3',6,6'-Hexachlorobiphenyl	38411-22-2	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.1

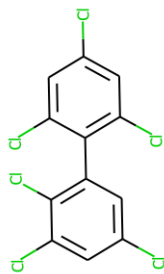
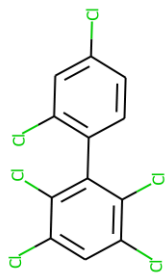
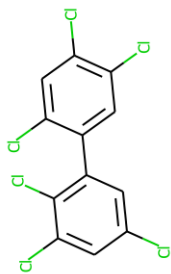
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,4',5-Hexachlorobiphenyl	35694-06-5	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.4
			
2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.2
			
2,2',3,4,4',6-Hexachlorobiphenyl	56030-56-9	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.9
			

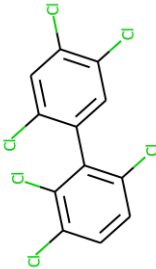
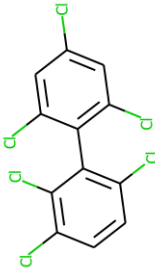
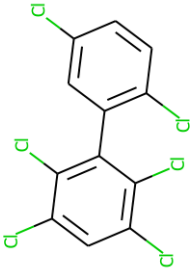


pcb	casrn	molecular_formula	x_log_pstructure
	59291-64-4	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.0
	52712-04-6	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.2
	41411-61-4	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.0

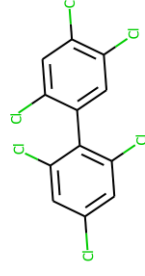
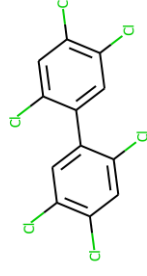
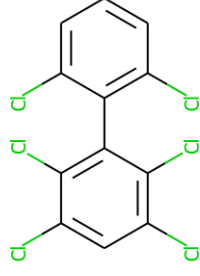
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,5,6'-Hexachlorobiphenyl	68194-15-0	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.9
			
2,2',3,4,5',6'-Hexachlorobiphenyl	68194-14-9	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.8
			
2,2',3,4,6,6'-Hexachlorobiphenyl	74472-40-5	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.7
			

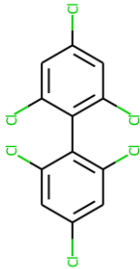
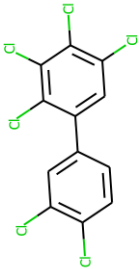
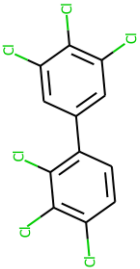
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4',5,5'-Hexachlorobiphenyl	51908-16-8	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.1
2,2',3,4',5,6'-Hexachlorobiphenyl	68194-13-8	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.9
2,2',3,4',5,6'-Hexachlorobiphenyl	74472-41-6	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.9

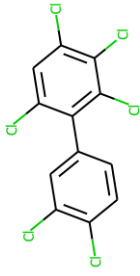
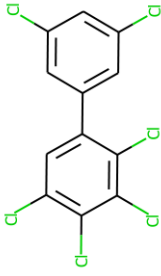
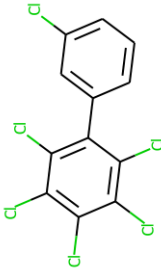


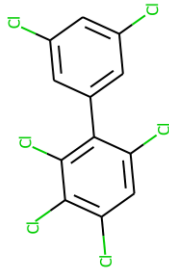
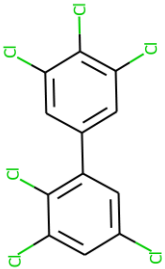
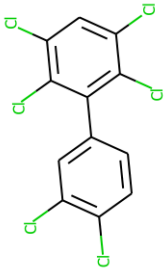
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4',5',6'-Hexachlorobiphenyl	38380-04-0	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.1
			
2,2',3,4',6,6'-Hexachlorobiphenyl	68194-08-1	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.7
			
2,2',3,5,5',6'-Hexachlorobiphenyl	52663-63-5	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.8
			

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,5,6,6'-Hexachlorobiphenyl	68194-09-2	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.5
2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.2
2,2',4,4',5,6'-Hexachlorobiphenyl	60145-22-4	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	6.9

