Chemical Structures of PCBs congeners

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PCB Chemical properties

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

```
C1=CC=~ C1=CC=~ 1,2-di~
                                                                                                                                                                                           C1=CC=\sim C1=CC=\sim 1,4-di\sim
                                                                                                                                                                                                            C1=CC=~ C1=CC=~ 1,3-di~
                  cid molec~3 molec~4 canon~5 isome~6 iupac~7
                                                    1-chlo~
                                                                      1-chlo~
                                                                                      C1=CC=~ C1=CC=~ 1-chlo~
                                                                                                       C1=CC=~ C1=CC=~ 1-chlo~
                                                                                                                                         C1=CC=~ C1=CC=~ 1-chlo~
                                                                                                                                                           2,4-di~
                                                                                                                                                                           C1=CC=~ C1=CC=~ 1-chlo~
                                                                                                                                                                                                                                                               h_bond_acceptor_count <dbl>, volume3d <dbl>, and abbreviated variable names
                                                                                                                                                                                                                             # ... with 199 more rows, 7 more variables: x_log_p <dbl>, exact_mass <dbl>,
                                                                      C1=CC=~ C1=CC=~
                                                                                                                                                          C1=CC=~ C1=CC=~
                                                    C1=CC=~ C1=CC=~
                                                                                                                                                                                                                                                                                  1: biphenyl, 2: category, 3: molecular_formula, 4: molecular_weight,
                                    <chr>
                                                                                                                                                                                                                                               monoisotopic_mass <dbl>, tpsa <dbl>, h_bond_donor_count <dbl>,
                                    5: canonical_smiles, 6: isomeric_smiles, 7: iupac_name
