

## Electronic Supplementary Information (ESI)

### Development of Polyparameter Linear Free Energy Relationships Models for Octanol-Air Partition Coefficients of Diverse Chemicals

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## Model validation

Multicollinearity in a multiple linear regression model means the linear dependence of one descriptor on all other descriptors. *VIF* can be used to detect multicollinearity:

$$VIF = 1 / (1 - R^2) \quad (s1)$$

$R^2$  is the coefficient of determination obtained by MLR for a descriptor against all the others. A *VIF* higher than 10 is regarded as an indicator of multicollinearity.

The internal and external predictive abilities can be assessed by the root-mean-square error (*RMSE*), which is defined as:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (s2)$$

Here,  $y_i$  and  $\hat{y}_i$  refers to the  $i$ th chemical's experimental and predicted values respectively;  $n$  is the total number of chemicals in the data set.

Regarding to the internal validation, for the purpose of robustness assessment we used leave-many-out cross validation and calculated cross-validation coefficient ( $Q^2_{CV}$ ). In the process of cross validation, firstly the original data with  $n$  data points is randomly partitioned into  $k$  equal sized subsets ( $m = n / k$ ). Of the  $k$  subsamples, a single subset with  $m$  data points is retained as the testing set, and the remaining  $k - 1$  subsets are used as the training set. The cross-validation process is then repeated  $k$  times (the *folds*), with each of the  $k$  subsamples used exactly once as the testing set.  $Q^2_{CV}$  can then be calculated as follows:

$$Q^2_{CV} = 1 - \frac{\sum_{i=1}^n (\hat{y}_i^{(n-m)} - y_i)^2}{\sum_{i=1}^n (y_i - \bar{y}^{(n-m,i)})^2} \quad (s3)$$

Here,  $\hat{y}_i^{(n-m)}$  is the predicted value of the  $i$ th chemical calculated from the model developed by the training set with  $n - m$  data points ( $i$  is included in the  $m$  data points).  $\bar{y}^{(n-m,i)}$  represents the average of all observed values in this training set. Generally,  $Q^2_{CV} > 0.5$  suggests good robustness and  $Q^2_{CV} > 0.9$  indicates outstanding robustness. In this study, the cross validation round ( $k$ ) is 10.

As for the external validation,  $Q^2_{EXT}$  as well as the  $RMSE_{EXT}$  which refers to *RMSE* of the validation set were used to evaluate the external predictive power of the two models.  $Q^2_{EXT}$  is defined as follows:

$$Q^2_{EXT} = 1 - \sum_{i=1}^n (y_i - \hat{y}_i)^2 / \sum_{i=1}^n (y_i - \bar{y}_i)^2 \quad (s4)$$

$\hat{y}_i$  is the predicted value of the  $i$ th chemical in the validation set;  $\bar{y}_i$  represents the average of all observed values in the validation set;  $Q^2_{\text{EXT}}$  verifies the external predictive power of the model based on evenly distributed data sets.

### Applicability domain definition

For the pp-LFER model (5), the applicability domain (AD) definition results for four respective approaches are: (1) For the ranges of descriptor spaces, the ranges are  $E$  (-1.87 ~ 4.07);  $S$  (-0.26 ~ 2.26);  $A$  (0 ~ 0.81);  $B$  (0 ~ 0.98);  $L$  (-1.741 ~ 13.264). (2) The Euclidean distances are in the range of 0.109 ~ 0.985. (3) The city-block distances are in the range of 0.182 ~ 1.729. (4) The probability densities are in the ranges of  $9.85 \times 10^{-4} \sim 379.771$ .

For the pp-LFER model (6), the AD definition results for four respective approaches are: (1) For the ranges of descriptor spaces, the ranges are  $E$  (-1.87 ~ 4.07);  $S$  (-0.26 ~ 2.26);  $A$  (0 ~ 0.81);  $B$  (0 ~ 0.98);  $L$  (-1.741 ~ 13.264). (2) The Euclidean distances are in the range of 0.104 ~ 0.989. (3) The city-block distances are in the range of 0.185 ~ 1.749. (4) The probability densities are in the ranges of  $5.15 \times 10^{-4} \sim 405.987$ .

For the pp-LFER- $T$  model (10), the AD definition results for four respective approaches are: (1) For the ranges of descriptor spaces, the ranges are  $E/T$  ( $-6.27 \times 10^{-3} \sim 0.0137$ );  $S/T$  ( $-6.71 \times 10^{-4} \sim 8.27 \times 10^{-3}$ );  $A/T$  ( $0 \sim 2.72 \times 10^{-3}$ );  $B/T$  ( $0 \sim 3.29 \times 10^{-3}$ );  $L/T$  ( $-5.84 \times 10^{-3} \sim 0.0445$ );  $1/T$  ( $3.09 \times 10^{-3} \sim 3.80 \times 10^{-3}$ ). (2) The Euclidean distances are in the range of 0.040 ~ 1.085. (3) The city-block distances are in the range of 0.086 ~ 2.283. (4) The probability densities are in the ranges of  $4.43 \times 10^{-5} \sim 5.64 \times 10^4$ .

For the pp-LFER- $T$  model (11), the AD definition results for four respective approaches are: (1) For the ranges of descriptor spaces, the ranges are  $E/T$  ( $-6.27 \times 10^{-3} \sim 0.0137$ );  $S/T$  ( $-6.71 \times 10^{-4} \sim 8.27 \times 10^{-3}$ );  $A/T$  ( $0 \sim 2.72 \times 10^{-3}$ );  $B/L$  ( $0 \sim 3.29 \times 10^{-3}$ );  $L/T$  ( $-5.84 \times 10^{-3} \sim 0.0445$ );  $1/T$  ( $3.09 \times 10^{-3} \sim 3.80 \times 10^{-3}$ ). (2) The Euclidean distances are in the range of 0.040 ~ 1.086. (3) The city-block distances are in the range of 0.082 ~ 2.287. (4) The probability densities are in the ranges of  $5.25 \times 10^{-5} \sim 5.55 \times 10^4$ .

**Table S1. List of the Abraham descriptors for chemicals used in this study.**

| CAS-RN   | Name          | $E$  | $S$  | $A$  | $B$  | $V$  | $L$  |
|----------|---------------|------|------|------|------|------|------|
| 109-74-0 | butanonitrile | 0.19 | 0.90 | 0.00 | 0.36 | 0.69 | 2.55 |
| 123-72-8 | butanal       | 0.19 | 0.65 | 0.00 | 0.45 | 0.69 | 2.27 |
| 111-43-3 | dipropylether | 0.01 | 0.25 | 0.00 | 0.45 | 1.01 | 2.95 |
| 71-36-3  | butan-1-ol    | 0.22 | 0.42 | 0.37 | 0.48 | 0.73 | 2.60 |

| <b>CAS-RN</b> | <b>Name</b>                       | <b><i>E</i></b> | <b><i>S</i></b> | <b><i>A</i></b> | <b><i>B</i></b> | <b><i>V</i></b> | <b><i>L</i></b> |
|---------------|-----------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 7440-59-7     | helium                            | 0.00            | 0.00            | 0.00            | 0.00            | 0.07            | -1.74           |
| 108-90-7      | chlorobenzene                     | 0.72            | 0.65            | 0.00            | 0.07            | 0.84            | 3.66            |
| 1333-74-0     | hydrogen                          | 0.00            | 0.00            | 0.00            | 0.00            | 0.11            | -1.20           |
| 74-87-3       | chloromethane                     | 0.25            | 0.43            | 0.00            | 0.08            | 0.37            | 1.16            |
| 141-78-6      | ethyl acetate                     | 0.11            | 0.62            | 0.00            | 0.45            | 0.75            | 2.31            |
| 107-12-0      | propionitrile                     | 0.16            | 0.90            | 0.02            | 0.36            | 0.55            | 2.08            |
| 103-30-0      | trans-stilbene                    | 1.45            | 1.04            | 0.00            | 0.34            | 1.56            | 7.53            |
| 69-72-7       | 2-hydroxybenzoic acid             | 0.90            | 0.85            | 0.73            | 0.37            | 0.99            | 4.73            |
| 91-20-3       | naphthalene                       | 1.34            | 0.92            | 0.00            | 0.20            | 1.09            | 5.16            |
| 78-83-1       | 2-methylpropan-1-ol               | 0.22            | 0.39            | 0.37            | 0.48            | 0.73            | 2.41            |
| 75-73-0       | tetrafluoromethane                | -0.58           | -0.26           | 0.00            | 0.00            | 0.32            | -0.82           |
| 7440-63-3     | xenon                             | 0.00            | 0.00            | 0.00            | 0.00            | 0.33            | 0.38            |
| 124-40-3      | dimethylamine                     | 0.19            | 0.30            | 0.08            | 0.66            | 0.49            | 1.60            |
| 7440-37-1     | argon                             | 0.00            | 0.00            | 0.00            | 0.00            | 0.19            | -0.69           |
| 10024-97-2    | nitrous oxide                     | 0.07            | 0.35            | 0.00            | 0.10            | 0.28            | 0.16            |
| 594-27-4      | tetramethyl tin                   | 0.32            | 0.11            | 0.00            | 0.10            | 1.04            | 2.65            |
| 75-09-2       | dichloromethane                   | 0.39            | 0.57            | 0.10            | 0.05            | 0.49            | 2.02            |
| 67-66-3       | trichloromethane                  | 0.43            | 0.49            | 0.15            | 0.02            | 0.62            | 2.48            |
| 71-55-6       | 1,1,1-trichloroethane             | 0.37            | 0.41            | 0.00            | 0.09            | 0.76            | 2.73            |
| 99-76-3       | methyl 4-hydroxybenzoate          | 0.90            | 1.37            | 0.69            | 0.45            | 1.13            | 5.67            |
| 7782-44-7     | oxygen                            | 0.00            | 0.00            | 0.00            | 0.00            | 0.18            | -0.72           |
| 1825-31-6     | 1,4-dichloronaphthalene           | 1.57            | 1.06            | 0.00            | 0.09            | 1.33            | 6.76            |
| 3432-57-3     | 1,4,5,8-tetrachloronaphthalene    | 1.81            | 1.18            | 0.00            | 0.00            | 1.58            | 9.14            |
| 150224-22-9   | 1,2,4,6,8-pentachloronaphthalene  | 1.93            | 1.30            | 0.00            | 0.00            | 1.70            | 9.28            |
| 150224-18-3   | 1,2,3,5,6-pentachloronaphthalene  | 1.93            | 1.36            | 0.00            | 0.00            | 1.70            | 9.22            |
| 2437-55-0     | 1,4,5-trichloronaphthalene        | 1.69            | 1.12            | 0.00            | 0.00            | 1.45            | 8.07            |
| 6733-54-6     | 1,2,4,5-tetrachloronaphthalene    | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.67            |
| 150224-25-2   | 1,2,4,5,8-pentachloronaphthalene  | 1.93            | 1.36            | 0.00            | 0.00            | 1.70            | 9.59            |
| 58877-88-6    | 1,2,3,4,5,6-hexachloronaphthalene | 2.05            | 1.42            | 0.00            | 0.00            | 1.82            | 10.54           |
| 103426-94-4   | 1,2,3,5,7,8-hexachloronaphthalene | 2.05            | 1.42            | 0.00            | 0.00            | 1.82            | 10.24           |
| 150224-21-8   | 1,2,4,7,8-pentachloronaphthalene  | 1.93            | 1.30            | 0.00            | 0.00            | 1.70            | 9.46            |
| 90948-28-0    | 1,2,4,5,6,8-hexachloronaphthalene | 2.05            | 1.42            | 0.00            | 0.00            | 1.82            | 10.30           |
| 67922-27-4    | 1,2,3,4,5,7-hexachloronaphthalene | 2.05            | 1.42            | 0.00            | 0.00            | 1.82            | 10.18           |
| 149864-80-2   | 1,2,5,8-tetrachloronaphthalene    | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.82            |

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|---------------|---------------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 103426-96-6   | 1,2,3,4,6,7-hexachloronaphthalene     | 2.05            | 1.42            | 0.00            | 0.00            | 1.82            | 10.04           |
| 150224-24-1   | 1,2,3,5,8-pentachloronaphthalene      | 1.93            | 1.36            | 0.00            | 0.00            | 1.70            | 9.50            |
| 51570-45-7    | 1,2,4,6-tetrachloronaphthalene        | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.27            |
| 55720-43-9    | 1,4,6,7-tetrachloronaphthalene        | 1.81            | 1.18            | 0.00            | 0.00            | 1.58            | 8.53            |
| 2437-54-9     | 1,4,6-trichloronaphthalene            | 1.69            | 1.12            | 0.00            | 0.00            | 1.45            | 7.65            |
| 150224-19-4   | 1,2,4,5,7-pentachloronaphthalene      | 1.93            | 1.30            | 0.00            | 0.00            | 1.70            | 9.23            |
| 67922-26-3    | 1,2,3,4,6-pentachloronaphthalene      | 1.93            | 1.36            | 0.00            | 0.00            | 1.70            | 9.20            |
| 51570-43-5    | 1,3,5-trichloronaphthalene            | 1.69            | 1.12            | 0.00            | 0.00            | 1.45            | 7.59            |
| 6529-87-9     | 1,2,4,8-tetrachloronaphthalene        | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.74            |
| 53555-65-0    | 1,2,3,5,7-pentachloronaphthalene      | 1.93            | 1.36            | 0.00            | 0.00            | 1.70            | 8.98            |
| 2198-77-8     | 2,7-dichloronaphthalene               | 1.57            | 1.06            | 0.00            | 0.08            | 1.33            | 6.79            |
| 55720-33-7    | 1,2,5-trichloronaphthalene            | 1.69            | 1.18            | 0.00            | 0.00            | 1.45            | 7.64            |
| 103426-93-3   | 1,2,3,4,5,8-hexachloronaphthalene     | 2.05            | 1.42            | 0.00            | 0.00            | 1.82            | 10.66           |
| 1825-30-5     | 1,5-dichloronaphthalene               | 1.57            | 1.06            | 0.00            | 0.09            | 1.33            | 6.78            |
| 51570-44-6    | 1,2,6-trichloronaphthalene            | 1.69            | 1.18            | 0.00            | 0.00            | 1.45            | 7.70            |
| 55720-34-8    | 1,2,7-trichloronaphthalene            | 1.69            | 1.18            | 0.00            | 0.00            | 1.45            | 7.76            |
| 2234-13-1     | 1,2,3,4,5,6,7,8-octachloronaphthalene | 2.29            | 1.54            | 0.00            | 0.00            | 2.07            | 12.88           |
| 58863-15-3    | 1,2,3,4,5,6,8-heptachloronaphthalene  | 2.17            | 1.48            | 0.00            | 0.00            | 1.94            | 11.41           |
| 58863-14-2    | 1,2,3,4,5,6,7-heptachloronaphthalene  | 2.17            | 1.48            | 0.00            | 0.00            | 1.94            | 11.39           |
| 149864-82-4   | 1,2,7,8-tetrachloronaphthalene        | 1.81            | 1.30            | 0.00            | 0.00            | 1.58            | 8.62            |
| 103426-97-7   | 1,2,3,5,6,7-hexachloronaphthalene     | 2.05            | 1.42            | 0.00            | 0.00            | 1.82            | 10.04           |
| 50402-52-3    | 1,2,3-trichloronaphthalene            | 1.69            | 1.24            | 0.00            | 0.01            | 1.45            | 7.67            |
| 2050-69-3     | 1,2-dichloronaphthalene               | 1.57            | 1.12            | 0.00            | 0.09            | 1.33            | 6.81            |
| 150224-23-0   | 1,2,3,6,8-pentachloronaphthalene      | 1.93            | 1.36            | 0.00            | 0.00            | 1.70            | 9.54            |
| 34588-40-4    | 2,3,6,7-tetrachloronaphthalene        | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.80            |
| 150224-15-0   | 1,3,6,8-tetrachloronaphthalene        | 1.81            | 1.18            | 0.00            | 0.00            | 1.58            | 8.66            |
| 67922-25-2    | 1,2,3,4,5-pentachloronaphthalene      | 1.93            | 1.36            | 0.00            | 0.00            | 1.70            | 9.66            |
| 67922-21-8    | 1,2,4,7-tetrachloronaphthalene        | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.27            |
| 31604-28-1    | 1,3,5,8-tetrachloronaphthalene        | 1.81            | 1.18            | 0.00            | 0.00            | 1.58            | 8.67            |
| 149864-79-9   | 1,2,6,7-tetrachloronaphthalene        | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.67            |
| 150224-16-1   | 1,2,3,6,7-pentachloronaphthalene      | 1.93            | 1.36            | 0.00            | 0.00            | 1.70            | 9.40            |
| 20020-02-4    | 1,2,3,4-tetrachloronaphthalene        | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.62            |
| 55720-41-7    | 1,2,3,7-tetrachloronaphthalene        | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.65            |
| 67922-22-9    | 1,2,5,6-tetrachloronaphthalene        | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.52            |