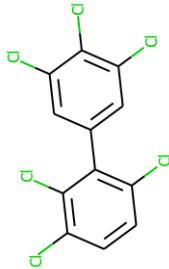
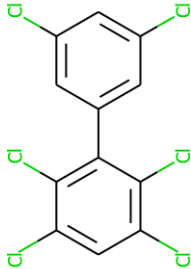
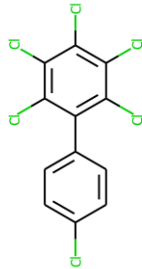


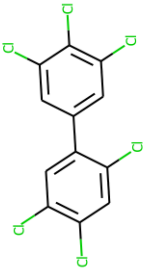
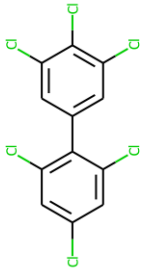
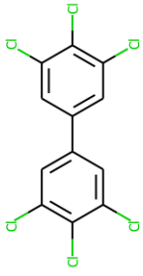
pcb	casrn	molecular_formula	x_log_pstructure
			
2,2',4,4',6,6'-Hexachlorobiphenyl	33979-03-2	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.3
			
2,3,3',4,4',5-Hexachlorobiphenyl	38380-08-4	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.6
			
2,3,3',4,4',5'-Hexachlorobiphenyl	69782-90-7	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.6

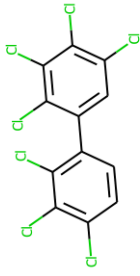
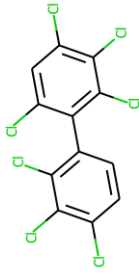
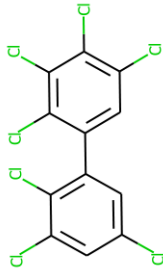
pcb	casrn	molecular_formula	x_log_pstructure
			
2,3,3',4,4',6-Hexachlorobiphenyl	74472-42-7	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.2
			
2,3,3',4,5,5'-Hexachlorobiphenyl	39635-35-3	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.4
			
2,3,3',4,5,6-Hexachlorobiphenyl	41411-62-5	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.3

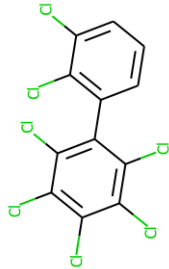
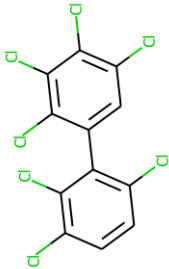
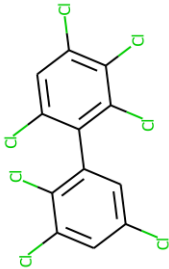
pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',4,5',6-Hexachlorobiphenyl	74472-43-8	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.1
			
2,3,3',4',5,5'-Hexachlorobiphenyl	39635-34-2	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.5
			
2,3,3',4',5,6-Hexachlorobiphenyl	74472-44-9	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.2
			

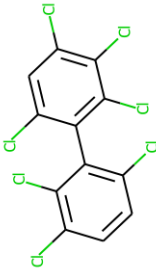
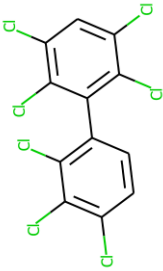
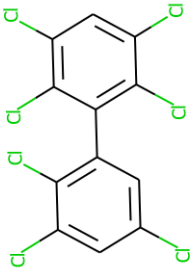


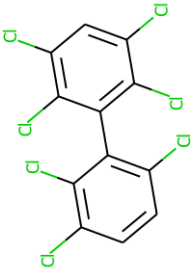
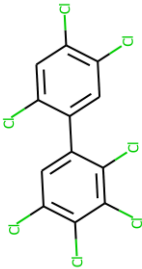
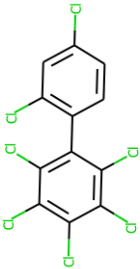
pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',4',5',6-Hexachlorobiphenyl	74472-45-0	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.2
			
2,3,3',5,5',6-Hexachlorobiphenyl	74472-46-1	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.4
			
2,3,4,4',5,6-Hexachlorobiphenyl	41411-63-6	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.3
			

pcb	casrn	molecular_formula	x_log_pstructure
2,3',4,4',5,5',6-Hexachlorobiphenyl	52663-72-6	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.5
			