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                                                                                                                       C12H8C~
                                                                                                                                         33100 C12H8C~
                                                                                                                                                          C12H8C~
                                                                                                                                                                           C12H8C~
                                                                                                                                                                                           36980 C12H8C~
                                                    249266 C12H9Cl
                                                                     C12H9C1
                                    <dbl> <dbl> <db><
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                                                                                                                      27959
                                                                                                                                                         36399
                                                                                     16323
                                                                                                      25622
                                                                     16322
                                                   1 Congen~
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                  casrn biphe~1 categ~2
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                                                                                                                                      6 Congen∼
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                                                                                                                                                                          8 Congen~
                                    <dbl> <dbl> <db><
# A tibble: 209 \times 17
                                    <chr>
                                                                                                                       5 2,3-Dic~ 1660~
                                                                                                                                                                         8 2,4'-Di~ 3488~
                                                                                                                                                                                          2,5-Dic~ 3488~
                                                                                                                                                                                                            2,6-Dic~ 3314~
                                                                     2051~
                                                                                      2051~
                                                                                                      4 2,2'-Di~ 1302~
                                                                                                                                         6 2,3'-Di~ 2556~
                                                                                                                                                          2,4-Dic~ 3328~
                                                    2051~
                                                                                     3 4-Chlor~
                                                    2-\mathrm{Chlor}^{\sim}
                                                                      3-Chlor~
                                    <chr>
                   pcb
                                                                      a
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Making chemically aware table

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

$x_\log_pstructure$	4.5
molecular_formula	C12H9Cl
casrn	2051-60-7
pcb	2-Chlorobiphenyl

pcb	casrn	molecular_formula	x_log_pstructure
3-Chlorobiphenyl	2051-61-8	C12H9Cl	4.6
4-Chlorobiphenyl	2051-62-9	C12H9Cl	4.6
2,2-Dichlorobiphenyl	13029-08-8	C12H8Cl2	5.0

pcb	casrn	molecular_formula	x_log_pstructure
9 9 Dishlowdinhown	1680 O 17	el Substantial	
2,3-Dichlorobiphenyl	7-16-60991	C12H8Cl2	4.8
2,3'-Dichlorobiphenyl	25569-80-6	C12H8Cl2	5.0
2,4-Dichlorobiphenyl	33284-50-3	C12H8Cl2	5.3

pcb	casrn	molecular_formula	x_log_pstructure
2,4'-Dichlorobiphenyl	34883-43-7	C12H8Cl2	5.1
	6000	or Cotto	
Z,5-Dichlorobiphenyi	34883-39-1	CIZHSCIZ	5.5 D
2,6-Dichlorobiphenyl	33146-45-1	C12H8Cl2	5.0

pcb	casrn	molecular_formula	$f{x}_{-}log_{-}pstructure$
3,3'-Dichlorobiphenyl	2050-67-1	C12H8Cl2	5.2
3,4-Dichlorobiphenyl	2974-92-7	C12H8Cl2	5.3
3,4'-Dichlorobiphenyl	2974-90-5	C12H8Cl2	5.2

pcb	casrn	molecular_formula	x_log_pstructure
3,5-Dichlorobiphenyl	34883-41-5	C12H8Cl2	4.8
4,4'-Dichlorobiphenyl	2050-68-2	C12H8Cl2	5.6
2,2',3-Trichlorobiphenyl	38444-78-9	C12H7Cl3	5.3

pcb	casrn	molecular_formula	x_log_pstructure
2,2,4-Trichlorobiphenyl	37680-66-3	C12H7Cl3	57.8
2,2',5-Trichlorobiphenyl	37680-65-2	C12H7Cl3	5.6
2,2,6-Trichlorobiphenyl	38444-73-4	C12H7Cl3	5.5

pcb	casrn	molecular_formula	x_log_pstructure
2,3,3'-Trichlorobiphenyl	38444-84-7	C12H7Cl3	5.6
2,3,4-Trichlorobiphenyl	55702-46-0	C12H7Cl3	5.9
2,3,4'-Trichlorobiphenyl	38444-85-8	C12H7Cl3	5.4

pcb	casrn	molecular_formula	x_log_pstructure
2, 3, 5- Trichlorobiphenyl	55720-44-0	C12H7Cl3	57.8
2, 3, 6- Trichlor obiphenyl	55702-45-9	C12H7Cl3	5.7
2,3',4-Trichlorobiphenyl	55712-37-3	C12H7Cl3	5.6

pcb	casrn	molecular_formula	$f{x_log_pstructure}$
2,3',5-Trichlorobiphenyl	38444-81-4	C12H7Cl3	57.8
2,3,6-Trichlorobiphenyl	38444-76-7	C12H7Cl3	5.7
2,4,4'- Trichlorobiphenyl	7012-37-5	C12H7Cl3	5.6

pcb	casrn	molecular_formula	x_log_pstructure
2,4,5-Trichlorobiphenyl	15862-07-4	C12H7Cl3	5.9
2,4,6-Trichlorobiphenyl	35693-92-6	C12H7Cl3	5.7
2,4',5-Trichlorobiphenyl	16606-02-3	C12H7Cl3	5.8

pcb	casrn	molecular_formula	${ m x_log_pstructure}$
$2,4',6- {\rm Trichlorobiphenyl}$	38444-77-8	C12H7Cl3	5.7
2,3',4'-Trichlorobiphenyl	38444-86-9	C12H7Cl3	5.9
2,3',5'-Trichlorobiphenyl	37680-68-5	C12H7Cl3	5.6