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|---------------|-----------------------------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 55720-39-3    | 1,6,7-trichloronaphthalene                          | 1.69            | 1.18            | 0.00            | 0.00            | 1.45            | 7.76            |
| 91-58-7       | 2-chloronaphthalene                                 | 1.45            | 1.00            | 0.00            | 0.14            | 1.21            | 5.83            |
| 53555-64-9    | 1,3,5,7-tetrachloronaphthalene                      | 1.81            | 1.18            | 0.00            | 0.00            | 1.58            | 8.19            |
| 53555-63-8    | 1,2,3,5-tetrachloronaphthalene                      | 1.81            | 1.24            | 0.00            | 0.00            | 1.58            | 8.54            |
| 35065-29-3    | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180)   | 2.29            | 1.87            | 0.00            | 0.09            | 2.18            | 10.42           |
| 57465-28-8    | 3,3',4,4',5-pentachlorobiphenyl<br>(PCB-126)        | 2.11            | 1.57            | 0.00            | 0.09            | 1.94            | 9.88            |
| 69782-90-7    | 2,3,3',4,4',5'-hexachlorobiphenyl<br>(PCB-157)      | 2.21            | 1.72            | 0.00            | 0.09            | 2.06            | 10.27           |
| 32774-16-6    | 3,4,5,3',4',5'-hexachlorobiphenyl<br>(PCB-169)      | 2.21            | 1.70            | 0.00            | 0.07            | 2.06            | 10.61           |
| 41464-41-9    | 2,2',5,6'-tetrachlorobiphenyl (PCB-53)              | 1.87            | 1.48            | 0.00            | 0.15            | 1.81            | 7.95            |
| 52663-72-6    | 2,3',4,4',5,5'-hexachlorobiphenyl<br>(PCB-167)      | 2.21            | 1.72            | 0.00            | 0.09            | 2.06            | 10.09           |
| 38380-08-4    | 2,3,3',4,4',5-hexachlorobiphenyl<br>(PCB-156)       | 2.21            | 1.72            | 0.00            | 0.09            | 2.06            | 10.20           |
| 32598-10-0    | 2,3',4,4'-tetrachlorobiphenyl (PCB-66)              | 1.91            | 1.46            | 0.00            | 0.13            | 1.81            | 8.72            |
| 39635-31-9    | 2,3,3',4,4',5,5'-heptachlorobiphenyl<br>(PCB-189)   | 2.36            | 1.87            | 0.00            | 0.07            | 2.18            | 10.89           |
| 38444-85-8    | 2,3,4'-trichlorobiphenyl (PCB-22)                   | 1.77            | 1.33            | 0.00            | 0.15            | 1.69            | 8.03            |
| 32690-93-0    | 2,4,4',5-tetrachlorobiphenyl (PCB-74)               | 1.91            | 1.46            | 0.00            | 0.13            | 1.81            | 8.58            |
| 74472-34-7    | 2,3,4',5-tetrachlorobiphenyl (PCB-63)               | 1.92            | 1.46            | 0.00            | 0.13            | 1.81            | 8.52            |
| 38444-84-7    | 2,3,3'-trichlorobiphenyl (PCB-20)                   | 1.78            | 1.33            | 0.00            | 0.15            | 1.69            | 7.98            |
| 38444-86-9    | 2',3,4-trichlorobiphenyl (PCB-33)                   | 1.77            | 1.33            | 0.00            | 0.15            | 1.69            | 8.01            |
| 15862-07-4    | 2,4,5-trichlorobiphenyl (PCB-29)                    | 1.77            | 1.33            | 0.00            | 0.15            | 1.69            | 7.72            |
| 73575-54-9    | 2,2',3,6,6'-pentachlorobiphenyl<br>(PCB-96)         | 1.99            | 1.61            | 0.00            | 0.13            | 1.94            | 8.44            |
| 32598-11-1    | 2,3',4',5-tetrachlorobiphenyl (PCB-70)              | 1.89            | 1.46            | 0.00            | 0.13            | 1.81            | 8.69            |
| 34883-41-5    | 3,5-dichlorobiphenyl (PCB-14)                       | 1.65            | 1.18            | 0.00            | 0.16            | 1.57            | 7.37            |
| 2136-99-4     | 2,2',3,3',5,5',6,6'-octachlorobiphenyl<br>(PCB-202) | 2.44            | 2.00            | 0.00            | 0.06            | 2.30            | 10.14           |
| 2050-67-1     | 3,3'-dichlorobiphenyl (PCB-11)                      | 1.66            | 1.18            | 0.00            | 0.16            | 1.57            | 7.48            |

| <b>CAS-RN</b> | <b>Name</b>                                         | <b><i>E</i></b> | <b><i>S</i></b> | <b><i>A</i></b> | <b><i>B</i></b> | <b><i>V</i></b> | <b><i>L</i></b> |
|---------------|-----------------------------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 52663-78-2    | 2,2',3,3',4,4',5,6-octachlorobiphenyl<br>(PCB-195)  | 2.45            | 2.00            | 0.00            | 0.06            | 2.30            | 10.83           |
| 38444-81-4    | 2,3',5-trichlorobiphenyl (PCB-26)                   | 1.78            | 1.33            | 0.00            | 0.15            | 1.69            | 7.81            |
| 37680-66-3    | 2,2',4-trichlorobiphenyl (PCB-17)                   | 1.74            | 1.35            | 0.00            | 0.17            | 1.69            | 7.52            |
| 74472-50-7    | 2,3,3',4,4',5',6-heptachlorobiphenyl<br>(PCB-191)   | 2.33            | 1.87            | 0.00            | 0.09            | 2.18            | 10.35           |
| 41464-40-8    | 2,2',4,5'-tetrachlorobiphenyl (PCB-49)              | 1.89            | 1.48            | 0.00            | 0.15            | 1.81            | 8.19            |
| 16605-91-7    | 2,3-dichlorobiphenyl (PCB-5)                        | 1.63            | 1.20            | 0.00            | 0.18            | 1.57            | 7.17            |
| 55712-37-3    | 2,3',4-trichlorobiphenyl (PCB-25)                   | 1.77            | 1.33            | 0.00            | 0.15            | 1.69            | 7.85            |
| 40186-71-8    | 2,2',3,3',4,5',6,6'-octachlorobiphenyl<br>(PCB-201) | 2.43            | 2.00            | 0.00            | 0.06            | 2.30            | 10.39           |
| 38380-05-1    | 2,2',3,3',4,6'-hexachlorobiphenyl<br>(PCB-132)      | 2.16            | 1.74            | 0.00            | 0.11            | 2.06            | 9.54            |
| 2051-62-9     | 4-chlorobiphenyl (PCB-3)                            | 1.50            | 1.05            | 0.00            | 0.18            | 1.45            | 6.72            |
| 61798-70-7    | 2,2',3,3',4,6-hexachlorobiphenyl<br>(PCB-131)       | 2.16            | 1.74            | 0.00            | 0.11            | 2.06            | 9.29            |
| 25569-80-6    | 2,3'-dichlorobiphenyl (PCB-6)                       | 1.63            | 1.20            | 0.00            | 0.18            | 1.57            | 7.15            |
| 2051-24-3     | decachlorobiphenyl (PCB-209)                        | 2.72            | 2.26            | 0.00            | 0.02            | 2.55            | 11.70           |
| 34883-39-1    | 2,5-dichlorobiphenyl (PCB-9)                        | 1.63            | 1.20            | 0.00            | 0.18            | 1.57            | 7.00            |
| 52663-67-9    | 2,2',3,3',5,5',6-heptachlorobiphenyl<br>(PCB-178)   | 2.31            | 1.87            | 0.00            | 0.09            | 2.18            | 9.81            |
| 2051-60-7     | 2-chlorobiphenyl                                    | 1.36            | 1.07            | 0.00            | 0.23            | 1.45            | 6.43            |
| 74472-44-9    | 2,3,3',4',5,6-hexachlorobiphenyl<br>(PCB-163)       | 2.19            | 1.74            | 0.00            | 0.11            | 2.06            | 9.67            |
| 35065-30-6    | 2,2',3,3',4,4',5-heptachlorobiphenyl<br>(PCB-170)   | 2.33            | 1.87            | 0.00            | 0.09            | 2.18            | 10.58           |
| 74472-42-7    | 2,3,3',4,4',6-hexachlorobiphenyl<br>(PCB-158)       | 2.18            | 1.74            | 0.00            | 0.11            | 2.06            | 9.65            |
| 52663-71-5    | 2,2',3,3',4,4',6-heptachlorobiphenyl<br>(PCB-171)   | 2.30            | 1.87            | 0.00            | 0.09            | 2.18            | 10.03           |
| 70362-47-9    | 2,2',4,5-tetrachlorobiphenyl (PCB-48)               | 1.89            | 1.48            | 0.00            | 0.15            | 1.81            | 8.20            |
| 38444-78-9    | 2,2',3-trichlorobiphenyl (PCB-16)                   | 1.75            | 1.35            | 0.00            | 0.17            | 1.69            | 7.65            |
| 41464-46-4    | 2,3',4,6-tetrachlorobiphenyl (PCB-71)               | 1.89            | 1.48            | 0.00            | 0.15            | 1.81            | 8.48            |

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|---------------|-------------------------------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 68194-16-1    | 2,2',3,3',4,5,6-heptachlorobiphenyl<br>(PCB-173)      | 2.31            | 1.87            | 0.00            | 0.09            | 2.18            | 10.09           |
| 51908-16-8    | 2,2',3,4',5,5'-hexachlorobiphenyl<br>(PCB-146)        | 2.19            | 1.74            | 0.00            | 0.11            | 2.06            | 9.53            |
| 52663-70-4    | 2,2',3,3',4',5,6-heptachlorobiphenyl<br>(PCB-177)     | 2.28            | 1.87            | 0.00            | 0.09            | 2.18            | 10.07           |
| 68194-14-9    | 2,2',3,4,5',6-hexachlorobiphenyl<br>(PCB-144)         | 2.16            | 1.74            | 0.00            | 0.11            | 2.06            | 9.12            |
| 38411-25-5    | 2,2',3,3',4,5,6'-heptachlorobiphenyl<br>(PCB-174)     | 2.31            | 1.87            | 0.00            | 0.09            | 2.18            | 10.16           |
| 40186-72-9    | 2,2',3,3',4,4',5,5',6-nonachlorobiphenyl<br>(PCB-206) | 2.60            | 2.13            | 0.00            | 0.04            | 2.43            | 11.45           |
| 52663-74-8    | 2,2',3,3',4,5,5'-heptachlorobiphenyl<br>(PCB-172)     | 2.34            | 1.87            | 0.00            | 0.09            | 2.18            | 10.33           |
| 68194-13-8    | 2,2',3,4',5,6-hexachlorobiphenyl<br>(PCB-147)         | 2.16            | 1.74            | 0.00            | 0.11            | 2.06            | 9.18            |
| 52663-77-1    | 2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl<br>(PCB-208) | 2.58            | 2.13            | 0.00            | 0.04            | 2.43            | 10.92           |
| 74472-53-0    | 2,3,3',4,4',5,5',6-octachlorobiphenyl<br>(PCB-205)    | 2.48            | 2.00            | 0.00            | 0.06            | 2.30            | 11.15           |
| 33284-50-3    | 2,4-dichlorobiphenyl (PCB-7)                          | 1.62            | 1.20            | 0.00            | 0.18            | 1.57            | 7.04            |
| 2437-79-8     | 2,2',4,4'-tetrachlorobiphenyl (PCB-47)                | 1.88            | 1.48            | 0.00            | 0.15            | 1.81            | 8.23            |
| 52663-79-3    | 2,2',3,3',4,4',5,6,6'-nonachlorobiphenyl<br>(PCB-207) | 2.57            | 2.13            | 0.00            | 0.04            | 2.43            | 10.90           |
| 69782-91-8    | 2,3,3',4',5,5',6-heptachlorobiphenyl<br>(PCB-193)     | 2.34            | 1.87            | 0.00            | 0.09            | 2.18            | 10.37           |
| 52663-64-6    | 2,2',3,3',5,6,6'-heptachlorobiphenyl<br>(PCB-179)     | 2.32            | 1.87            | 0.00            | 0.09            | 2.18            | 9.61            |
| 60145-20-2    | 2,2',3,3',5-pentachlorobiphenyl<br>(PCB-83)           | 2.05            | 1.61            | 0.00            | 0.13            | 1.94            | 8.97            |
| 2974-92-7     | 3,4-dichlorobiphenyl (PCB-12)                         | 1.65            | 1.18            | 0.00            | 0.16            | 1.57            | 7.53            |
| 52663-76-0    | 2,2',3,4,4',5,5',6-octachlorobiphenyl<br>(PCB-203)    | 2.48            | 2.00            | 0.00            | 0.06            | 2.30            | 10.63           |

| <b>CAS-RN</b> | <b>Name</b>                                         | <b><i>E</i></b> | <b><i>S</i></b> | <b><i>A</i></b> | <b><i>B</i></b> | <b><i>V</i></b> | <b><i>L</i></b> |
|---------------|-----------------------------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 38411-22-2    | 2,2',3,3',6,6'-hexachlorobiphenyl<br>(PCB-136)      | 2.14            | 1.74            | 0.00            | 0.11            | 2.06            | 9.12            |
| 41464-51-1    | 2,2',3',4,5-pentachlorobiphenyl<br>(PCB-97)         | 2.04            | 1.61            | 0.00            | 0.13            | 1.94            | 9.03            |
| 68194-17-2    | 2,2',3,3',4,5,5',6-octachlorobiphenyl<br>(PCB-198)  | 2.46            | 2.00            | 0.00            | 0.06            | 2.30            | 10.58           |
| 52663-75-9    | 2,2',3,3',4,5,5',6'-octachlorobiphenyl<br>(PCB-199) | 2.46            | 2.00            | 0.00            | 0.06            | 2.30            | 10.67           |
| 52663-65-7    | 2,2',3,3',4,6,6'-heptachlorobiphenyl<br>(PCB-176)   | 2.31            | 1.87            | 0.00            | 0.09            | 2.18            | 9.59            |
| 52704-70-8    | 2,2',3,3',5,6-hexachlorobiphenyl<br>(PCB-134)       | 2.17            | 1.74            | 0.00            | 0.11            | 2.06            | 9.31            |
| 42740-50-1    | 2,2',3,3',4,4',5,6'-octachlorobiphenyl<br>(PCB-196) | 2.45            | 2.00            | 0.00            | 0.06            | 2.30            | 10.65           |
| 52663-63-5    | 2,2',3,5,5',6-hexachlorobiphenyl<br>(PCB-151)       | 2.17            | 1.74            | 0.00            | 0.11            | 2.06            | 9.14            |
| 52744-13-5    | 2,2',3,3',5,6'-hexachlorobiphenyl<br>(PCB-135)      | 2.17            | 1.74            | 0.00            | 0.11            | 2.06            | 9.29            |
| 41411-64-7    | 2,3,3',4,4',5,6-heptachlorobiphenyl<br>(PCB-190)    | 2.33            | 1.87            | 0.00            | 0.09            | 2.18            | 10.45           |
| 52712-04-6    | 2,2',3,4,5,5'-hexachlorobiphenyl<br>(PCB-141)       | 2.19            | 1.74            | 0.00            | 0.11            | 2.06            | 9.67            |
| 40186-70-7    | 2,2',3,3',4,5',6-heptachlorobiphenyl<br>(PCB-175)   | 2.31            | 1.87            | 0.00            | 0.09            | 2.18            | 9.78            |
| 52663-73-7    | 2,2',3,3',4,5,6,6'-octachlorobiphenyl<br>(PCB-200)  | 2.43            | 2.00            | 0.00            | 0.06            | 2.30            | 10.41           |
| 33091-17-7    | 2,2',3,3',4,4',6,6'-octachlorobiphenyl<br>(PCB-197) | 2.42            | 2.00            | 0.00            | 0.06            | 2.30            | 10.10           |
| 52663-69-1    | 2,2',3,4,4',5',6-heptachlorobiphenyl<br>(PCB-183)   | 2.30            | 1.87            | 0.00            | 0.09            | 2.18            | 9.85            |
| 32598-13-3    | 3,3',4,4'-tetrachlorobiphenyl (PCB-77)              | 1.94            | 1.44            | 0.00            | 0.11            | 1.81            | 9.21            |
| 74472-47-2    | 2,2',3,4,4',5,6-heptachlorobiphenyl<br>(PCB-181)    | 2.30            | 1.87            | 0.00            | 0.09            | 2.18            | 9.97            |
| 13029-08-8    | 2,2'-dichlorobiphenyl (PCB-4)                       | 1.60            | 1.22            | 0.00            | 0.20            | 1.57            | 6.82            |