2,3',4,4',5',6-Hexachlorobiphenyl	59291-65-5	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.2
			
3,3',4,4',5,5',6-Hexachlorobiphenyl	32774-16-6	C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub>	7.4
			

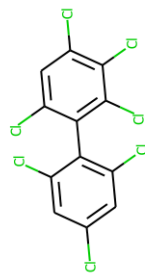
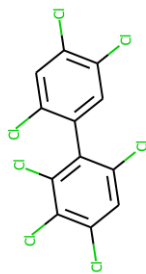
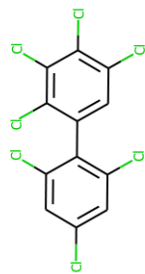
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,4',5-Heptachlorobiphenyl	35065-30-6	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.9
			
2,2',3,3',4,4',6-Heptachlorobiphenyl	52663-71-5	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.4
			
2,2',3,3',4,5,5'-Heptachlorobiphenyl	52663-74-8	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	8.0
			

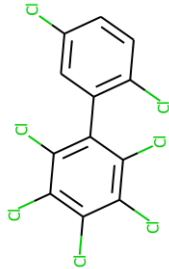
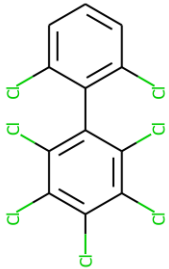
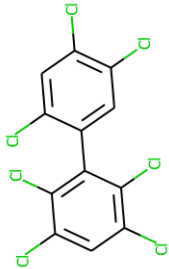
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,5,6-Heptachlorobiphenyl	68194-16-1	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.4
			
2,2',3,3',4,5,6'-Heptachlorobiphenyl	38411-25-5	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.5
			
2,2',3,3',4,5',6-Heptachlorobiphenyl	40186-70-7	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.8
			

pcb	casrn	molecular_formula	x_log_pstructure
			
2,2',3,3',4,6,6'-Heptachlorobiphenyl	52663-65-7	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.3
			
2,2',3,3',4,5',6'-Heptachlorobiphenyl	52663-70-4	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.4
			
2,2',3,3',5,5',6'-Heptachlorobiphenyl	52663-67-9	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.8

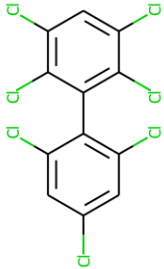
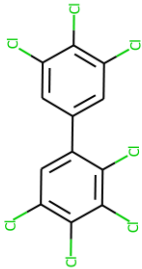
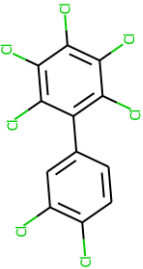
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',5,6,6'-Heptachlorobiphenyl	52663-64-6	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.1
			
2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.9
			
2,2',3,4,4',5,6-Heptachlorobiphenyl	74472-47-2	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.6
			

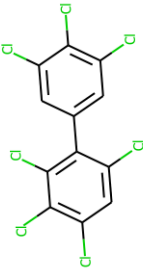
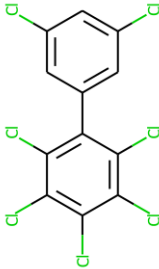
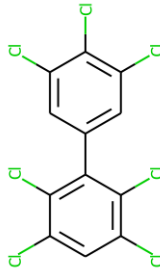
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,4',5,6'-Heptachlorobiphenyl	60145-23-5	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.5
2,2',3,4,4',5',6'-Heptachlorobiphenyl	52663-69-1	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.4
2,2',3,4,4',6,6'-Heptachlorobiphenyl	74472-48-3	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.3

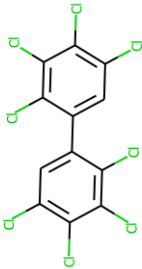
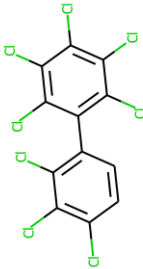
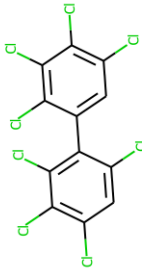