pcb	casrn	molecular_formula	x_log_pstructure
3,3',4-Trichlorobiphenyl	37680-69-6	C12H7Cl3	5.9
3.3'.5-Trichlorobiphenvl	38444-87-0	C12H7Cl3	8.50
3,4,4'-1richlorobiphenyl	38444-90-5	CIZH7CI3	9.6

pcb	casrn	molecular_formula	x_log_pstructure
3,4,5-Trichlorobiphenyl	53555-66-1	C12H7Cl3	6.0
3,4',5-Trichlorobiphenyl	38444-88-1	C12H7Cl3	5.4
2,2',3,3'-Tetrachlorobiphenyl	38444-93-8	C12H6Cl4	6.2

pcb	casrn	molecular_formula	x_log_pstructure
2.2'.3.4-Tetrachlorobiphenyl	52663-59-9	C12H6Cl4	6.1
2,2,3,4'-Tetrachlorobiphenyl	36559-22-5	C12H6Cl4	6.0
2,2',3,5-Tetrachlorobiphenyl	70362-46-8	C12H6Cl4	5.8

pcb	casrn	molecular_formula	${f x_log_pstructure}$
2,2,3,5-Tetrachlorobiphenyl	41464-39-5	C12H6Cl4	57.8
2,2',3,6-Tetrachlorobiphenyl	70362-45-7	C12H6Cl4	5.4
2,2',3,6'-Tetrachlorobiphenyl	41464-47-5	C12H6Cl4	5.4

pcb	casrn	molecular_formula	x_log_pstructure
2,2',4,4'-Tetrachlorobiphenyl	2437-79-8	C12H6Cl4	6.3
2,2',4,5-Tetrachlorobiphenyl	70362-47-9	C12H6Cl4	9.9
2,2',4,5'-Tetrachlorobiphenyl	41464-40-8	C12H6Cl4	6.4

pcb	casrn	molecular_formula	${f x_log_pstructure}$
2,2',4,6-Tetrachlorobiphenyl	62796-65-0	C12H6Cl4	6.1
2,2',4,6'-Tetrachlorobiphenyl	68194-04-7	C12H6C14	6.1
2,2',5,5'-Tetrachlorobiphenyl	35693-99-3	C12H6Cl4	6.1

pcb	casrn	molecular_formula	x_log_pstructure
2,2',5,6'-Tetrachlorobiphenyl	41464-41-9	C12H6Cl4	5.6
2,2',6,6'-Tetrachlorobiphenyl	15968-05-5	C12H6Cl4	5.9
2,3,3',4-Tetrachlorobiphenyl	74338-24-2	C12H6Cl4	6.2

pcb	casrn	molecular_formula	x_\log_{-} pstructure
2,3,3',4'-Tetrachlorobiphenyl	41464-43-1	C12H6Cl4	6.0
2,3,3',5-Tetrachlorobiphenyl	70424-67-8	C12H6Cl4	6.2
2,3,3',5'-Tetrachlorobiphenyl	41464-49-7	C12H6Cl4	6.2

pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',6-Tetrachlorobiphenyl	74472-33-6	C12H6Cl4	6.3
2,3,4,4'-Tetrachlorobiphenyl	33025-41-1	C12H6Cl4	6.5
2, 3, 4, 5-Tetrachlorobiphenyl	33284-53-6	C12H6Cl4	6.4

pcb	casrn	molecular_formula	x_log_pstructure
2.3.4 6-Tetrachlorohinhenvl	54930-99-7	C19H6Cl4	X LT
		TO OTTO PO	
2,3,4',5-1etrachlorobiphenyl	(44/2-34-7	CIZHBCI4	0.2
2,3,4',6-Tetrachlorobiphenyl	52663-58-8	C12H6Cl4	6.3

pcb	casrn	molecular_formula	x_log_pstructure
$2, 3, 5, 6\text{-}\mathrm{Tetrachlorobiphenyl}$	33284-54-7	C12H6Cl4	5.9
2,3,4,4-Tetrachlorobiphenyl	32598-10-0	C12H6Cl4	6.3
2,3',4,5-Tetrachlorobiphenyl	73575-53-8	C12H6Cl4	6.5

pcb	casrn	molecular_formula	${ m x_log_pstructure}$
$2,3,4,5\text{-}\mathrm{Tetrachlorobiphenyl}$	73575-52-7	C12H6Cl4	9.9
2,3',4,6-Tetrachlorobiphenyl	60233-24-1	C12H6C14	6.3
2,3',4',5-Tetrachlorobiphenyl	32598-11-1	C12H6Cl4	6.2

x_log_pstructure	6.5	6.4	6.1
molecular_formula	C12H6Cl4	C12H6Cl4	C12H6Cl4
casrn	41464-46-4	41464-42-0	74338-23-1
pcb	$2, 3, 4, 6. {\it Tetrachlorobiphenyl}$	2,3',5,5'-Tetrachlorobiphenyl	$2, 3, 5, 6. {\it Tetrachlorobiphenyl}$

pcb	casrn	molecular_formula	x_log_pstructure
2 4 4' 5-Tetrachlorohinhenvl	39690-93-0	C19H6C14	
2,4,4,0-retracmonomphenyi	0-08-08070	O12110O14	0.7
2,4,4',6-Tetrachlorobiphenyl	32598-12-2	C12H6Cl4	6.3
2,3,4',5'-Tetrachlorobiphenyl	70362-48-0	C12H6Cl4	6.5

bcb	casrn	molecular_formula	${ m x_log_pstructure}$
3,3',5,5'-Tetrachlorobiphenyl	33284-52-5	C12H6Cl4	6.1
3,4,4',5-Tetrachlorobiphenyl	70362-50-4	C12H6Cl4	
2,2',3,3',4-Pentachlorobiphenyl	52663-62-4	C12H5Cl5	6.7

x_log_pstructure	6.8	0.9	9.9
molecular_formula	C12H5Cl5	C12H5Cl5	C12H5Cl5