| <b>CAS-RN</b> | <b>Name</b>                                       | <b><i>E</i></b> | <b><i>S</i></b> | <b><i>A</i></b> | <b><i>B</i></b> | <b><i>V</i></b> | <b><i>L</i></b> |
|---------------|---------------------------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 34883-43-7    | 2,4'-dichlorobiphenyl (PCB-8)                     | 1.62            | 1.20            | 0.00            | 0.18            | 1.57            | 7.20            |
| 38379-99-6    | 2,2',3,5',6-pentachlorobiphenyl<br>(PCB-95)       | 2.02            | 1.61            | 0.00            | 0.13            | 1.94            | 8.63            |
| 38380-04-0    | 2,2',3,4',5',6-hexachlorobiphenyl<br>(PCB-149)    | 2.16            | 1.74            | 0.00            | 0.11            | 2.06            | 9.35            |
| 38380-03-9    | 2,3,3',4',6-pentachlorobiphenyl<br>(PCB-110)      | 2.04            | 1.61            | 0.00            | 0.13            | 1.94            | 9.16            |
| 52663-60-2    | 2,2',3,3',6-pentachlorobiphenyl<br>(PCB-84)       | 2.02            | 1.61            | 0.00            | 0.13            | 1.94            | 8.80            |
| 52663-59-9    | 2,2',3,4-tetrachlorobiphenyl (PCB-41)             | 1.89            | 1.48            | 0.00            | 0.15            | 1.81            | 8.39            |
| 52663-58-8    | 2,3,4',6-tetrachlorobiphenyl (PCB-64)             | 1.89            | 1.48            | 0.00            | 0.15            | 1.81            | 8.35            |
| 52663-68-0    | 2,2',3,4',5,5',6-heptachlorobiphenyl<br>(PCB-187) | 2.31            | 1.87            | 0.00            | 0.09            | 2.18            | 9.86            |
| 41464-47-5    | 2,2',3,6'-tetrachlorobiphenyl (PCB-46)            | 1.87            | 1.48            | 0.00            | 0.15            | 1.81            | 8.12            |
| 38444-77-8    | 2,4',6-trichlorobiphenyl (PCB-32)                 | 1.74            | 1.35            | 0.00            | 0.17            | 1.69            | 7.67            |
| 37680-65-2    | 2,2',5-trichlorobiphenyl (PCB-18)                 | 1.75            | 1.35            | 0.00            | 0.17            | 1.69            | 7.48            |
| 41464-39-5    | 2,2',3,5'-tetrachlorobiphenyl (PCB-44)            | 1.90            | 1.48            | 0.00            | 0.15            | 1.81            | 8.31            |
| 2051-61-8     | 3-chlorobiphenyl                                  | 1.51            | 1.05            | 0.00            | 0.18            | 1.45            | 6.67            |
| 124-13-0      | octanal                                           | 0.16            | 0.65            | 0.00            | 0.45            | 1.25            | 4.36            |
| 142-84-7      | dipropylamine                                     | 0.12            | 0.30            | 0.08            | 0.68            | 1.05            | 3.35            |
| 79-24-3       | nitroethane                                       | 0.27            | 0.95            | 0.02            | 0.33            | 0.57            | 2.41            |
| 563-80-4      | 3-methylbutan-2-one                               | 0.13            | 0.65            | 0.00            | 0.51            | 0.83            | 2.69            |
| 110-82-7      | cyclohexane                                       | 0.31            | 0.10            | 0.00            | 0.00            | 0.85            | 2.96            |
| 74-88-4       | iodomethane                                       | 0.68            | 0.43            | 0.00            | 0.13            | 0.51            | 2.11            |
| 109-67-1      | 1-pentene                                         | 0.09            | 0.08            | 0.00            | 0.07            | 0.77            | 2.05            |
| 79-20-9       | methyl acetate                                    | 0.14            | 0.64            | 0.00            | 0.45            | 0.61            | 1.91            |
| 111-66-0      | 1-octene                                          | 0.09            | 0.08            | 0.00            | 0.07            | 1.19            | 3.57            |
| 592-41-6      | 1-hexene                                          | 0.08            | 0.08            | 0.00            | 0.07            | 0.91            | 2.57            |
| 85-01-8       | phenanthrene                                      | 2.06            | 1.29            | 0.00            | 0.26            | 1.45            | 7.63            |
| 100-47-0      | benzonitrile                                      | 0.74            | 1.11            | 0.00            | 0.33            | 0.87            | 4.04            |
| 110-59-8      | pentanonitrile                                    | 0.18            | 0.90            | 0.00            | 0.36            | 0.83            | 3.11            |
| 75-50-3       | trimethylamine                                    | 0.14            | 0.20            | 0.00            | 0.67            | 0.63            | 1.62            |
| 95-47-6       | o-xylene                                          | 0.66            | 0.56            | 0.00            | 0.16            | 1.00            | 3.94            |
| 100-41-4      | ethylbenzene                                      | 0.61            | 0.51            | 0.00            | 0.15            | 1.00            | 3.78            |

| CAS-RN    | Name                                                           | <i>E</i> | <i>S</i> | <i>A</i> | <i>B</i> | <i>V</i> | <i>L</i> |
|-----------|----------------------------------------------------------------|----------|----------|----------|----------|----------|----------|
| 108-93-0  | cyclohexanol                                                   | 0.46     | 0.54     | 0.32     | 0.57     | 0.90     | 3.76     |
| 74-98-6   | propane                                                        | 0.00     | 0.00     | 0.00     | 0.00     | 0.53     | 1.05     |
| 142-92-7  | hexyl acetate                                                  | 0.06     | 0.60     | 0.00     | 0.45     | 1.31     | 4.35     |
| 634-90-2  | 1,2,3,5-tetrachlorobenzene                                     | 1.16     | 0.85     | 0.00     | 0.00     | 1.21     | 5.92     |
| 108-21-4  | isopropyl acetate                                              | 0.06     | 0.57     | 0.00     | 0.47     | 0.89     | 2.55     |
| 111-87-5  | 1-octanol                                                      | 0.20     | 0.42     | 0.37     | 0.48     | 1.30     | 4.62     |
| 124-38-9  | carbon dioxide                                                 | 0.15     | 0.42     | 0.00     | 0.10     | 0.28     | 0.06     |
| 108-20-3  | diisopropylether                                               | 0.00     | 0.19     | 0.00     | 0.45     | 1.01     | 2.48     |
| 7440-01-9 | neon                                                           | 0.00     | 0.00     | 0.00     | 0.00     | 0.09     | -1.58    |
| 319-85-7  | $\beta$ -hexachlorocyclohexane ( $\beta$ -HCH)                 | 1.45     | 0.88     | 0.00     | 0.69     | 1.58     | 7.49     |
| 319-86-8  | $\delta$ -hexachlorocyclohexane ( $\delta$ -HCH)               | 1.45     | 0.94     | 0.00     | 0.63     | 1.58     | 7.63     |
| 319-84-6  | $\alpha$ -hexachlorocyclohexane ( $\alpha$ -HCH)               | 1.45     | 0.73     | 0.00     | 0.71     | 1.58     | 7.32     |
| 1746-01-6 | 2,3,7,8-tetrachlorodibenzo- <i>p</i> -dioxin<br>(2,3,7,8-TCDD) | 2.05     | 1.69     | 0.00     | 0.00     | 1.82     | 9.76     |
| 127-19-5  | dimethylacetamide                                              | 0.36     | 1.35     | 0.00     | 0.77     | 0.79     | 3.64     |
| 107-06-2  | 1,2-dichloroethane                                             | 0.42     | 0.64     | 0.10     | 0.11     | 0.64     | 2.57     |
| 108-87-2  | methylcyclohexane                                              | 0.24     | 0.06     | 0.00     | 0.00     | 0.99     | 3.32     |
| 67-72-1   | hexachloroethane                                               | 0.68     | 0.68     | 0.00     | 0.00     | 1.13     | 4.72     |
| 110-83-8  | cyclohexene                                                    | 0.40     | 0.28     | 0.00     | 0.09     | 0.80     | 2.95     |
| 64-19-7   | acetic acid                                                    | 0.27     | 0.64     | 0.62     | 0.44     | 0.47     | 1.82     |
| 103-65-1  | propylbenzene                                                  | 0.60     | 0.50     | 0.00     | 0.15     | 1.14     | 4.23     |
| 123-51-3  | 3-methylbutan-1-ol                                             | 0.19     | 0.39     | 0.37     | 0.48     | 0.87     | 3.01     |
| 7439-90-9 | krypton                                                        | 0.00     | 0.00     | 0.00     | 0.00     | 0.25     | -0.21    |
| 123-92-2  | isopentyl acetate                                              | 0.05     | 0.57     | 0.00     | 0.47     | 1.17     | 3.74     |
| 123-86-4  | butyl acetate                                                  | 0.07     | 0.60     | 0.00     | 0.45     | 1.03     | 3.35     |
| 191-24-2  | benzo[g,h,i]perylene                                           | 4.07     | 1.90     | 0.00     | 0.45     | 2.08     | 13.26    |
| 129-00-0  | pyrene                                                         | 2.81     | 1.71     | 0.00     | 0.28     | 1.59     | 8.83     |
| 608-93-5  | pentachlorobenzene                                             | 1.33     | 0.92     | 0.06     | 0.00     | 1.33     | 6.63     |
| 205-99-2  | benzo[b]fluoranthene                                           | 3.19     | 1.82     | 0.00     | 0.40     | 1.95     | 11.63    |
| 75-05-8   | acetonitrile                                                   | 0.24     | 0.90     | 0.07     | 0.32     | 0.40     | 1.74     |
| 207-08-9  | benzo[k]fluoranthene                                           | 3.19     | 1.91     | 0.00     | 0.33     | 1.95     | 11.61    |
| 110-74-7  | propyl formate                                                 | 0.13     | 0.63     | 0.00     | 0.38     | 0.75     | 2.43     |
| 193-39-5  | indeno[1,2,3-cd]pyrene                                         | 3.61     | 1.93     | 0.00     | 0.42     | 2.08     | 12.70    |
| 74-82-8   | methane                                                        | 0.00     | 0.00     | 0.00     | 0.00     | 0.25     | -0.32    |

| CAS-RN    | Name                                          | <i>E</i> | <i>S</i> | <i>A</i> | <i>B</i> | <i>V</i> | <i>L</i> |
|-----------|-----------------------------------------------|----------|----------|----------|----------|----------|----------|
| 67-63-0   | propan-2-ol                                   | 0.21     | 0.36     | 0.33     | 0.56     | 0.59     | 1.76     |
| 50-32-8   | benzo[a]pyrene                                | 3.63     | 1.96     | 0.00     | 0.37     | 1.95     | 11.74    |
| 74-95-3   | dibromomethane                                | 0.71     | 0.69     | 0.00     | 0.11     | 0.60     | 2.89     |
| 107-87-9  | pentan-2-one                                  | 0.14     | 0.68     | 0.00     | 0.51     | 0.83     | 2.76     |
| 75-03-6   | Iodoethane                                    | 0.64     | 0.40     | 0.00     | 0.15     | 0.65     | 2.57     |
| 110-43-0  | heptan-2-one                                  | 0.12     | 0.68     | 0.00     | 0.51     | 1.11     | 3.76     |
| 111-27-3  | hexan-1-ol                                    | 0.21     | 0.42     | 0.37     | 0.48     | 1.01     | 3.61     |
| 107-31-3  | methyl formate                                | 0.19     | 0.68     | 0.00     | 0.38     | 0.47     | 1.29     |
| 540-54-5  | 1-chloropropane                               | 0.22     | 0.40     | 0.00     | 0.10     | 0.65     | 2.20     |
| 109-69-3  | 1-chlorobutane                                | 0.21     | 0.40     | 0.00     | 0.10     | 0.80     | 2.72     |
| 71-43-2   | Benzene                                       | 0.61     | 0.52     | 0.00     | 0.14     | 0.72     | 2.79     |
| 78-87-5   | 1,2-dichloropropane                           | 0.37     | 0.63     | 0.00     | 0.17     | 0.78     | 2.84     |
| 74-96-4   | Bromoethane                                   | 0.37     | 0.40     | 0.00     | 0.12     | 0.57     | 2.12     |
| 647-42-7  | 1h,1h,2h,2h-perfluorooctan-1-ol<br>(6:2 FTOH) | -0.81    | 0.02     | 0.52     | 0.20     | 1.53     | 3.38     |
| 106-97-8  | butane                                        | 0.00     | 0.00     | 0.00     | 0.00     | 0.67     | 1.62     |
| 74-85-1   | ethene                                        | 0.11     | 0.10     | 0.00     | 0.07     | 0.35     | 0.29     |
| 1634-04-4 | t-butyl methyl ether                          | 0.02     | 0.21     | 0.00     | 0.59     | 0.87     | 2.38     |
| 109-60-4  | propyl acetate                                | 0.09     | 0.60     | 0.00     | 0.45     | 0.89     | 2.82     |
| 120-82-1  | 1,2,4-trichlorobenzene                        | 0.98     | 0.81     | 0.00     | 0.00     | 1.08     | 5.25     |
| 79-01-6   | trichloroethene                               | 0.52     | 0.37     | 0.08     | 0.03     | 0.72     | 3.00     |
| 108-03-2  | nitropropane                                  | 0.24     | 0.95     | 0.00     | 0.31     | 0.71     | 2.89     |
| 78-79-5   | 2-methyl-1,3-butadiene                        | 0.31     | 0.23     | 0.00     | 0.10     | 0.73     | 2.10     |
| 78-93-3   | butanone                                      | 0.17     | 0.70     | 0.00     | 0.51     | 0.69     | 2.29     |
| 630-08-0  | carbon monoxide                               | 0.00     | 0.00     | 0.00     | 0.04     | 0.22     | -0.84    |
| 628-63-7  | pentyl acetate                                | 0.07     | 0.60     | 0.00     | 0.45     | 1.17     | 3.84     |
| 66-25-1   | hexanal                                       | 0.15     | 0.65     | 0.00     | 0.45     | 0.97     | 3.36     |
| 95-50-1   | 1,2-dichlorobenzene                           | 0.87     | 0.78     | 0.00     | 0.04     | 0.96     | 4.52     |
| 96-22-0   | pentan-3-one                                  | 0.15     | 0.66     | 0.00     | 0.51     | 0.83     | 2.81     |
| 62-44-2   | 4-ethoxyacetanilide                           | 0.94     | 1.48     | 0.48     | 0.86     | 1.45     | 6.89     |
| 771-56-2  | pentafluorotoluene                            | 0.16     | 0.59     | 0.00     | 0.01     | 0.95     | 3.24     |
| 67-56-1   | methanol                                      | 0.28     | 0.44     | 0.43     | 0.47     | 0.31     | 0.97     |
| 78-92-2   | 2-butanol                                     | 0.22     | 0.36     | 0.33     | 0.56     | 0.73     | 2.34     |
| 105-37-3  | ethyl propanoate                              | 0.09     | 0.58     | 0.00     | 0.45     | 0.89     | 2.81     |

| CAS-RN    | Name                                             | <i>E</i> | <i>S</i> | <i>A</i> | <i>B</i> | <i>V</i> | <i>L</i> |
|-----------|--------------------------------------------------|----------|----------|----------|----------|----------|----------|
| 111-65-9  | octane                                           | 0.00     | 0.00     | 0.00     | 0.00     | 1.24     | 3.68     |
| 79-00-5   | 1,1,2-trichloroethane                            | 0.50     | 0.68     | 0.13     | 0.08     | 0.76     | 3.29     |
| 75-15-0   | carbon disulfide                                 | 0.88     | 0.21     | 0.00     | 0.07     | 0.49     | 2.35     |
| 156-59-2  | cis-1,2-dichloroethene                           | 0.44     | 0.61     | 0.11     | 0.05     | 0.59     | 2.44     |
| 75-34-3   | 1,1-dichloroethane                               | 0.32     | 0.49     | 0.10     | 0.10     | 0.64     | 2.32     |
| 2551-62-4 | sulfur hexafluoride                              | -0.60    | -0.20    | 0.00     | 0.00     | 0.46     | -0.12    |
| 109-94-4  | ethyl formate                                    | 0.15     | 0.66     | 0.00     | 0.38     | 0.61     | 1.85     |
| 108-88-3  | toluene                                          | 0.60     | 0.52     | 0.00     | 0.04     | 0.86     | 3.33     |
| 71-23-8   | propan-1-ol                                      | 0.24     | 0.42     | 0.37     | 0.48     | 0.59     | 2.03     |
| 142-82-5  | heptane                                          | 0.00     | 0.00     | 0.00     | 0.00     | 1.10     | 3.17     |
| 7727-37-9 | nitrogen                                         | 0.00     | 0.00     | 0.00     | 0.00     | 0.22     | -0.98    |
| 109-66-0  | pentane                                          | 0.00     | 0.00     | 0.00     | 0.00     | 0.81     | 2.16     |
| 110-54-3  | hexane                                           | 0.00     | 0.00     | 0.00     | 0.00     | 0.95     | 2.67     |
| 84-74-2   | dibutyl phthalate                                | 0.70     | 1.27     | 0.00     | 0.95     | 2.27     | 8.97     |
| 84-66-2   | diethyl phthalate                                | 0.73     | 1.26     | 0.00     | 0.90     | 1.71     | 7.21     |
| 131-11-3  | dimethyl phthalate                               | 0.78     | 1.26     | 0.00     | 0.88     | 1.43     | 6.28     |
| 141-62-8  | decamethyltetrasiloxane (L <sub>4</sub> )        | -0.72    | -0.17    | 0.00     | 0.56     | 2.68     | 4.92     |
| 107-46-0  | hexamethyldisiloxane (L <sub>2</sub> )           | -0.27    | -0.19    | 0.00     | 0.30     | 1.50     | 3.12     |
| 92-86-4   | 4,4'-dibrombiphenyl (PBB-15)                     | 2.15     | 1.18     | 0.00     | 0.25     | 1.67     | 8.66     |
| 53-70-3   | dibenz[a,h]anthracene                            | 3.83     | 2.26     | 0.00     | 0.55     | 2.19     | 12.55    |
| 218-01-9  | chrysene                                         | 2.59     | 1.66     | 0.00     | 0.29     | 1.82     | 10.14    |
| 208-96-8  | acenaphthylene                                   | 1.55     | 1.13     | 0.00     | 0.21     | 1.22     | 6.40     |
| 56-55-3   | benz[a]anthracene                                | 2.74     | 1.68     | 0.00     | 0.37     | 1.82     | 10.12    |
| 92-52-4   | biphenyl                                         | 1.36     | 0.99     | 0.00     | 0.26     | 1.32     | 6.01     |
| 206-44-0  | fluoranthene                                     | 2.23     | 1.51     | 0.00     | 0.24     | 1.59     | 8.70     |
| 556-67-2  | octamethylcyclotetrasiloxane (D <sub>4</sub> )   | -0.47    | -0.08    | 0.00     | 0.51     | 2.35     | 4.47     |
| 107-51-7  | octamethyltrisiloxane (L <sub>3</sub> )          | -0.50    | -0.07    | 0.00     | 0.37     | 2.09     | 3.94     |
| 540-97-6  | dodecamethylcyclohexasiloxane (D <sub>6</sub> )  | -0.88    | -0.12    | 0.00     | 0.74     | 3.52     | 6.08     |
| 2043-47-2 | 1h,1h,2h,2h-perfluorohexan-1-ol<br>(4:2 FTOH)    | -0.67    | 0.18     | 0.62     | 0.31     | 1.35     | 2.52     |
| 541-02-6  | decamethylcyclopentasiloxane (D <sub>5</sub> )   | -0.70    | -0.10    | 0.00     | 0.50     | 2.93     | 5.24     |
| 865-86-1  | 1h,1h,2h,2h-perfluorododecan-1-ol<br>(10:2 FTOH) | -1.87    | 0.20     | 0.55     | 0.25     | 2.65     | 3.90     |