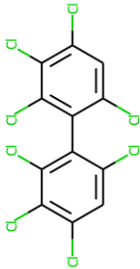
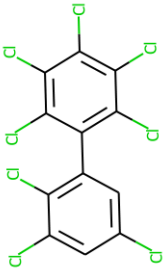
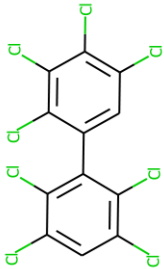
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,5,5',6-Heptachlorobiphenyl	52712-05-7	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.5
			
2,2',3,4,5,6,6'-Heptachlorobiphenyl	74472-49-4	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.1
			
2,2',3,4',5,5',6-Heptachlorobiphenyl	52663-68-0	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.5
			

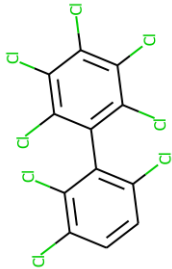
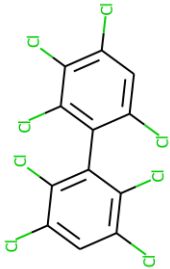
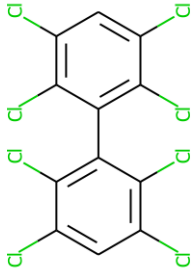


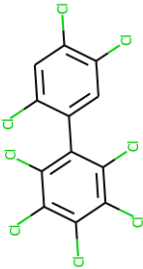
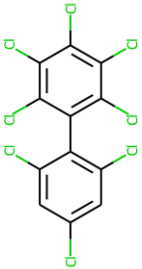
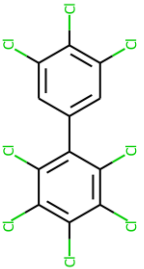
pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4',5,6,6'-Heptachlorobiphenyl	74487-85-7	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.1
			
2,3,3',4,4',5,5'-Heptachlorobiphenyl	39635-31-9	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	8.1
			
2,3,3',4,4',5,6-Heptachlorobiphenyl	41411-64-7	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.9
			

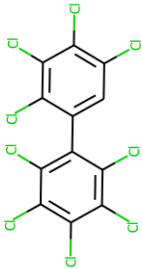
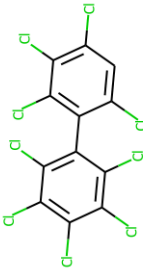
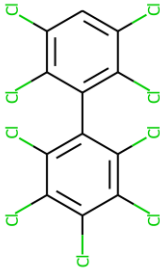
pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',4,4',5',6-Heptachlorobiphenyl	74472-50-7	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	7.7
			
2,3,3',4,5,5',6-Heptachlorobiphenyl	74472-51-8	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	8.0
			
2,3,3',4',5,5',6-Heptachlorobiphenyl	69782-91-8	C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub>	8.0
			

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	35694-08-7	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.6
			
2,2',3,3',4,4',5,6-Octachlorobiphenyl	52663-78-2	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.2
			
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	42740-50-1	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.2
			

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,4',6,6'-Octachlorobiphenyl	33091-17-7	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.0
			
2,2',3,3',4,5,5',6-Octachlorobiphenyl	68194-17-2	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.1
			
2,2',3,3',4,5,5',6'-Octachlorobiphenyl	52663-75-9	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.2
			

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,5,6,6'-Octachlorobiphenyl	52663-73-7	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.4
			
2,2',3,3',4,5',6,6'-Octachlorobiphenyl	40186-71-8	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	7.7
			
2,2',3,3',5,5',6,6'-Octachlorobiphenyl	2136-99-4	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	7.7
			

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,4',5,5',6-Octachlorobiphenyl	52663-76-0	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.1
			
2,2',3,4,4',5,6,6'-Octachlorobiphenyl	74472-52-9	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	7.5
			
2,3,3',4,4',5,5',6-Octachlorobiphenyl	74472-53-0	C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub>	8.5
			

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	40186-72-9	C <sub>12</sub> HCl <sub>9</sub>	8.8
			
2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	52663-79-3	C <sub>12</sub> HCl <sub>9</sub>	8.2
			
2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	52663-77-1	C <sub>12</sub> HCl <sub>9</sub>	8.2
			

pcb	casrn	molecular_formula	x_log_pstructure
Decachlorobiphenyl	2051-24-3	C <sub>12</sub> Cl <sub>10</sub>	8.3