casrn	60145-20-2	52663-60-2	65510-45-4
pcb	2,2',3,3',5-Pentachlorobiphenyl	2,2',3,3',6-Pentachlorobiphenyl	$2.2^{\circ}, 3.4.4^{\circ} - Pentachlorobiphenyl$

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,5-Pentachlorobiphenyl	55312-69-1	C12H5Cl5	6.7
2,2,3,4,5-Pentachlorobiphenyl	38380-02-8	C12H5Cl5	6.4
$2,2^{\circ},3,4,6\text{-Pentachlorobiphenyl}$	55215-17-3	C12H5Cl5	6.3

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,6'-Pentachlorobiphenyl	73575-57-2	C12H5Cl5	6.3
2,2',3,4',5-Pentachlorobiphenyl	68194-07-0	C12H5Cl5	6.8
2,2',3,4',6-Pentachlorobiphenyl	68194-05-8	C12H5Cl5	6.3

pcb	casrn	molecular_formula	x_log_pstructure
2,2,3,5,5-Pentachlorobiphenyl	52663-61-3	C12H5Cl5	7.0
2,2,3,5,6-Pentachlorobiphenyl	73575-56-1	C12H5Cl5	6.2
$2,2^{\prime},3,5,6^{\prime}\text{-Pentachlorobiphenyl}$	73575-55-0	C12H5Cl5	6.2

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,5',6-Pentachlorobiphenyl	38379-99-6	C12H5Cl5	6.5
2,2',3,6,6'-Pentachlorobiphenyl	73575-54-9	C12H5Cl5	6.1
$2,2',3,4',5'\hbox{-Pentachlorobiphenyl}$	41464-51-1	C12H5Cl5	6.7

pcb	casrn	molecular_formula	x_log_pstructure
2,2,3,4,6'- Pentachlor obiphenyl	60233-25-2	C12H5Cl5	6.3
2,2,4,4',5 - Pentachlorobiphenyl	38380-01-7	C12H5Cl5	7.2
2,2',4,4',6-Pentachlorobiphenyl	39485-83-1	C12H5Cl5	6.3

pcb	casrn	molecular_formula	x_log_pstructure
$2,2',4,5,5'- {\rm Pentachlorobiphenyl}$	37680-73-2	C12H5Cl5	6.5
2,2',4,5,6'-Pentachlorobiphenyl	68194-06-9	C12H5Cl5	6.3
2,2',4,5',6-Pentachlorobiphenyl	60145-21-3	C12H5Cl5	6.2

pcb	casrn	molecular_formula	$f{x_log_pstructure}$
$2,2,4,6,6'\text{-}\operatorname{Pentachlorobiphenyl}$	56558-16-8	C12H5Cl5	5.8
2, 3, 3, 4.4-Pentachlorobiphenyl	32598-14-4	C12H5Cl5	9.9
2, 3, 3, 4, 5-Pentachlorobiphenyl	70424-69-0	C12H5Cl5	6.9

pcb	casrn	molecular_formula	x_log_pstructure
$2,3,3,4',5 - \mathrm{Pentachlorobiphenyl}$	70424-68-9	C12H5Cl5	6.9
2,3,3',4,5'-Pentachlorobiphenyl	70362-41-3	C12H5Cl5	2.0
2,3,3,4,6-Pentachlorobiphenyl	74472-35-8	C12H5Cl5	6.6

pcb	casrn	molecular_formula	x_log_pstructure
2,3,3,4,6-Pentachlorobiphenyl	38380-03-9	C12H5Cl5	9.9
2,3,3',5,5'-Pentachlorobiphenyl	39635-32-0	C12H5Cl5	6.8
2,3,3',5,6-Pentachlorobiphenyl	74472-36-9	C12H5Cl5	6.7

pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',5',6-Pentachlorobiphenyl	68194-10-5	C12H5Cl5	6.6
2, 3, 4, 4', 5-Pentachlorobiphenyl	74472-37-0	C12H5Cl5	7.0
2, 3, 4, 4', 6-Pentachlorobiphenyl	74472-38-1	C12H5Cl5	9.9

pcb	casrn	molecular_formula	$f{x_log_pstructure}$
2, 3, 4, 5, 6-Pentachlorobiphenyl	18259-05-7	C12H5Cl5	G.7
2,3,4',5,6-Pentachlorobiphenyl	68194-11-6	C12H5Cl5	6.5
2, 3, 4, 4, 5- Pentachlor obiphenyl	31508-00-6	C12H5Cl5	7.1

$f{x}_\log_pstructure$	6.6	6.9	6.5
molecular_formula	C12H5Cl5	C12H5Cl5	C12H5Cl5
casrn	56558-17-9	68194-12-7	56558-18-0
pcb	2, 3, 4, 4', 6-Pentachlorobiphenyl	2,3,4,5,5-Pentachlorobiphenyl	2,3',4,5',6-Pentachlorobiphenyl

pcb	casrn	molecular_formula	x_log_pstructure
2,3,3',4',5'-Pentachlorobiphenyl	76842-07-4	C12H5Cl5	7.0
2,3',4,4',5'-Pentachlorobiphenyl	65510-44-3	C12H5Cl5	6.9
2,3',4',5,5'-Pentachlorobiphenyl	70424-70-3	C12H5Cl5	6.9

pcb	casrn	molecular_formula	$f{x}_log_pstructure$
2.3', 4', 5', 6-Pentachlorobiphenyl	74472-39-2	C12H5Cl5	6.5
3,3',4,4',5-Pentachlorobiphenyl	57465-28-8	C12H5Cl5	7.3
3,3',4,5,5'-Pentachlorobiphenyl	39635-33-1	C12H5Cl5	6.8