| <b>CAS-RN</b> | <b>Name</b>                                         | <b><i>E</i></b> | <b><i>S</i></b> | <b><i>A</i></b> | <b><i>B</i></b> | <b><i>V</i></b> | <b><i>L</i></b> |
|---------------|-----------------------------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 678-39-7      | 1h,1h,2h,2h-perfluorodecan-1-ol<br>(8:2 FTOH)       | -1.56           | 0.20            | 0.55            | 0.25            | 2.22            | 3.47            |
| 109-99-9      | tetrahydrofuran                                     | 0.29            | 0.52            | 0.00            | 0.48            | 0.62            | 2.64            |
| 67-68-5       | dimethylsulfoxide                                   | 0.52            | 1.74            | 0.00            | 0.88            | 0.61            | 3.46            |
| 122-39-4      | diphenylamine                                       | 1.70            | 1.28            | 0.15            | 0.53            | 1.42            | 6.80            |
| 117-84-0      | dioctyl phthalate                                   | 0.66            | 1.28            | 0.00            | 1.13            | 3.40            | 11.96           |
| 123-91-1      | dioxane                                             | 0.33            | 0.74            | 0.00            | 0.58            | 0.68            | 2.83            |
| 86-73-7       | fluorene                                            | 1.66            | 1.12            | 0.00            | 0.25            | 1.36            | 6.92            |
| 120-12-7      | anthracene                                          | 1.92            | 1.31            | 0.00            | 0.25            | 1.45            | 7.69            |
| 100-66-3      | anisole                                             | 0.71            | 0.77            | 0.00            | 0.31            | 0.92            | 3.81            |
| 90-13-1       | 1-chloronaphthalene                                 | 1.42            | 0.95            | 0.00            | 0.14            | 1.21            | 6.18            |
| 109-73-9      | n-butylamine                                        | 0.22            | 0.35            | 0.16            | 0.61            | 0.77            | 2.62            |
| 60-57-1       | dieldrin                                            | 2.09            | 2.05            | 0.03            | 0.63            | 2.01            | 8.49            |
| 72-20-8       | endrin                                              | 2.09            | 1.60            | 0.09            | 0.71            | 2.01            | 7.69            |
| 309-00-2      | aldrin                                              | 2.07            | 0.95            | 0.00            | 0.42            | 2.01            | 8.58            |
| 72-54-8       | p,p'-dichlorodiphenyldichloroethane<br>(p,p'-DDD)   | 1.76            | 1.71            | 0.02            | 0.22            | 2.10            | 9.86            |
| 32598-14-4    | 2,3,3',4,4'-pentachlorobiphenyl<br>(PCB-105)        | 2.04            | 1.59            | 0.00            | 0.11            | 1.94            | 9.59            |
| 33284-53-6    | 2,3,4,5-tetrachlorobiphenyl (PCB-61)                | 1.92            | 1.46            | 0.00            | 0.13            | 1.81            | 8.69            |
| 50-29-3       | p,p'-dichlorodiphenyltrichloroethane<br>(p,p'-DDT)  | 1.81            | 1.76            | 0.00            | 0.16            | 2.22            | 10.02           |
| 33979-03-2    | 2,2',4,4',6,6'-hexachlorobiphenyl<br>(PCB-155)      | 2.12            | 1.74            | 0.00            | 0.11            | 2.06            | 8.72            |
| 634-66-2      | 1,2,3,4-tetrachlorobenzene                          | 1.18            | 0.92            | 0.00            | 0.00            | 1.21            | 6.17            |
| 87-61-6       | 1,2,3-trichlorobenzene                              | 1.03            | 0.86            | 0.00            | 0.00            | 1.08            | 5.42            |
| 629-96-9      | 1-eicosanol                                         | 0.14            | 0.42            | 0.37            | 0.48            | 2.99            | 10.67           |
| 110-89-4      | piperidine                                          | 0.42            | 0.40            | 0.06            | 0.77            | 0.80            | 3.08            |
| 37680-73-2    | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)        | 2.04            | 1.61            | 0.00            | 0.13            | 1.94            | 8.87            |
| 7012-37-5     | 2,4,4'-trichlorobiphenyl (PCB-28)                   | 1.76            | 1.33            | 0.00            | 0.15            | 1.69            | 7.90            |
| 72-55-9       | p,p'-dichlorodiphenyldichloroethylene<br>(p,p'-DDE) | 1.80            | 1.40            | 0.06            | 0.14            | 2.05            | 9.73            |
| 78-82-0       | 2-cyanopropane                                      | 0.14            | 0.87            | 0.00            | 0.40            | 0.69            | 2.47            |

| CAS-RN     | Name                                                | <i>E</i> | <i>S</i> | <i>A</i> | <i>B</i> | <i>V</i> | <i>L</i> |
|------------|-----------------------------------------------------|----------|----------|----------|----------|----------|----------|
| 123-75-1   | pyrrolidine                                         | 0.41     | 0.95     | 0.24     | 0.42     | 0.66     | 2.88     |
| 118-74-1   | hexachlorobenzene (HCB)                             | 1.49     | 0.99     | 0.00     | 0.00     | 1.45     | 7.39     |
| 959-98-8   | $\alpha$ -endosulfan                                | 2.23     | 0.98     | 0.00     | 0.87     | 2.08     | 8.56     |
| 87-85-4    | hexamethylbenzene                                   | 0.95     | 0.72     | 0.00     | 0.28     | 1.56     | 6.56     |
| 75-52-5    | nitromethane                                        | 0.31     | 0.95     | 0.06     | 0.31     | 0.42     | 1.89     |
| 120-92-3   | cyclopentanone                                      | 0.37     | 0.86     | 0.00     | 0.52     | 0.72     | 3.22     |
| 2050-68-2  | 4,4'-dichlorobiphenyl (PCB-15)                      | 1.64     | 1.18     | 0.00     | 0.16     | 1.57     | 7.58     |
| 5103-71-9  | cis-chlordane                                       | 2.10     | 1.47     | 0.00     | 0.45     | 2.13     | 8.73     |
| 75-65-0    | 2-methylpropan-2-ol                                 | 0.18     | 0.30     | 0.31     | 0.60     | 0.73     | 1.96     |
| 112-92-5   | 1-octadecanol                                       | 0.15     | 0.42     | 0.37     | 0.48     | 2.70     | 9.66     |
| 83-32-9    | acenaphthene                                        | 1.60     | 1.05     | 0.00     | 0.22     | 1.26     | 6.47     |
| 58-89-9    | $\gamma$ -hexachlorocyclohexane ( $\gamma$ -HCH)    | 1.45     | 0.91     | 0.00     | 0.68     | 1.58     | 7.47     |
| 120-94-5   | n-methylpyrrolidine                                 | 0.30     | 0.98     | 0.00     | 0.40     | 0.80     | 3.13     |
| 124-11-8   | nonene                                              | 0.09     | 0.08     | 0.00     | 0.07     | 1.33     | 4.07     |
| 35694-08-7 | 2,2',3,3',4,4',5,5'-octachlorobiphenyl<br>(PCB-194) | 2.48     | 2.00     | 0.00     | 0.06     | 2.30     | 11.19    |
| 142-68-7   | tetrahydropyran                                     | 0.30     | 0.49     | 0.00     | 0.48     | 0.76     | 3.01     |
| 99-96-7    | 4-hydroxybenzoic acid                               | 0.93     | 0.90     | 0.81     | 0.56     | 0.99     | 4.87     |
| 628-73-9   | hexanonitrile                                       | 0.17     | 0.90     | 0.00     | 0.36     | 0.97     | 3.61     |
| 36653-82-4 | 1-hexadecanol                                       | 0.15     | 0.42     | 0.37     | 0.48     | 2.42     | 8.65     |
| 19670-15-6 | $\beta$ -endosulfan                                 | 2.23     | 0.94     | 0.00     | 0.98     | 2.08     | 9.28     |
| 68-12-2    | dimethylformamide                                   | 0.37     | 1.31     | 0.00     | 0.74     | 0.65     | 3.17     |
| 106-37-6   | 1,4-dibromobenzene                                  | 1.15     | 0.86     | 0.00     | 0.04     | 1.07     | 5.32     |
| 107-07-3   | 2-chloroethanol                                     | 0.42     | 0.77     | 0.39     | 0.50     | 0.57     | 2.44     |
| 103-29-7   | 1,2-diphenylethane                                  | 1.22     | 1.04     | 0.00     | 0.33     | 1.61     | 6.76     |
| 108-95-2   | phenol                                              | 0.81     | 0.89     | 0.60     | 0.30     | 0.78     | 3.77     |
| 74-89-5    | methylamine                                         | 0.25     | 0.35     | 0.16     | 0.58     | 0.35     | 1.30     |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                   | 1.77     | 1.33     | 0.00     | 0.15     | 1.69     | 7.86     |
| 628-55-7   | diisobutylether                                     | 0.00     | 0.19     | 0.00     | 0.45     | 1.30     | 3.49     |
| 142-96-1   | dibutylether                                        | 0.00     | 0.25     | 0.00     | 0.45     | 1.30     | 3.92     |
| 693-65-2   | dipentyl ether                                      | 0.00     | 0.25     | 0.00     | 0.45     | 1.58     | 4.88     |
| 76-44-8    | heptachlor                                          | 2.08     | 0.85     | 0.00     | 0.56     | 1.96     | 8.05     |
| 115-10-6   | dimethyl ether                                      | 0.00     | 0.27     | 0.00     | 0.41     | 0.45     | 1.29     |
| 106-46-7   | 1,4-dichlorobenzene                                 | 0.83     | 0.75     | 0.00     | 0.02     | 0.96     | 4.44     |

| CAS-RN     | Name                                           | <i>E</i> | <i>S</i> | <i>A</i> | <i>B</i> | <i>V</i> | <i>L</i> |
|------------|------------------------------------------------|----------|----------|----------|----------|----------|----------|
| 105-54-4   | ethyl butanoate                                | 0.07     | 0.58     | 0.00     | 0.45     | 1.03     | 3.27     |
| 1024-57-3  | heptachlor epoxide                             | 2.22     | 1.20     | 0.00     | 0.61     | 1.96     | 8.51     |
| 60-29-7    | diethylether                                   | 0.04     | 0.25     | 0.00     | 0.45     | 0.73     | 2.02     |
| 108-70-3   | 1,3,5-trichlorobenzene                         | 0.98     | 0.73     | 0.00     | 0.00     | 1.08     | 5.05     |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)         | 1.90     | 1.48     | 0.00     | 0.15     | 1.81     | 8.14     |
| 5103-74-2  | trans-chlordane                                | 2.06     | 1.25     | 0.00     | 0.53     | 2.13     | 9.11     |
| 65510-44-3 | 2,3,4,4',5-pentachlorobiphenyl<br>(PCB-123)    | 2.06     | 1.59     | 0.00     | 0.11     | 1.94     | 9.39     |
| 56-23-5    | tetrachloromethane                             | 0.46     | 0.38     | 0.00     | 0.00     | 0.74     | 2.82     |
| 127-18-4   | tetrachloroethene                              | 0.64     | 0.44     | 0.00     | 0.00     | 0.84     | 3.58     |
| 591-78-6   | hexan-2-one                                    | 0.14     | 0.68     | 0.00     | 0.51     | 0.97     | 3.29     |
| 67-64-1    | propanone                                      | 0.18     | 0.70     | 0.04     | 0.49     | 0.55     | 1.70     |
| 64-17-5    | ethanol                                        | 0.25     | 0.42     | 0.37     | 0.48     | 0.45     | 1.49     |
| 124-48-1   | dibromochloromethane                           | 0.78     | 0.68     | 0.12     | 0.10     | 0.72     | 3.30     |
| 71-41-0    | pentan-1-ol                                    | 0.22     | 0.42     | 0.37     | 0.48     | 0.87     | 3.11     |
| 108-38-3   | m-xylene                                       | 0.62     | 0.52     | 0.00     | 0.16     | 1.00     | 3.84     |
| 110-19-0   | isobutyl acetate                               | 0.05     | 0.57     | 0.00     | 0.47     | 1.03     | 3.16     |
| 541-73-1   | 1,3-dichlorobenzene                            | 0.85     | 0.73     | 0.00     | 0.02     | 0.96     | 4.41     |
| 31508-00-6 | 2',3,4,4',5'-pentachlorobiphenyl<br>(PCB-118)  | 2.06     | 1.59     | 0.00     | 0.11     | 1.94     | 9.40     |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138) | 2.18     | 1.74     | 0.00     | 0.11     | 2.06     | 9.77     |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl<br>(PCB-153) | 2.18     | 1.74     | 0.00     | 0.11     | 2.06     | 9.59     |
| 95-94-3    | 1,2,4,5-tetrachlorobenzene                     | 1.16     | 0.86     | 0.00     | 0.00     | 1.21     | 5.93     |
| 106-42-3   | p-xylene                                       | 0.61     | 0.52     | 0.00     | 0.16     | 1.00     | 3.84     |
| 98-82-8    | isopropylbenzene                               | 0.60     | 0.49     | 0.00     | 0.16     | 1.14     | 4.08     |
| 123-38-6   | propanal                                       | 0.20     | 0.65     | 0.00     | 0.45     | 0.55     | 1.82     |
| 198-55-0   | perylene                                       | 3.26     | 1.76     | 0.00     | 0.40     | 1.95     | 12.05    |
| 74-84-0    | ethane                                         | 0.00     | 0.00     | 0.00     | 0.00     | 0.39     | 0.49     |

**Table S2. Experimental  $\log K_{OA}$  values at different temperatures in the training and validation sets.**

| CAS-RN | Name | <i>T/K</i> | $\log K_{OA}(\text{Exp})$ |
|--------|------|------------|---------------------------|
|--------|------|------------|---------------------------|

| CAS-RN      | Name                              | T/K    | logK <sub>OA</sub> (Exp) |
|-------------|-----------------------------------|--------|--------------------------|
| 68-12-2     | dimethylformamide                 | 298.15 | 4.38                     |
| 75-03-6     | iodoethane                        | 298.15 | 2.59                     |
| 75-05-8     | acetonitrile                      | 298.15 | 2.31                     |
| 75-09-2     | dichloromethane                   | 298.15 | 2.27                     |
| 79-01-6     | trichloroethene                   | 298.15 | 2.99                     |
| 85-01-8     | phenanthrene                      | 313.15 | 6.93                     |
| 85-01-8     | phenanthrene                      | 303.15 | 7.42                     |
| 85-01-8     | phenanthrene                      | 298.15 | 7.57                     |
| 85-01-8     | phenanthrene                      | 293.15 | 7.9                      |
| 85-01-8     | phenanthrene                      | 283.15 | 8.27                     |
| 85-01-8     | phenanthrene                      | 273.15 | 8.81                     |
| 7440-01-9   | neon                              | 298.15 | -1.57                    |
| 92-86-4     | 4,4'-dibromobiphenyl (PBB-15)     | 298.15 | 8.5                      |
| 92-86-4     | 4,4'-dibromobiphenyl (PBB-15)     | 283.15 | 9.05                     |
| 10024-97-2  | nitrous oxide                     | 298.15 | 0.33                     |
| 100-41-4    | ethylbenzene                      | 298.15 | 3.72                     |
| 100-47-0    | benzonitrile                      | 298.15 | 4.46                     |
| 100-66-3    | anisole                           | 298.15 | 4.01                     |
| 1024-57-3   | heptachlor epoxide                | 298.15 | 8.59                     |
| 103-29-7    | 1,2-diphenylethane                | 298.15 | 6.45                     |
| 103-30-0    | trans-stilbene                    | 298.15 | 7.48                     |
| 103426-93-3 | 1,2,3,4,5,8-hexachloronaphthalene | 323.15 | 9.03                     |
| 103426-93-3 | 1,2,3,4,5,8-hexachloronaphthalene | 313.15 | 9.56                     |
| 103426-93-3 | 1,2,3,4,5,8-hexachloronaphthalene | 303.15 | 10.21                    |
| 103426-93-3 | 1,2,3,4,5,8-hexachloronaphthalene | 298.15 | 10.37                    |
| 103426-93-3 | 1,2,3,4,5,8-hexachloronaphthalene | 293.15 | 10.62                    |
| 103426-94-4 | 1,2,3,5,7,8-hexachloronaphthalene | 323.15 | 8.57                     |
| 103426-94-4 | 1,2,3,5,7,8-hexachloronaphthalene | 313.15 | 8.99                     |
| 103426-94-4 | 1,2,3,5,7,8-hexachloronaphthalene | 303.15 | 9.62                     |
| 103426-94-4 | 1,2,3,5,7,8-hexachloronaphthalene | 298.15 | 9.83                     |
| 103426-94-4 | 1,2,3,5,7,8-hexachloronaphthalene | 293.15 | 10.09                    |
| 103426-96-6 | 1,2,3,4,6,7-hexachloronaphthalene | 323.15 | 8.42                     |
| 103426-96-6 | 1,2,3,4,6,7-hexachloronaphthalene | 313.15 | 8.84                     |
| 103426-96-6 | 1,2,3,4,6,7-hexachloronaphthalene | 303.15 | 9.46                     |
| 103426-96-6 | 1,2,3,4,6,7-hexachloronaphthalene | 298.15 | 9.7                      |
| 103426-96-6 | 1,2,3,4,6,7-hexachloronaphthalene | 293.15 | 10.01                    |
| 103426-96-6 | 1,2,3,4,6,7-hexachloronaphthalene | 283.15 | 10.58                    |
| 103426-97-7 | 1,2,3,5,6,7-hexachloronaphthalene | 298.15 | 9.58                     |
| 103-65-1    | propylbenzene                     | 298.15 | 4.09                     |
| 105-37-3    | ethyl propanoate                  | 298.15 | 3.15                     |
| 105-54-4    | ethyl butanoate                   | 298.15 | 3.56                     |
| 106-37-6    | 1,4-dibromobenzene                | 298.15 | 5.21                     |
| 106-42-3    | p-xylene                          | 298.15 | 3.79                     |

| CAS-RN   | Name                                    | T/K    | logK <sub>OA</sub> (Exp) |
|----------|-----------------------------------------|--------|--------------------------|
| 106-46-7 | 1,4-dichlorobenzene                     | 298.15 | 4.46                     |
| 106-97-8 | butane                                  | 298.15 | 1.53                     |
| 107-06-2 | 1,2-dichloroethane                      | 298.15 | 2.78                     |
| 107-07-3 | 2-chloroethanol                         | 298.15 | 4.3                      |
| 107-12-0 | propionitrile                           | 298.15 | 2.69                     |
| 107-31-3 | methyl formate                          | 298.15 | 1.75                     |
| 107-46-0 | hexamethyldisiloxane (L <sub>2</sub> )  | 298.15 | 2.98                     |
| 107-51-7 | octamethyltrisiloxane (L <sub>3</sub> ) | 298.15 | 3.77                     |
| 107-87-9 | pentan-2-one                            | 298.15 | 3.19                     |
| 108-03-2 | nitropropane                            | 298.15 | 3.25                     |
| 108-20-3 | diisopropylether                        | 298.15 | 2.66                     |
| 108-21-4 | isopropyl acetate                       | 298.15 | 2.93                     |
| 108-38-3 | m-xylene                                | 298.15 | 3.78                     |
| 108-70-3 | 1,3,5-trichlorobenzene                  | 298.15 | 4.85                     |
| 108-87-2 | methylcyclohexane                       | 298.15 | 3.05                     |
| 108-88-3 | toluene                                 | 298.15 | 3.31                     |
| 108-90-7 | chlorobenzene                           | 298.15 | 3.31                     |
| 108-93-0 | cyclohexanol                            | 298.15 | 5.18                     |
| 108-95-2 | phenol                                  | 298.15 | 5.68                     |
| 109-60-4 | propyl acetate                          | 298.15 | 3.17                     |
| 109-66-0 | pentane                                 | 298.15 | 1.95                     |
| 109-67-1 | 1-pentene                               | 298.15 | 1.93                     |
| 109-69-3 | 1-chlorobutane                          | 298.15 | 2.72                     |
| 109-73-9 | n-butylamine                            | 298.15 | 3.61                     |
| 109-74-0 | butanonitrile                           | 298.15 | 3.12                     |
| 109-94-4 | ethyl formate                           | 298.15 | 2.19                     |
| 109-99-9 | tetrahydrofuran                         | 298.15 | 2.86                     |
| 110-19-0 | isobutyl acetate                        | 298.15 | 3.45                     |
| 110-43-0 | heptan-2-one                            | 298.15 | 4.15                     |
| 110-54-3 | hexane                                  | 298.15 | 2.44                     |
| 110-59-8 | pentanonitrile                          | 298.15 | 3.6                      |
| 110-74-7 | propyl formate                          | 298.15 | 2.66                     |
| 110-82-7 | cyclohexane                             | 298.15 | 2.71                     |
| 110-83-8 | cyclohexene                             | 298.15 | 2.83                     |
| 110-89-4 | piperidine                              | 298.15 | 4.04                     |
| 111-27-3 | hexan-1-ol                              | 298.15 | 5.18                     |
| 111-43-3 | dipropylether                           | 298.15 | 2.97                     |
| 111-65-9 | octane                                  | 298.15 | 3.3                      |
| 111-66-0 | 1-octene                                | 298.15 | 3.35                     |
| 111-87-5 | 1-octanol                               | 298.15 | 6.03                     |
| 112-92-5 | 1-octadecanol                           | 298.15 | 10.93                    |
| 115-10-6 | dimethyl ether                          | 298.15 | 1.37                     |
| 117-84-0 | dioctyl phthalate                       | 298.15 | 11.18                    |

| CAS-RN      | Name                                      | T/K    | logK <sub>OA</sub> (Exp) |
|-------------|-------------------------------------------|--------|--------------------------|
| 118-74-1    | hexachlorobenzene (HCB)                   | 298.15 | 6.9                      |
| 118-74-1    | hexachlorobenzene (HCB)                   | 293.15 | 7.56                     |
| 118-74-1    | hexachlorobenzene (HCB)                   | 288.15 | 7.7                      |
| 118-74-1    | hexachlorobenzene (HCB)                   | 283.15 | 7.89                     |
| 118-74-1    | hexachlorobenzene (HCB)                   | 278.15 | 8.1                      |
| 120-12-7    | anthracene                                | 298.15 | 7.55                     |
| 120-82-1    | 1,2,4-trichlorobenzene                    | 298.15 | 4.95                     |
| 120-92-3    | cyclopentanone                            | 298.15 | 3.67                     |
| 120-94-5    | n-methylpyrrolidine                       | 298.15 | 3.64                     |
| 122-39-4    | diphenylamine                             | 298.15 | 7.64                     |
| 123-38-6    | propanal                                  | 298.15 | 3.02                     |
| 123-51-3    | 3-methylbutan-1-ol                        | 298.15 | 4.52                     |
| 123-72-8    | butanal                                   | 298.15 | 3.39                     |
| 123-75-1    | pyrrolidine                               | 298.15 | 4.07                     |
| 123-86-4    | butyl acetate                             | 298.15 | 3.65                     |
| 123-91-1    | dioxane                                   | 298.15 | 3.17                     |
| 123-92-2    | isopentyl acetate                         | 298.15 | 3.94                     |
| 124-11-8    | nonene                                    | 298.15 | 3.83                     |
| 124-13-0    | octanal                                   | 298.15 | 5.36                     |
| 124-38-9    | carbon dioxide                            | 298.15 | 0.16                     |
| 124-40-3    | dimethylamine                             | 298.15 | 2                        |
| 124-48-1    | dibromochloromethane                      | 298.15 | 3.59                     |
| 127-18-4    | tetrachloroethene                         | 298.15 | 3.48                     |
| 127-19-5    | dimethylacetamide                         | 298.15 | 5.33                     |
| 129-00-0    | pyrene                                    | 313.15 | 8.12                     |
| 129-00-0    | pyrene                                    | 303.15 | 8.55                     |
| 129-00-0    | pyrene                                    | 298.15 | 8.8                      |
| 129-00-0    | pyrene                                    | 293.15 | 9.16                     |
| 129-00-0    | pyrene                                    | 283.15 | 9.53                     |
| 129-00-0    | pyrene                                    | 273.15 | 9.97                     |
| 13029-08-8  | 2,2'-dichlorobiphenyl (PCB-4)             | 298.15 | 7.18                     |
| 131-11-3    | dimethyl phthalate                        | 298.15 | 7                        |
| 1333-74-0   | hydrogen                                  | 298.15 | -1.29                    |
| 141-62-8    | decamethyltetrasiloxane (L <sub>4</sub> ) | 298.15 | 4.66                     |
| 141-78-6    | ethyl acetate                             | 298.15 | 2.7                      |
| 142-68-7    | tetrahydropyran                           | 298.15 | 3.22                     |
| 142-82-5    | heptane                                   | 298.15 | 2.95                     |
| 142-84-7    | dipropylamine                             | 298.15 | 3.59                     |
| 142-92-7    | hexyl acetate                             | 298.15 | 4.58                     |
| 142-96-1    | dibutylether                              | 298.15 | 3.89                     |
| 149864-79-9 | 1,2,6,7-tetrachloronaphthalene            | 298.15 | 8.34                     |
| 149864-80-2 | 1,2,5,8-tetrachloronaphthalene            | 323.15 | 7.36                     |
| 149864-80-2 | 1,2,5,8-tetrachloronaphthalene            | 313.15 | 7.68                     |

| CAS-RN      | Name                             | T/K    | logK <sub>OA</sub> (Exp) |
|-------------|----------------------------------|--------|--------------------------|
| 149864-80-2 | 1,2,5,8-tetrachloronaphthalene   | 303.15 | 8.14                     |
| 149864-80-2 | 1,2,5,8-tetrachloronaphthalene   | 298.15 | 8.4                      |
| 149864-80-2 | 1,2,5,8-tetrachloronaphthalene   | 293.15 | 8.7                      |
| 149864-80-2 | 1,2,5,8-tetrachloronaphthalene   | 283.15 | 9.14                     |
| 149864-82-4 | 1,2,7,8-tetrachloronaphthalene   | 298.15 | 8.65                     |
| 150224-15-0 | 1,3,6,8-tetrachloronaphthalene   | 298.15 | 8.28                     |
| 150224-16-1 | 1,2,3,6,7-pentachloronaphthalene | 298.15 | 9.15                     |
| 150224-18-3 | 1,2,3,5,6-pentachloronaphthalene | 323.15 | 7.91                     |
| 150224-18-3 | 1,2,3,5,6-pentachloronaphthalene | 313.15 | 8.3                      |
| 150224-18-3 | 1,2,3,5,6-pentachloronaphthalene | 303.15 | 8.8                      |
| 150224-18-3 | 1,2,3,5,6-pentachloronaphthalene | 298.15 | 9.15                     |
| 150224-18-3 | 1,2,3,5,6-pentachloronaphthalene | 293.15 | 9.48                     |
| 150224-18-3 | 1,2,3,5,6-pentachloronaphthalene | 283.15 | 10.08                    |
| 150224-19-4 | 1,2,4,5,7-pentachloronaphthalene | 323.15 | 7.76                     |
| 150224-19-4 | 1,2,4,5,7-pentachloronaphthalene | 313.15 | 8.1                      |
| 150224-19-4 | 1,2,4,5,7-pentachloronaphthalene | 303.15 | 8.59                     |
| 150224-19-4 | 1,2,4,5,7-pentachloronaphthalene | 298.15 | 8.86                     |
| 150224-19-4 | 1,2,4,5,7-pentachloronaphthalene | 293.15 | 9.17                     |
| 150224-19-4 | 1,2,4,5,7-pentachloronaphthalene | 283.15 | 9.63                     |
| 150224-21-8 | 1,2,4,7,8-pentachloronaphthalene | 323.15 | 7.93                     |
| 150224-21-8 | 1,2,4,7,8-pentachloronaphthalene | 313.15 | 8.27                     |
| 150224-21-8 | 1,2,4,7,8-pentachloronaphthalene | 303.15 | 8.83                     |
| 150224-21-8 | 1,2,4,7,8-pentachloronaphthalene | 298.15 | 9.06                     |
| 150224-21-8 | 1,2,4,7,8-pentachloronaphthalene | 293.15 | 9.42                     |
| 150224-21-8 | 1,2,4,7,8-pentachloronaphthalene | 283.15 | 9.81                     |
| 150224-22-9 | 1,2,4,6,8-pentachloronaphthalene | 323.15 | 7.67                     |
| 150224-22-9 | 1,2,4,6,8-pentachloronaphthalene | 313.15 | 8                        |
| 150224-22-9 | 1,2,4,6,8-pentachloronaphthalene | 303.15 | 8.52                     |
| 150224-22-9 | 1,2,4,6,8-pentachloronaphthalene | 298.15 | 8.78                     |
| 150224-22-9 | 1,2,4,6,8-pentachloronaphthalene | 293.15 | 9.11                     |
| 150224-22-9 | 1,2,4,6,8-pentachloronaphthalene | 283.15 | 9.54                     |
| 150224-23-0 | 1,2,3,6,8-pentachloronaphthalene | 298.15 | 9.25                     |
| 150224-24-1 | 1,2,3,5,8-pentachloronaphthalene | 323.15 | 7.96                     |
| 150224-24-1 | 1,2,3,5,8-pentachloronaphthalene | 313.15 | 8.34                     |
| 150224-24-1 | 1,2,3,5,8-pentachloronaphthalene | 303.15 | 8.86                     |
| 150224-24-1 | 1,2,3,5,8-pentachloronaphthalene | 298.15 | 9.13                     |
| 150224-24-1 | 1,2,3,5,8-pentachloronaphthalene | 293.15 | 9.44                     |
| 150224-24-1 | 1,2,3,5,8-pentachloronaphthalene | 283.15 | 9.97                     |
| 150224-25-2 | 1,2,4,5,8-pentachloronaphthalene | 323.15 | 7.98                     |
| 150224-25-2 | 1,2,4,5,8-pentachloronaphthalene | 313.15 | 8.35                     |
| 150224-25-2 | 1,2,4,5,8-pentachloronaphthalene | 303.15 | 8.89                     |
| 150224-25-2 | 1,2,4,5,8-pentachloronaphthalene | 298.15 | 9.18                     |
| 150224-25-2 | 1,2,4,5,8-pentachloronaphthalene | 293.15 | 9.49                     |