pcb	casrn	molecular_formula	x_log_pstructure
2.2.3.3.44'-Hexachlorohinhenvl	38380-07-3	C12H4Cl6	
2,2',3,3',4,5-Hexachlorobiphenyl	55215-18-4	C12H4Cl6	7.3
2,2,3,3,4,5'- Hexachlor obiphenyl	52663-66-8	C12H4Cl6	7.4

pcb	casrn	molecular_formula	${f x_log_pstructure}$
2,2,3,3,4,6- Hexachlor obiphenyl	61798-70-7	C12H4Cl6	6.8
2,2',3,3',4,6'-Hexachlorobiphenyl	38380-05-1	C12H4Cl6	7.0
2,2',3,3',5,5'-Hexachlorobiphenyl	35694-04-3	C12H4Cl6	7.1

pcb	casrn	molecular_formula	x_log_pstructure
$2,2,3,3,5,6. {\rm Hexachlorobiphenyl}$	52704-70-8	C12H4Cl6	6.8
2,2',3,3',5,6'-Hexachlorobiphenyl	52744-13-5	C12H4Cl6	7.1
2,2,3,3,6,6 Hexachlor obiphenyl	38411-22-2	C12H4Cl6	7.1

pcb	casrn	molecular_formula	x_log_pstructure
9.97. 2.4.47 5 Hovershlowshimhound	2 7 6 7 7	C19H4Cl6	
2,2,3,4,4,3-nexacnioropipnenyl	33094-00-3	C12H4Cl0	1.4
2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2	C12H4Cl6	7.2
$2,2^{\circ},3,4,4^{\circ},6\text{-Hexachlorobiphenyl}$	56030-56-9	C12H4Cl6	6.9

mula x_log_pstructure	7.0	7.2	7.0
molecular_formula	C12H4Cl6	C12H4Cl6	C12H4Cl6
casrn	59291-64-4	52712-04-6	41411-61-4
pcb	2,2,3,4,4,6'- Hexachlorobiphenyl	2,2',3,4,5,5'-Hexachlorobiphenyl	2,2,3,4,5,6-Hexachlorobiphenyl

pcb	casrn	molecular_formula	x_log_pstructure
$2,2,3,4,5,6'-{\rm Hexachlorobiphenyl}$	68194-15-0	C12H4Cl6	6.9
2,2',3,4,5',6-Hexachlorobiphenyl	68194-14-9	C12H4Cl6	6.8
$2,2,3,4,6,6'- {\rm Hexachlorobiphenyl}$	74472-40-5	C12H4Cl6	6.7

pcb	casrn	molecular_formula	$f{x_log_pstructure}$
2,2',3,4',5,5'- Hexachlor objphenyl	51908-16-8	C12H4Cl6	7.1
2,2',3,4',5,6-Hexachlorobiphenyl	68194-13-8	C12H4Cl6	6.9
2,2',3,4',5,6'-Hexachlorobiphenyl	74472-41-6	C12H4Cl6	6.9

pcb	casrn	molecular_formula	${f x_log_pstructure}$
2,2,3,4,5,6-Hexachlorobiphenyl	38380-04-0	C12H4Cl6	7.1
2,2,3,4',6,6'- Hexachlor obiphenyl	68194-08-1	C12H4Cl6	6.7
$2,2^{\prime},3,5,5^{\prime},6\text{-Hexachlorobiphenyl}$	52663-63-5	C12H4Cl6	6.8

pcb	casrn	molecular_formula	${ m x_log_pstructure}$
2,2,3,5,6,6-Hexachlorobiphenyl	68194-09-2	C12H4Cl6	6.5
2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1	C12H4Cl6	7.2
2,2',4,4',5,6'-Hexachlorobiphenyl	60145-22-4	C12H4Cl6	6.9

la x_log_pstructure	7.3	2.6	2.6
molecular_formula	C12H4Cl6	C12H4Cl6	C12H4Cl6
casrn	33979-03-2	38380-08-4	69782-90-7
pcb	2,2',4,4',6,6'- Hexachlorobiphenyl	2,3,3',4,4',5-Hexachlorobiphenyl	2,3,3',4,4',5'-Hexachlorobiphenyl

ula x_log_pstructure	7.2	7.7	7.3
molecular_formula	C12H4Cl6	C12H4Cl6	C12H4Cl6
casrn	74472-42-7	39635-35-3	41411-62-5
pcb	$2,3,3,4,4',6-{\rm Hexachlorobiphenyl}$	2,3,3',4,5,5'-Hexachlorobiphenyl	2, 3, 3, 4, 5, 6- Hexachlor objphenyl

pcb	casrn	molecular_formula	$x_\log_pstructure$
0.0.0, 4.5.0.11	7. 6. 6. 6. 6.	STO THE FO	
2,3,3',4,5',6-Hexachlorobiphenyl	74472-43-8	C12H4Cl6	7.1
2,3,3,4,5,5-Hexachlorobiphenyl	39635-34-2	C12H4Cl6	7.5
2,3,3,4',5,6- Hexachlorobip henyl	74472-44-9	C12H4Cl6	7.2

pcb	casrn	molecular_formula	x_log_pstructure
2, 3, 3', 4', 5', 6-Hexachlorobiphenyl	74472-45-0	C12H4Cl6	7.2
2,3,3',5,5',6-Hexachlorobiphenyl	74472-46-1	C12H4Cl6	7.4
2, 3, 4, 4', 5, 6- Hexa chlorobip henyl	41411-63-6	C12H4Cl6	7.3

pcb	casrn	molecular_formula	x_log_pstructure
2.3' 4.4'.5.5'-Hexachlorobiphenvl	52663-72-6	C12H4Cl6	
2,3,4,4,5,6-Hexachlorobiphenyl	59291-65-5	C12H4Cl6	7.2
3,3,4,4',5,5'-Hexachlorobiphenyl	32774-16-6	C12H4Cl6	7.4

pcb	casrn	molecular_formula	$f{x_log_pstructure}$