| CAS-RN     | Name                                                  | T/K    | logK <sub>OA</sub> (Exp) |
|------------|-------------------------------------------------------|--------|--------------------------|
| 156-59-2   | cis-1,2-dichloroethene                                | 298.15 | 2.56                     |
| 15862-07-4 | 2,4,5-trichlorobiphenyl (PCB-29)                      | 298.15 | 8                        |
| 15862-07-4 | 2,4,5-trichlorobiphenyl (PCB-29)                      | 293.15 | 8.03                     |
| 15862-07-4 | 2,4,5-trichlorobiphenyl (PCB-29)                      | 283.15 | 8.51                     |
| 15862-07-4 | 2,4,5-trichlorobiphenyl (PCB-29)                      | 273.15 | 8.97                     |
| 15862-07-4 | 2,4,5-trichlorobiphenyl (PCB-29)                      | 263.15 | 9.5                      |
| 1634-04-4  | t-butyl methyl ether                                  | 298.15 | 2.58                     |
| 16605-91-7 | 2,3-dichlorobiphenyl (PCB-5)                          | 293.15 | 7.59                     |
| 16605-91-7 | 2,3-dichlorobiphenyl (PCB-5)                          | 273.15 | 8.55                     |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                     | 316.15 | 7.13                     |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                     | 308.15 | 7.48                     |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                     | 298.15 | 7.92                     |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                     | 297.15 | 7.98                     |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                     | 293.15 | 8.4                      |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                     | 286.15 | 8.52                     |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                     | 283.15 | 8.68                     |
| 16606-02-3 | 2,4',5-trichlorobiphenyl (PCB-31)                     | 273.15 | 9.43                     |
| 1746-01-6  | 2,3,7,8-tetrachlorodibenzo-p-dioxin<br>(2,3,7,8-TCDD) | 323.15 | 8.78                     |
| 1746-01-6  | 2,3,7,8-tetrachlorodibenzo-p-dioxin<br>(2,3,7,8-TCDD) | 313.15 | 9.28                     |
| 1746-01-6  | 2,3,7,8-tetrachlorodibenzo-p-dioxin<br>(2,3,7,8-TCDD) | 298.15 | 10.05                    |
| 1746-01-6  | 2,3,7,8-tetrachlorodibenzo-p-dioxin<br>(2,3,7,8-TCDD) | 293.15 | 10.32                    |
| 1825-30-5  | 1,5-dichloronaphthalene                               | 298.15 | 6.65                     |
| 1825-31-6  | 1,4-dichloronaphthalene                               | 323.15 | 6.13                     |
| 1825-31-6  | 1,4-dichloronaphthalene                               | 313.15 | 6.38                     |
| 1825-31-6  | 1,4-dichloronaphthalene                               | 303.15 | 6.72                     |
| 1825-31-6  | 1,4-dichloronaphthalene                               | 298.15 | 6.93                     |
| 1825-31-6  | 1,4-dichloronaphthalene                               | 293.15 | 7.13                     |
| 1825-31-6  | 1,4-dichloronaphthalene                               | 283.15 | 7.52                     |
| 191-24-2   | benzo[g,h,i]perylene                                  | 298.15 | 12.55                    |
| 193-39-5   | indeno[1,2,3-cd]pyrene                                | 298.15 | 12.43                    |
| 19670-15-6 | β-endosulfan                                          | 298.15 | 9.53                     |
| 198-55-0   | perylene                                              | 298.15 | 11.7                     |
| 20020-02-4 | 1,2,3,4-tetrachloronaphthalene                        | 298.15 | 8.3                      |
| 2043-47-2  | 1h,1h,2h,2h-perfluorohexan-1-ol<br>(4:2 FTOH)         | 298.15 | 4.8                      |
| 2050-67-1  | 3,3'-dichlorobiphenyl (PCB-11)                        | 293.15 | 7.9                      |
| 2050-67-1  | 3,3'-dichlorobiphenyl (PCB-11)                        | 273.15 | 8.86                     |
| 2050-68-2  | 4,4'-dichlorobiphenyl (PCB-15)                        | 298.15 | 7.68                     |
| 2050-68-2  | 4,4'-dichlorobiphenyl (PCB-15)                        | 293.15 | 7.88                     |

| CAS-RN    | Name                                             | T/K    | logK <sub>OA</sub> (Exp) |
|-----------|--------------------------------------------------|--------|--------------------------|
| 2050-68-2 | 4,4'-dichlorobiphenyl (PCB-15)                   | 283.15 | 8.35                     |
| 2050-68-2 | 4,4'-dichlorobiphenyl (PCB-15)                   | 273.15 | 8.83                     |
| 2050-68-2 | 4,4'-dichlorobiphenyl (PCB-15)                   | 263.15 | 9.36                     |
| 2050-69-3 | 1,2-dichloronaphthalene                          | 298.15 | 6.83                     |
| 2051-24-3 | decachlorobiphenyl (PCB-209)                     | 293.15 | 11.96                    |
| 2051-24-3 | decachlorobiphenyl (PCB-209)                     | 273.15 | 13.36                    |
| 2051-60-7 | 2-chlorobiphenyl                                 | 293.15 | 6.65                     |
| 2051-60-7 | 2-chlorobiphenyl                                 | 273.15 | 7.54                     |
| 2051-61-8 | 3-chlorobiphenyl                                 | 303.15 | 6.63                     |
| 2051-61-8 | 3-chlorobiphenyl                                 | 298.15 | 6.82                     |
| 2051-61-8 | 3-chlorobiphenyl                                 | 293.15 | 7                        |
| 2051-61-8 | 3-chlorobiphenyl                                 | 283.15 | 7.43                     |
| 2051-61-8 | 3-chlorobiphenyl                                 | 273.15 | 7.9                      |
| 2051-61-8 | 3-chlorobiphenyl                                 | 263.15 | 8.37                     |
| 2051-62-9 | 4-chlorobiphenyl (PCB-3)                         | 303.15 | 6.62                     |
| 2051-62-9 | 4-chlorobiphenyl (PCB-3)                         | 298.15 | 6.8                      |
| 2051-62-9 | 4-chlorobiphenyl (PCB-3)                         | 293.15 | 7.01                     |
| 2051-62-9 | 4-chlorobiphenyl (PCB-3)                         | 283.15 | 7.43                     |
| 2051-62-9 | 4-chlorobiphenyl (PCB-3)                         | 273.15 | 7.91                     |
| 2051-62-9 | 4-chlorobiphenyl (PCB-3)                         | 263.15 | 8.34                     |
| 205-99-2  | benzo[b]fluoranthene                             | 298.15 | 11.34                    |
| 206-44-0  | fluoranthene                                     | 313.15 | 8.16                     |
| 206-44-0  | fluoranthene                                     | 303.15 | 8.65                     |
| 206-44-0  | fluoranthene                                     | 298.15 | 8.88                     |
| 206-44-0  | fluoranthene                                     | 293.15 | 9.12                     |
| 207-08-9  | benzo[k]fluoranthene                             | 298.15 | 11.37                    |
| 208-96-8  | acenaphthylene                                   | 298.15 | 6.34                     |
| 2136-99-4 | 2,2',3,3',5,5',6,6'-octachlorobiphenyl (PCB-202) | 293.15 | 10.38                    |
| 2136-99-4 | 2,2',3,3',5,5',6,6'-octachlorobiphenyl (PCB-202) | 273.15 | 11.57                    |
| 218-01-9  | chrysene                                         | 298.15 | 10.3                     |
| 2198-77-8 | 2,7-dichloronaphthalene                          | 298.15 | 6.7                      |
| 2234-13-1 | 1,2,3,4,5,6,7,8-octachloronaphthalene            | 298.15 | 11.05                    |
| 2437-54-9 | 1,4,6-trichloronaphthalene                       | 323.15 | 6.36                     |
| 2437-54-9 | 1,4,6-trichloronaphthalene                       | 313.15 | 6.64                     |
| 2437-54-9 | 1,4,6-trichloronaphthalene                       | 303.15 | 7.03                     |
| 2437-54-9 | 1,4,6-trichloronaphthalene                       | 298.15 | 7.27                     |
| 2437-54-9 | 1,4,6-trichloronaphthalene                       | 293.15 | 7.55                     |
| 2437-54-9 | 1,4,6-trichloronaphthalene                       | 283.15 | 7.91                     |
| 2437-55-0 | 1,4,5-trichloronaphthalene                       | 323.15 | 6.59                     |
| 2437-55-0 | 1,4,5-trichloronaphthalene                       | 313.15 | 6.88                     |
| 2437-55-0 | 1,4,5-trichloronaphthalene                       | 303.15 | 7.29                     |

| CAS-RN     | Name                                             | T/K    | logK <sub>OA</sub> (Exp) |
|------------|--------------------------------------------------|--------|--------------------------|
| 2437-55-0  | 1,4,5-trichloronaphthalene                       | 298.15 | 7.56                     |
| 2437-55-0  | 1,4,5-trichloronaphthalene                       | 293.15 | 7.85                     |
| 2437-55-0  | 1,4,5-trichloronaphthalene                       | 283.15 | 8.24                     |
| 2437-79-8  | 2,2',4,4'-tetrachlorobiphenyl (PCB-47)           | 293.15 | 8.56                     |
| 2437-79-8  | 2,2',4,4'-tetrachlorobiphenyl (PCB-47)           | 273.15 | 9.55                     |
| 2551-62-4  | sulfur hexafluoride                              | 298.15 | -0.3                     |
| 25569-80-6 | 2,3'-dichlorobiphenyl (PCB-6)                    | 293.15 | 7.55                     |
| 25569-80-6 | 2,3'-dichlorobiphenyl (PCB-6)                    | 273.15 | 8.51                     |
| 2974-92-7  | 3,4-dichlorobiphenyl (PCB-12)                    | 293.15 | 7.8                      |
| 2974-92-7  | 3,4-dichlorobiphenyl (PCB-12)                    | 273.15 | 8.71                     |
| 309-00-2   | aldrin                                           | 298.15 | 8.08                     |
| 309-00-2   | aldrin                                           | 293.15 | 8.3                      |
| 309-00-2   | aldrin                                           | 288.15 | 8.54                     |
| 309-00-2   | aldrin                                           | 283.15 | 8.68                     |
| 309-00-2   | aldrin                                           | 278.15 | 9.01                     |
| 31508-00-6 | 2',3,4,4',5'-pentachlorobiphenyl (PCB-118)       | 303.15 | 9.57                     |
| 31508-00-6 | 2',3,4,4',5'-pentachlorobiphenyl (PCB-118)       | 298.15 | 9.82                     |
| 31508-00-6 | 2',3,4,4',5'-pentachlorobiphenyl (PCB-118)       | 293.15 | 10.08                    |
| 31508-00-6 | 2',3,4,4',5'-pentachlorobiphenyl (PCB-118)       | 283.15 | 10.64                    |
| 31508-00-6 | 2',3,4,4',5'-pentachlorobiphenyl (PCB-118)       | 273.15 | 11.23                    |
| 31508-00-6 | 2',3,4,4',5'-pentachlorobiphenyl (PCB-118)       | 263.15 | 11.93                    |
| 31604-28-1 | 1,3,5,8-tetrachloronaphthalene                   | 298.15 | 8.28                     |
| 319-84-6   | $\alpha$ -hexachlorocyclohexane ( $\alpha$ -HCH) | 298.15 | 7.61                     |
| 319-84-6   | $\alpha$ -hexachlorocyclohexane ( $\alpha$ -HCH) | 293.15 | 7.81                     |
| 319-84-6   | $\alpha$ -hexachlorocyclohexane ( $\alpha$ -HCH) | 288.15 | 7.97                     |
| 319-84-6   | $\alpha$ -hexachlorocyclohexane ( $\alpha$ -HCH) | 283.15 | 8.18                     |
| 319-84-6   | $\alpha$ -hexachlorocyclohexane ( $\alpha$ -HCH) | 278.15 | 8.41                     |
| 319-85-7   | $\beta$ -hexachlorocyclohexane ( $\beta$ -HCH)   | 308.15 | 8.37                     |
| 319-85-7   | $\beta$ -hexachlorocyclohexane ( $\beta$ -HCH)   | 298.15 | 8.88                     |
| 319-85-7   | $\beta$ -hexachlorocyclohexane ( $\beta$ -HCH)   | 293.15 | 8.99                     |
| 319-85-7   | $\beta$ -hexachlorocyclohexane ( $\beta$ -HCH)   | 288.15 | 9.44                     |
| 319-85-7   | $\beta$ -hexachlorocyclohexane ( $\beta$ -HCH)   | 278.15 | 10.07                    |
| 319-86-8   | $\delta$ -hexachlorocyclohexane ( $\delta$ -HCH) | 308.15 | 8.44                     |
| 319-86-8   | $\delta$ -hexachlorocyclohexane ( $\delta$ -HCH) | 298.15 | 8.84                     |
| 319-86-8   | $\delta$ -hexachlorocyclohexane ( $\delta$ -HCH) | 293.15 | 8.93                     |
| 319-86-8   | $\delta$ -hexachlorocyclohexane ( $\delta$ -HCH) | 288.15 | 9.46                     |
| 319-86-8   | $\delta$ -hexachlorocyclohexane ( $\delta$ -HCH) | 278.15 | 10.04                    |

| CAS-RN     | Name                                             | T/K    | logK <sub>OA</sub> (Exp) |
|------------|--------------------------------------------------|--------|--------------------------|
| 32598-10-0 | 2,3',4,4'-tetrachlorobiphenyl (PCB-66)           | 303.15 | 8.82                     |
| 32598-10-0 | 2,3',4,4'-tetrachlorobiphenyl (PCB-66)           | 298.15 | 9.02                     |
| 32598-10-0 | 2,3',4,4'-tetrachlorobiphenyl (PCB-66)           | 293.15 | 9.22                     |
| 32598-10-0 | 2,3',4,4'-tetrachlorobiphenyl (PCB-66)           | 283.15 | 9.65                     |
| 32598-10-0 | 2,3',4,4'-tetrachlorobiphenyl (PCB-66)           | 273.15 | 10.21                    |
| 32598-11-1 | 2,3',4',5-tetrachlorobiphenyl (PCB-70)           | 293.15 | 9.22                     |
| 32598-11-1 | 2,3',4',5-tetrachlorobiphenyl (PCB-70)           | 273.15 | 10.29                    |
| 32598-13-3 | 3,3',4,4'-tetrachlorobiphenyl (PCB-77)           | 303.15 | 9.47                     |
| 32598-13-3 | 3,3',4,4'-tetrachlorobiphenyl (PCB-77)           | 298.15 | 9.7                      |
| 32598-13-3 | 3,3',4,4'-tetrachlorobiphenyl (PCB-77)           | 293.15 | 9.96                     |
| 32598-13-3 | 3,3',4,4'-tetrachlorobiphenyl (PCB-77)           | 283.15 | 10.36                    |
| 32598-13-3 | 3,3',4,4'-tetrachlorobiphenyl (PCB-77)           | 273.15 | 10.88                    |
| 32598-14-4 | 2,3,3',4,4'-pentachlorobiphenyl (PCB-105)        | 303.15 | 9.77                     |
| 32598-14-4 | 2,3,3',4,4'-pentachlorobiphenyl (PCB-105)        | 298.15 | 10                       |
| 32598-14-4 | 2,3,3',4,4'-pentachlorobiphenyl (PCB-105)        | 293.15 | 10.27                    |
| 32598-14-4 | 2,3,3',4,4'-pentachlorobiphenyl (PCB-105)        | 283.15 | 10.84                    |
| 32598-14-4 | 2,3,3',4,4'-pentachlorobiphenyl (PCB-105)        | 273.15 | 11.43                    |
| 32598-14-4 | 2,3,3',4,4'-pentachlorobiphenyl (PCB-105)        | 263.15 | 12.12                    |
| 32690-93-0 | 2,4,4',5-tetrachlorobiphenyl (PCB-74)            | 293.15 | 9.14                     |
| 32690-93-0 | 2,4,4',5-tetrachlorobiphenyl (PCB-74)            | 273.15 | 10.25                    |
| 32774-16-6 | 3,4,5,3',4',5'-hexachlorobiphenyl (PCB-169)      | 293.15 | 11.32                    |
| 32774-16-6 | 3,4,5,3',4',5'-hexachlorobiphenyl (PCB-169)      | 273.15 | 12.51                    |
| 33091-17-7 | 2,2',3,3',4,4',6,6'-octachlorobiphenyl (PCB-197) | 293.15 | 10.52                    |
| 33091-17-7 | 2,2',3,3',4,4',6,6'-octachlorobiphenyl (PCB-197) | 273.15 | 11.74                    |
| 33284-50-3 | 2,4-dichlorobiphenyl (PCB-7)                     | 293.15 | 7.39                     |
| 33284-50-3 | 2,4-dichlorobiphenyl (PCB-7)                     | 273.15 | 8.37                     |
| 33284-53-6 | 2,3,4,5-tetrachlorobiphenyl (PCB-61)             | 298.15 | 8.74                     |
| 33284-53-6 | 2,3,4,5-tetrachlorobiphenyl (PCB-61)             | 293.15 | 8.9                      |
| 33284-53-6 | 2,3,4,5-tetrachlorobiphenyl (PCB-61)             | 283.15 | 9.4                      |
| 33284-53-6 | 2,3,4,5-tetrachlorobiphenyl (PCB-61)             | 273.15 | 9.8                      |
| 33284-53-6 | 2,3,4,5-tetrachlorobiphenyl (PCB-61)             | 263.15 | 10.27                    |
| 33979-03-2 | 2,2',4,4',6,6'-hexachlorobiphenyl (PCB-155)      | 298.15 | 8.99                     |

| CAS-RN     | Name                                        | T/K    | logK <sub>OA</sub> (Exp) |
|------------|---------------------------------------------|--------|--------------------------|
| 33979-03-2 | 2,2',4,4',6,6'-hexachlorobiphenyl (PCB-155) | 293.15 | 9.16                     |
| 33979-03-2 | 2,2',4,4',6,6'-hexachlorobiphenyl (PCB-155) | 283.15 | 9.64                     |
| 33979-03-2 | 2,2',4,4',6,6'-hexachlorobiphenyl (PCB-155) | 273.15 | 9.97                     |
| 33979-03-2 | 2,2',4,4',6,6'-hexachlorobiphenyl (PCB-155) | 263.15 | 10.49                    |
| 3432-57-3  | 1,4,5,8-tetrachloronaphthalene              | 323.15 | 7.4                      |
| 3432-57-3  | 1,4,5,8-tetrachloronaphthalene              | 313.15 | 7.72                     |
| 3432-57-3  | 1,4,5,8-tetrachloronaphthalene              | 303.15 | 8.19                     |
| 3432-57-3  | 1,4,5,8-tetrachloronaphthalene              | 298.15 | 8.45                     |
| 3432-57-3  | 1,4,5,8-tetrachloronaphthalene              | 293.15 | 8.75                     |
| 3432-57-3  | 1,4,5,8-tetrachloronaphthalene              | 283.15 | 9.19                     |
| 34588-40-4 | 2,3,6,7-tetrachloronaphthalene              | 298.15 | 8.45                     |
| 34883-39-1 | 2,5-dichlorobiphenyl (PCB-9)                | 293.15 | 7.4                      |
| 34883-39-1 | 2,5-dichlorobiphenyl (PCB-9)                | 273.15 | 8.37                     |
| 34883-41-5 | 3,5-dichlorobiphenyl (PCB-14)               | 293.15 | 7.78                     |
| 34883-41-5 | 3,5-dichlorobiphenyl (PCB-14)               | 273.15 | 8.82                     |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 316.15 | 6.67                     |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 308.15 | 6.99                     |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 298.15 | 7.4                      |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 297.15 | 7.45                     |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 293.15 | 7.61                     |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 286.15 | 7.94                     |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 283.15 | 8.08                     |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 273.15 | 8.58                     |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl (PCB-153) | 308.15 | 8.89                     |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl (PCB-153) | 303.15 | 9.39                     |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl (PCB-153) | 298.15 | 9.73                     |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl (PCB-153) | 297.15 | 9.42                     |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl (PCB-153) | 293.15 | 10.04                    |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl (PCB-153) | 286.15 | 9.99                     |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl (PCB-153) | 283.15 | 10.62                    |
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl (PCB-153) | 273.15 | 11.25                    |

| CAS-RN     | Name                                              | T/K    | logK <sub>OA</sub> (Exp) |
|------------|---------------------------------------------------|--------|--------------------------|
| 35065-27-1 | 2,4,5,2',4',5'-hexachlorobiphenyl<br>(PCB-153)    | 263.15 | 11.73                    |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 323.15 | 8.78                     |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 316.15 | 8.68                     |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 313.15 | 9.22                     |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 308.15 | 9.04                     |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 303.15 | 9.53                     |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 298.15 | 9.51                     |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 297.15 | 9.57                     |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 293.15 | 10.09                    |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 286.15 | 10.14                    |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 283.15 | 10.61                    |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 273.15 | 11.27                    |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl<br>(PCB-138)    | 263.15 | 11.81                    |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180) | 308.15 | 9.44                     |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180) | 303.15 | 10.23                    |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180) | 298.15 | 9.88                     |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180) | 297.15 | 9.92                     |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180) | 293.15 | 10.75                    |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180) | 286.15 | 10.42                    |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180) | 283.15 | 11.38                    |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl<br>(PCB-180) | 273.15 | 12                       |
| 35065-29-3 | 2,2',3,4,4',5,5'-heptachlorobiphenyl              | 263.15 | 12.46                    |

| CAS-RN     | Name                                                           | T/K    | logK <sub>OA</sub> (Exp) |
|------------|----------------------------------------------------------------|--------|--------------------------|
| 35065-30-6 | (PCB-180)<br>2,2',3,3',4,4',5-heptachlorobiphenyl<br>(PCB-170) | 293.15 | 11.07                    |
| 35065-30-6 | 2,2',3,3',4,4',5-heptachlorobiphenyl<br>(PCB-170)              | 273.15 | 12.24                    |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)                         | 316.15 | 7.39                     |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)                         | 308.15 | 7.74                     |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)                         | 298.15 | 8.22                     |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)                         | 297.15 | 8.27                     |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)                         | 293.15 | 8.49                     |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)                         | 283.15 | 8.99                     |
| 35694-08-7 | 2,2',3,3',4,4',5,5'-octachlorobiphenyl<br>(PCB-194)            | 298.15 | 11.13                    |
| 35694-08-7 | 2,2',3,3',4,4',5,5'-octachlorobiphenyl<br>(PCB-194)            | 293.15 | 11.59                    |
| 35694-08-7 | 2,2',3,3',4,4',5,5'-octachlorobiphenyl<br>(PCB-194)            | 273.15 | 12.83                    |
| 36653-82-4 | 1-hexadecanol                                                  | 298.15 | 9.9                      |
| 37680-65-2 | 2,2',5-trichlorobiphenyl (PCB-18)                              | 298.15 | 7.6                      |
| 37680-65-2 | 2,2',5-trichlorobiphenyl (PCB-18)                              | 293.15 | 7.79                     |
| 37680-65-2 | 2,2',5-trichlorobiphenyl (PCB-18)                              | 273.15 | 8.7                      |
| 37680-66-3 | 2,2',4-trichlorobiphenyl (PCB-17)                              | 293.15 | 7.74                     |
| 37680-66-3 | 2,2',4-trichlorobiphenyl (PCB-17)                              | 273.15 | 8.66                     |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 308.15 | 8.31                     |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 303.15 | 8.78                     |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 298.15 | 9.06                     |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 297.15 | 8.83                     |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 293.15 | 9.31                     |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 286.15 | 9.4                      |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 283.15 | 9.78                     |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 273.15 | 10.31                    |
| 37680-73-2 | 2,2',4,5,5'-pentachlorobiphenyl<br>(PCB-101)                   | 263.15 | 10.7                     |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl<br>(PCB-95)                    | 303.15 | 8.55                     |

| CAS-RN     | Name                                           | T/K    | logK <sub>OA</sub> (Exp) |
|------------|------------------------------------------------|--------|--------------------------|
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)       | 298.15 | 8.71                     |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)       | 293.15 | 9.06                     |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)       | 283.15 | 9.51                     |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)       | 273.15 | 10.02                    |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)       | 263.15 | 10.51                    |
| 38380-03-9 | 2,3,3',4',6-pentachlorobiphenyl (PCB-110)      | 298.15 | 9.06                     |
| 38380-03-9 | 2,3,3',4',6-pentachlorobiphenyl (PCB-110)      | 293.15 | 9.58                     |
| 38380-03-9 | 2,3,3',4',6-pentachlorobiphenyl (PCB-110)      | 273.15 | 10.61                    |
| 38380-04-0 | 2,2',3,4',5',6-hexachlorobiphenyl (PCB-149)    | 298.15 | 9.27                     |
| 38380-04-0 | 2,2',3,4',5',6-hexachlorobiphenyl (PCB-149)    | 293.15 | 9.74                     |
| 38380-04-0 | 2,2',3,4',5',6-hexachlorobiphenyl (PCB-149)    | 273.15 | 10.83                    |
| 38380-05-1 | 2,2',3,3',4,6'-hexachlorobiphenyl (PCB-132)    | 293.15 | 10.07                    |
| 38380-05-1 | 2,2',3,3',4,6'-hexachlorobiphenyl (PCB-132)    | 273.15 | 11.16                    |
| 38380-08-4 | 2,3,3',4,4',5-hexachlorobiphenyl (PCB-156)     | 293.15 | 10.87                    |
| 38380-08-4 | 2,3,3',4,4',5-hexachlorobiphenyl (PCB-156)     | 273.15 | 12.07                    |
| 38411-22-2 | 2,2',3,3',6,6'-hexachlorobiphenyl (PCB-136)    | 293.15 | 9.53                     |
| 38411-22-2 | 2,2',3,3',6,6'-hexachlorobiphenyl (PCB-136)    | 273.15 | 10.59                    |
| 38411-25-5 | 2,2',3,3',4,5,6'-heptachlorobiphenyl (PCB-174) | 293.15 | 10.51                    |
| 38411-25-5 | 2,2',3,3',4,5,6'-heptachlorobiphenyl (PCB-174) | 273.15 | 11.67                    |
| 38444-77-8 | 2,4',6-trichlorobiphenyl (PCB-32)              | 298.15 | 7.72                     |
| 38444-77-8 | 2,4',6-trichlorobiphenyl (PCB-32)              | 293.15 | 7.97                     |
| 38444-77-8 | 2,4',6-trichlorobiphenyl (PCB-32)              | 273.15 | 8.89                     |
| 38444-78-9 | 2,2',3-trichlorobiphenyl (PCB-16)              | 293.15 | 7.98                     |
| 38444-78-9 | 2,2',3-trichlorobiphenyl (PCB-16)              | 273.15 | 8.87                     |

| CAS-RN     | Name                                               | T/K    | logK <sub>OA</sub> (Exp) |
|------------|----------------------------------------------------|--------|--------------------------|
| 38444-81-4 | 2,3,5-trichlorobiphenyl (PCB-26)                   | 293.15 | 8.27                     |
| 38444-81-4 | 2,3,5-trichlorobiphenyl (PCB-26)                   | 273.15 | 9.3                      |
| 38444-84-7 | 2,3,3'-trichlorobiphenyl (PCB-20)                  | 293.15 | 8.49                     |
| 38444-84-7 | 2,3,3'-trichlorobiphenyl (PCB-20)                  | 273.15 | 9.51                     |
| 38444-85-8 | 2,3,4'-trichlorobiphenyl (PCB-22)                  | 293.15 | 8.58                     |
| 38444-85-8 | 2,3,4'-trichlorobiphenyl (PCB-22)                  | 273.15 | 9.6                      |
| 38444-86-9 | 2',3,4-trichlorobiphenyl (PCB-33)                  | 293.15 | 8.52                     |
| 38444-86-9 | 2',3,4-trichlorobiphenyl (PCB-33)                  | 273.15 | 9.52                     |
| 39635-31-9 | 2,3,3',4,4',5,5'-heptachlorobiphenyl (PCB-189)     | 293.15 | 11.54                    |
| 39635-31-9 | 2,3,3',4,4',5,5'-heptachlorobiphenyl (PCB-189)     | 273.15 | 12.81                    |
| 40186-70-7 | 2,2',3,3',4,5',6-heptachlorobiphenyl (PCB-175)     | 293.15 | 10.17                    |
| 40186-70-7 | 2,2',3,3',4,5',6-heptachlorobiphenyl (PCB-175)     | 273.15 | 11.35                    |
| 40186-71-8 | 2,2',3,3',4,5',6,6'-octachlorobiphenyl (PCB-201)   | 293.15 | 10.98                    |
| 40186-71-8 | 2,2',3,3',4,5',6,6'-octachlorobiphenyl (PCB-201)   | 273.15 | 12.22                    |
| 40186-72-9 | 2,2',3,3',4,4',5,5',6-nonachlorobiphenyl (PCB-206) | 293.15 | 11.79                    |
| 40186-72-9 | 2,2',3,3',4,4',5,5',6-nonachlorobiphenyl (PCB-206) | 273.15 | 13.09                    |
| 41411-64-7 | 2,3,3',4,4',5,6-heptachlorobiphenyl (PCB-190)      | 293.15 | 10.87                    |
| 41411-64-7 | 2,3,3',4,4',5,6-heptachlorobiphenyl (PCB-190)      | 273.15 | 12.09                    |
| 41464-39-5 | 2,2',3,5'-tetrachlorobiphenyl (PCB-44)             | 298.15 | 8.36                     |
| 41464-39-5 | 2,2',3,5'-tetrachlorobiphenyl (PCB-44)             | 293.15 | 8.71                     |
| 41464-39-5 | 2,2',3,5'-tetrachlorobiphenyl (PCB-44)             | 273.15 | 9.67                     |
| 41464-40-8 | 2,2',4,5'-tetrachlorobiphenyl (PCB-49)             | 303.15 | 8.21                     |
| 41464-40-8 | 2,2',4,5'-tetrachlorobiphenyl (PCB-49)             | 298.15 | 8.39                     |
| 41464-40-8 | 2,2',4,5'-tetrachlorobiphenyl (PCB-49)             | 293.15 | 8.57                     |
| 41464-40-8 | 2,2',4,5'-tetrachlorobiphenyl (PCB-49)             | 283.15 | 9.08                     |
| 41464-40-8 | 2,2',4,5'-tetrachlorobiphenyl (PCB-49)             | 273.15 | 9.64                     |
| 41464-41-9 | 2,2',5,6'-tetrachlorobiphenyl (PCB-53)             | 303.15 | 7.84                     |
| 41464-41-9 | 2,2',5,6'-tetrachlorobiphenyl (PCB-53)             | 298.15 | 8.45                     |
| 41464-41-9 | 2,2',5,6'-tetrachlorobiphenyl (PCB-53)             | 293.15 | 8.24                     |
| 41464-41-9 | 2,2',5,6'-tetrachlorobiphenyl (PCB-53)             | 283.15 | 8.7                      |
| 41464-41-9 | 2,2',5,6'-tetrachlorobiphenyl (PCB-53)             | 273.15 | 9.28                     |
| 41464-46-4 | 2,3',4,6-tetrachlorobiphenyl (PCB-71)              | 293.15 | 8.84                     |
| 41464-46-4 | 2,3',4,6-tetrachlorobiphenyl (PCB-71)              | 273.15 | 9.78                     |

| CAS-RN     | Name                                                | T/K    | logK <sub>OA</sub> (Exp) |
|------------|-----------------------------------------------------|--------|--------------------------|
| 41464-47-5 | 2,2',3,6'-tetrachlorobiphenyl (PCB-46)              | 293.15 | 8.56                     |
| 41464-47-5 | 2,2',3,6'-tetrachlorobiphenyl (PCB-46)              | 273.15 | 9.49                     |
| 41464-51-1 | 2,2',3',4,5-pentachlorobiphenyl<br>(PCB-97)         | 293.15 | 9.44                     |
| 41464-51-1 | 2,2',3',4,5-pentachlorobiphenyl<br>(PCB-97)         | 273.15 | 10.49                    |
| 42740-50-1 | 2,2',3,3',4,4',5,6'-octachlorobiphenyl<br>(PCB-196) | 293.15 | 11.03                    |
| 42740-50-1 | 2,2',3,3',4,4',5,6'-octachlorobiphenyl<br>(PCB-196) | 273.15 | 12.27                    |
| 50-29-3    | p,p'-dichlorodiphenyltrichloroethane<br>(p,p'-DDT)  | 298.15 | 9.82                     |
| 50-32-8    | benzo[a]pyrene                                      | 298.15 | 11.56                    |
| 50402-52-3 | 1,2,3-trichloronaphthalene                          | 298.15 | 7.66                     |
| 5103-71-9  | cis-chlordane                                       | 298.15 | 8.92                     |
| 5103-71-9  | cis-chlordane                                       | 293.15 | 9.09                     |
| 5103-71-9  | cis-chlordane                                       | 288.15 | 9.49                     |
| 5103-71-9  | cis-chlordane                                       | 283.15 | 9.8                      |
| 5103-71-9  | cis-chlordane                                       | 278.15 | 10.22                    |
| 5103-74-2  | trans-chlordane                                     | 298.15 | 8.83                     |
| 51570-43-5 | 1,3,5-trichloronaphthalene                          | 323.15 | 6.38                     |
| 51570-43-5 | 1,3,5-trichloronaphthalene                          | 313.15 | 6.66                     |
| 51570-43-5 | 1,3,5-trichloronaphthalene                          | 303.15 | 7.04                     |
| 51570-43-5 | 1,3,5-trichloronaphthalene                          | 298.15 | 7.32                     |
| 51570-43-5 | 1,3,5-trichloronaphthalene                          | 293.15 | 7.63                     |
| 51570-43-5 | 1,3,5-trichloronaphthalene                          | 283.15 | 7.97                     |
| 51570-44-6 | 1,2,6-trichloronaphthalene                          | 298.15 | 7.5                      |
| 51570-45-7 | 1,2,4,6-tetrachloronaphthalene                      | 323.15 | 7.09                     |
| 51570-45-7 | 1,2,4,6-tetrachloronaphthalene                      | 313.15 | 7.39                     |
| 51570-45-7 | 1,2,4,6-tetrachloronaphthalene                      | 303.15 | 7.82                     |
| 51570-45-7 | 1,2,4,6-tetrachloronaphthalene                      | 298.15 | 8.08                     |
| 51570-45-7 | 1,2,4,6-tetrachloronaphthalene                      | 293.15 | 8.36                     |
| 51570-45-7 | 1,2,4,6-tetrachloronaphthalene                      | 283.15 | 8.79                     |
| 51908-16-8 | 2,2',3,4',5,5'-hexachlorobiphenyl<br>(PCB-146)      | 293.15 | 9.84                     |
| 51908-16-8 | 2,2',3,4',5,5'-hexachlorobiphenyl<br>(PCB-146)      | 273.15 | 10.96                    |
| 52663-58-8 | 2,3,4',6-tetrachlorobiphenyl (PCB-64)               | 298.15 | 8.41                     |
| 52663-58-8 | 2,3,4',6-tetrachlorobiphenyl (PCB-64)               | 293.15 | 8.63                     |
| 52663-58-8 | 2,3,4',6-tetrachlorobiphenyl (PCB-64)               | 273.15 | 9.62                     |
| 52663-59-9 | 2,2',3,4-tetrachlorobiphenyl (PCB-41)               | 293.15 | 8.82                     |
| 52663-59-9 | 2,2',3,4-tetrachlorobiphenyl (PCB-41)               | 273.15 | 9.79                     |
| 52663-60-2 | 2,2',3,3',6-pentachlorobiphenyl                     | 298.15 | 8.8                      |