$2,2^{\prime},3,3^{\prime},4,4^{\prime},5\text{-Heptachlorobiphenyl}$	35065-30-6	C12H3Cl7	7.9
2.2'.3.3'.4.4'.6-Heptachlorobiphenvl	52663-71-5	C12H3Cl7	7.4
2,2',3,3',4,5,5'-Heptachlorobiphenyl	52663-74-8	C12H3Cl7	8.0

pcb	casrn	molecular_formula	x_log_pstructure
9.97.3.37.45.6-Hentachlorohinhenvl	68194.16.1	C19H3Cl7	74
2,2,9,9,4,9,0-11eptacmorooipmeny1	00134-10-1	CIZIISCII	1.4
2,2',3,3',4,5,6'-Heptachlorobiphenyl	38411-25-5	C12H3Cl7	7.5
2,2',3,3',4,5',6-Heptachlorobiphenyl	40186-70-7	C12H3Cl7	7.8

pcb	casrn	molecular_formula	x_log_pstructure
2.2.3.3.4.6.6'-Hentachlorobinhenvl	52663-65-7	C12H3Cl7	
2,2',3,3',4,5',6'-Heptachlorobiphenyl	52663-70-4	C12H3Cl7	7.4
2,2,3,3,5,5,6. Heptachlorobiphenyl	52663-67-9	C12H3Cl7	7.8

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',5',6,6'-Heptachlorobiphenyl	52663-64-6	C12H3Cl7	7.1
2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3	C12H3Cl7	7.9
2,2',3,4,4',5.6- Heptachlorobip henyl	74472-47-2	C12H3Cl7	7.6

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,4',5,6'-Heptachlorobiphenyl	60145-23-5	C12H3Cl7	7.5
2.2',3,4,4',5',6-Heptachlorobiphenyl	52663-69-1	C12H3Cl7	7.4
2,2,3,4,4',6,6'- Heptachlorobiphenyl	74472-48-3	C12H3Cl7	7.3

pcb	casrn	molecular_formula	${f x_log_pstructure}$
2,2',3,4,5,5',6-Heptachlorobiphenyl	52712-05-7	C12H3Cl7	7.5
2,2',3,4,5,6,6'-Heptachlorobiphenyl	74472-49-4	C12H3Cl7	7.1
2,2,3,4',5,5',6- Heptachlorobiphenyl	52663-68-0	C12H3Cl7	7.5

pcb	casrn	molecular_formula	x_log_pstructure
2.2',3,4',5,6'd'-Heptachlorobiphenyl	74487-85-7	C12H3Cl7	7.1
2,3,3',4,4',5,5'-Heptachlorobiphenyl	39635-31-9	C12H3Cl7	8.1
2,3,3',4,4',5,6-Heptachlorobiphenyl	41411-64-7	C12H3Cl7	6.7

pcb	casrn	molecular_formula	x_log_pstructure
2.3.3'.4.4'.5'.6-Heptachlorobiphenyl	74472-50-7	C12H3Cl7	
2,3,3',4,5,5',6-Heptachlorobiphenyl	74472-51-8	C12H3Cl7	8.0
2,3,3',4',5,5',6-Heptachlorobiphenyl	69782-91-8	C12H3Cl7	8.0

pcb	casrn	molecular_formula	x_log_pstructure
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2,2,3,3,4,4,3,3 -Octacnioroniphenyl	33094-08-1	CIZHZCI8	8.0
2,2',3,3',4,4',5,6-Octachlorobiphenyl	52663-78-2	C12H2Cl8	8.2
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	42740-50-1	C12H2Cl8	8.2

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,4',6,6'-Octachlorobiphenyl	33091-17-7	C12H2Cl8	8.0
2,2',3,3',4,5,5',6-Octachlorobiphenyl	68194-17-2	C12H2Cl8	8.1
2,2',3,3',4,5,5',6'-Octachlorobiphenyl	52663-75-9	C12H2Cl8	8.2

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,5,6,6'-Octachlorobiphenyl	52663-73-7	C12H2Cl8	8.4
2,2',3,3',4,5',6,6'-Octachlorobiphenyl	40186-71-8	C12H2Cl8	7.7
2,2',3,3',5,5',6,6'-Octachlorobiphenyl	2136-99-4	C12H2Cl8	7.7

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,4,4',5,5',6-Octachlorobiphenyl	52663-76-0	C12H2Cl8	8.1
$2,2^{\prime},3,4,4^{\prime},5,6,6^{\prime}-Octachlorobiphenyl$	74472-52-9	C12H2Cl8	7.5
$2,3,3^{\prime},4,4^{\prime},5,5^{\prime},6\text{-}Octachlorobiphenyl}$	74472-53-0	C12H2Cl8	8.5

pcb	casrn	molecular_formula	x_log_pstructure
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	40186-72-9	C12HCl9	8.8
2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	52663-79-3	C12HCl9	8.2
2,2,3,3,4,5,5,6,6-Nonachlorobiphenyl	52663-77-1	C12HCl9	8.2

pcb	casrn	molecular_formula	$x_\log_{pstructure}$
Decachlorobiphenyl	2051-24-3	C12C110	8.3