| CAS-RN     | Name                                              | T/K    | logK <sub>OA</sub> (Exp) |
|------------|---------------------------------------------------|--------|--------------------------|
| 52663-60-2 | (PCB-84)<br>2,2',3,3',6-pentachlorobiphenyl       | 293.15 | 9.28                     |
| 52663-60-2 | (PCB-84)<br>2,2',3,3',6-pentachlorobiphenyl       | 273.15 | 10.28                    |
| 52663-63-5 | 2,2',3,5,5',6-hexachlorobiphenyl<br>(PCB-151)     | 293.15 | 9.58                     |
| 52663-63-5 | 2,2',3,5,5',6-hexachlorobiphenyl<br>(PCB-151)     | 273.15 | 10.68                    |
| 52663-64-6 | 2,2',3,3',5,6,6'-heptachlorobiphenyl<br>(PCB-179) | 293.15 | 10.1                     |
| 52663-64-6 | 2,2',3,3',5,6,6'-heptachlorobiphenyl<br>(PCB-179) | 273.15 | 11.26                    |
| 52663-65-7 | 2,2',3,3',4,6,6'-heptachlorobiphenyl<br>(PCB-176) | 293.15 | 10.06                    |
| 52663-65-7 | 2,2',3,3',4,6,6'-heptachlorobiphenyl<br>(PCB-176) | 273.15 | 11.22                    |
| 52663-67-9 | 2,2',3,3',5,5',6-heptachlorobiphenyl<br>(PCB-178) | 293.15 | 10.12                    |
| 52663-67-9 | 2,2',3,3',5,5',6-heptachlorobiphenyl<br>(PCB-178) | 273.15 | 11.28                    |
| 52663-68-0 | 2,2',3,4',5,5',6-heptachlorobiphenyl<br>(PCB-187) | 298.15 | 9.87                     |
| 52663-68-0 | 2,2',3,4',5,5',6-heptachlorobiphenyl<br>(PCB-187) | 293.15 | 10.22                    |
| 52663-68-0 | 2,2',3,4',5,5',6-heptachlorobiphenyl<br>(PCB-187) | 273.15 | 11.38                    |
| 52663-69-1 | 2,2',3,4,4',5',6-heptachlorobiphenyl<br>(PCB-183) | 293.15 | 10.26                    |
| 52663-69-1 | 2,2',3,4,4',5',6-heptachlorobiphenyl<br>(PCB-183) | 273.15 | 11.44                    |
| 52663-70-4 | 2,2',3,3',4',5,6-heptachlorobiphenyl<br>(PCB-177) | 293.15 | 10.58                    |
| 52663-70-4 | 2,2',3,3',4',5,6-heptachlorobiphenyl<br>(PCB-177) | 273.15 | 11.74                    |
| 52663-71-5 | 2,2',3,3',4,4',6-heptachlorobiphenyl<br>(PCB-171) | 303.15 | 9.96                     |
| 52663-71-5 | 2,2',3,3',4,4',6-heptachlorobiphenyl<br>(PCB-171) | 298.15 | 10.24                    |
| 52663-71-5 | 2,2',3,3',4,4',6-heptachlorobiphenyl<br>(PCB-171) | 293.15 | 10.51                    |
| 52663-71-5 | 2,2',3,3',4,4',6-heptachlorobiphenyl<br>(PCB-171) | 283.15 | 11.14                    |

| CAS-RN     | Name                                                  | T/K    | logK <sub>OA</sub> (Exp) |
|------------|-------------------------------------------------------|--------|--------------------------|
| 52663-71-5 | 2,2',3,3',4,4',6-heptachlorobiphenyl<br>(PCB-171)     | 273.15 | 11.78                    |
| 52663-71-5 | 2,2',3,3',4,4',6-heptachlorobiphenyl<br>(PCB-171)     | 263.15 | 12.31                    |
| 52663-72-6 | 2,3',4,4',5,5'-hexachlorobiphenyl<br>(PCB-167)        | 293.15 | 10.77                    |
| 52663-72-6 | 2,3',4,4',5,5'-hexachlorobiphenyl<br>(PCB-167)        | 273.15 | 11.96                    |
| 52663-73-7 | 2,2',3,3',4,5,6,6'-octachlorobiphenyl<br>(PCB-200)    | 293.15 | 10.82                    |
| 52663-73-7 | 2,2',3,3',4,5,6,6'-octachlorobiphenyl<br>(PCB-200)    | 273.15 | 12.05                    |
| 52663-74-8 | 2,2',3,3',4,5,5'-heptachlorobiphenyl<br>(PCB-172)     | 293.15 | 10.67                    |
| 52663-74-8 | 2,2',3,3',4,5,5'-heptachlorobiphenyl<br>(PCB-172)     | 273.15 | 11.84                    |
| 52663-75-9 | 2,2',3,3',4,5,5',6'-octachlorobiphenyl<br>(PCB-199)   | 293.15 | 11.05                    |
| 52663-75-9 | 2,2',3,3',4,5,5',6'-octachlorobiphenyl<br>(PCB-199)   | 273.15 | 12.28                    |
| 52663-76-0 | 2,2',3,4,4',5,5',6-octachlorobiphenyl<br>(PCB-203)    | 293.15 | 11.1                     |
| 52663-76-0 | 2,2',3,4,4',5,5',6-octachlorobiphenyl<br>(PCB-203)    | 273.15 | 12.36                    |
| 52663-77-1 | 2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl<br>(PCB-208) | 293.15 | 11.26                    |
| 52663-77-1 | 2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl<br>(PCB-208) | 273.15 | 12.57                    |
| 52663-78-2 | 2,2',3,3',4,4',5,6-octachlorobiphenyl<br>(PCB-195)    | 293.15 | 11.44                    |
| 52663-78-2 | 2,2',3,3',4,4',5,6-octachlorobiphenyl<br>(PCB-195)    | 273.15 | 12.72                    |
| 52663-79-3 | 2,2',3,3',4,4',5,6,6'-nonachlorobiphenyl<br>(PCB-207) | 293.15 | 11.26                    |
| 52663-79-3 | 2,2',3,3',4,4',5,6,6'-nonachlorobiphenyl<br>(PCB-207) | 273.15 | 12.6                     |
| 52704-70-8 | 2,2',3,3',5,6-hexachlorobiphenyl<br>(PCB-134)         | 293.15 | 9.71                     |
| 52704-70-8 | 2,2',3,3',5,6-hexachlorobiphenyl<br>(PCB-134)         | 273.15 | 10.8                     |
| 52712-04-6 | 2,2',3,4,5,5'-hexachlorobiphenyl<br>(PCB-141)         | 293.15 | 10.07                    |
| 52712-04-6 | 2,2',3,4,5,5'-hexachlorobiphenyl                      | 273.15 | 11.18                    |

| CAS-RN     | Name                                            | T/K    | logK <sub>OA</sub> (Exp) |
|------------|-------------------------------------------------|--------|--------------------------|
|            | (PCB-141)                                       |        |                          |
| 52744-13-5 | 2,2',3,3',5,6'-hexachlorobiphenyl<br>(PCB-135)  | 293.15 | 9.69                     |
| 52744-13-5 | 2,2',3,3',5,6'-hexachlorobiphenyl<br>(PCB-135)  | 273.15 | 10.78                    |
| 53555-63-8 | 1,2,3,5-tetrachloronaphthalene                  | 298.15 | 8.29                     |
| 53555-64-9 | 1,3,5,7-tetrachloronaphthalene                  | 298.15 | 7.9                      |
| 53555-65-0 | 1,2,3,5,7-pentachloronaphthalene                | 323.15 | 7.63                     |
| 53555-65-0 | 1,2,3,5,7-pentachloronaphthalene                | 313.15 | 7.97                     |
| 53555-65-0 | 1,2,3,5,7-pentachloronaphthalene                | 303.15 | 8.47                     |
| 53555-65-0 | 1,2,3,5,7-pentachloronaphthalene                | 298.15 | 8.73                     |
| 53555-65-0 | 1,2,3,5,7-pentachloronaphthalene                | 293.15 | 9.04                     |
| 53555-65-0 | 1,2,3,5,7-pentachloronaphthalene                | 283.15 | 9.5                      |
| 53-70-3    | dibenz[a,h]anthracene                           | 298.15 | 12.59                    |
| 540-54-5   | 1-chloropropane                                 | 298.15 | 2.24                     |
| 540-97-6   | dodecamethylcyclohexasiloxane (D <sub>6</sub> ) | 298.15 | 5.86                     |
| 541-02-6   | decamethylcyclopentasiloxane (D <sub>5</sub> )  | 298.15 | 4.95                     |
| 541-73-1   | 1,3-dichlorobenzene                             | 298.15 | 4.12                     |
| 556-67-2   | octamethylcyclotetrasiloxane (D <sub>4</sub> )  | 298.15 | 4.31                     |
| 55712-37-3 | 2,3',4-trichlorobiphenyl (PCB-25)               | 293.15 | 8.28                     |
| 55712-37-3 | 2,3',4-trichlorobiphenyl (PCB-25)               | 273.15 | 9.31                     |
| 55720-33-7 | 1,2,5-trichloronaphthalene                      | 298.15 | 7.5                      |
| 55720-34-8 | 1,2,7-trichloronaphthalene                      | 298.15 | 7.54                     |
| 55720-39-3 | 1,6,7-trichloronaphthalene                      | 298.15 | 7.5                      |
| 55720-41-7 | 1,2,3,7-tetrachloronaphthalene                  | 298.15 | 8.35                     |
| 55720-43-9 | 1,4,6,7-tetrachloronaphthalene                  | 323.15 | 7.12                     |
| 55720-43-9 | 1,4,6,7-tetrachloronaphthalene                  | 313.15 | 7.43                     |
| 55720-43-9 | 1,4,6,7-tetrachloronaphthalene                  | 303.15 | 7.87                     |
| 55720-43-9 | 1,4,6,7-tetrachloronaphthalene                  | 298.15 | 8.13                     |
| 55720-43-9 | 1,4,6,7-tetrachloronaphthalene                  | 293.15 | 8.42                     |
| 55720-43-9 | 1,4,6,7-tetrachloronaphthalene                  | 283.15 | 8.85                     |
| 56-23-5    | tetrachloromethane                              | 298.15 | 2.79                     |
| 563-80-4   | 3-methylbutan-2-one                             | 298.15 | 3.04                     |
| 56-55-3    | benz[a]anthracene                               | 298.15 | 10.28                    |
| 57465-28-8 | 3,3',4,4',5-pentachlorobiphenyl<br>(PCB-126)    | 303.15 | 10.1                     |
| 57465-28-8 | 3,3',4,4',5-pentachlorobiphenyl<br>(PCB-126)    | 298.15 | 10.35                    |
| 57465-28-8 | 3,3',4,4',5-pentachlorobiphenyl<br>(PCB-126)    | 293.15 | 10.61                    |
| 57465-28-8 | 3,3',4,4',5-pentachlorobiphenyl<br>(PCB-126)    | 283.15 | 11.24                    |
| 57465-28-8 | 3,3',4,4',5-pentachlorobiphenyl                 | 273.15 | 11.81                    |

| CAS-RN     | Name                                          | T/K    | logK <sub>OA</sub> (Exp) |
|------------|-----------------------------------------------|--------|--------------------------|
|            | (PCB-126)                                     |        |                          |
| 57465-28-8 | 3,3',4,4',5-pentachlorobiphenyl<br>(PCB-126)  | 263.15 | 12.55                    |
| 58863-14-2 | 1,2,3,4,5,6,7-heptachloronaphthalene          | 298.15 | 10.5                     |
| 58863-15-3 | 1,2,3,4,5,6,8-heptachloronaphthalene          | 323.15 | 9.261                    |
| 58863-15-3 | 1,2,3,4,5,6,8-heptachloronaphthalene          | 313.15 | 9.667                    |
| 58863-15-3 | 1,2,3,4,5,6,8-heptachloronaphthalene          | 303.15 | 10.1                     |
| 58863-15-3 | 1,2,3,4,5,6,8-heptachloronaphthalene          | 298.15 | 10.68                    |
| 58863-15-3 | 1,2,3,4,5,6,8-heptachloronaphthalene          | 283.15 | 11.076                   |
| 58877-88-6 | 1,2,3,4,5,6-hexachloronaphthalene             | 323.15 | 8.87                     |
| 58877-88-6 | 1,2,3,4,5,6-hexachloronaphthalene             | 313.15 | 9.35                     |
| 58877-88-6 | 1,2,3,4,5,6-hexachloronaphthalene             | 303.15 | 9.94                     |
| 58877-88-6 | 1,2,3,4,5,6-hexachloronaphthalene             | 298.15 | 10.11                    |
| 58877-88-6 | 1,2,3,4,5,6-hexachloronaphthalene             | 293.15 | 10.33                    |
| 58-89-9    | γ-hexachlorocyclohexane (γ-HCH)               | 298.15 | 7.85                     |
| 58-89-9    | γ-hexachlorocyclohexane (γ-HCH)               | 293.15 | 8.06                     |
| 58-89-9    | γ-hexachlorocyclohexane (γ-HCH)               | 288.15 | 8.22                     |
| 58-89-9    | γ-hexachlorocyclohexane (γ-HCH)               | 283.15 | 8.45                     |
| 58-89-9    | γ-hexachlorocyclohexane (γ-HCH)               | 278.15 | 8.68                     |
| 591-78-6   | hexan-2-one                                   | 298.15 | 3.68                     |
| 592-41-6   | 1-hexene                                      | 298.15 | 2.41                     |
| 594-27-4   | tetramethyl tin                               | 298.15 | 2.62                     |
| 60145-20-2 | 2,2',3,3',5-pentachlorobiphenyl<br>(PCB-83)   | 293.15 | 9.39                     |
| 60145-20-2 | 2,2',3,3',5-pentachlorobiphenyl<br>(PCB-83)   | 273.15 | 10.44                    |
| 60-29-7    | diethylether                                  | 298.15 | 2.19                     |
| 60-57-1    | dieldrin                                      | 318.15 | 8.08                     |
| 60-57-1    | dieldrin                                      | 308.15 | 8.55                     |
| 60-57-1    | dieldrin                                      | 298.15 | 8.9                      |
| 60-57-1    | dieldrin                                      | 288.15 | 9.36                     |
| 608-93-5   | pentachlorobenzene                            | 298.15 | 6.27                     |
| 608-93-5   | pentachlorobenzene                            | 293.15 | 6.54                     |
| 608-93-5   | pentachlorobenzene                            | 283.15 | 6.93                     |
| 608-93-5   | pentachlorobenzene                            | 273.15 | 7.42                     |
| 608-93-5   | pentachlorobenzene                            | 263.15 | 7.93                     |
| 61798-70-7 | 2,2',3,3',4,6-hexachlorobiphenyl<br>(PCB-131) | 293.15 | 9.83                     |
| 61798-70-7 | 2,2',3,3',4,6-hexachlorobiphenyl<br>(PCB-131) | 273.15 | 10.92                    |
| 62-44-2    | 4-ethoxyacetanilide                           | 298.15 | 9.59                     |
| 628-55-7   | diisobutylether                               | 298.15 | 3.4                      |
| 628-63-7   | pentyl acetate                                | 298.15 | 4.12                     |

| CAS-RN     | Name                                          | T/K    | logK <sub>OA</sub> (Exp) |
|------------|-----------------------------------------------|--------|--------------------------|
| 628-73-9   | hexanonitrile                                 | 298.15 | 4.08                     |
| 629-96-9   | 1-eicosanol                                   | 298.15 | 12.06                    |
| 630-08-0   | carbon monoxide                               | 298.15 | -0.88                    |
| 634-66-2   | 1,2,3,4-tetrachlorobenzene                    | 298.15 | 5.64                     |
| 634-66-2   | 1,2,3,4-tetrachlorobenzene                    | 293.15 | 5.82                     |
| 634-66-2   | 1,2,3,4-tetrachlorobenzene                    | 283.15 | 6.21                     |
| 634-66-2   | 1,2,3,4-tetrachlorobenzene                    | 273.15 | 6.64                     |
| 634-66-2   | 1,2,3,4-tetrachlorobenzene                    | 263.15 | 7.08                     |
| 634-90-2   | 1,2,3,5-tetrachlorobenzene                    | 298.15 | 5.55                     |
| 64-17-5    | ethanol                                       | 298.15 | 3.2                      |
| 64-19-7    | acetic acid                                   | 298.15 | 4.31                     |
| 647-42-7   | 1h,1h,2h,2h-perfluorooctan-1-ol<br>(6:2 FTOH) | 298.15 | 5.26                     |
| 6529-87-9  | 1,2,4,8-tetrachloronaphthalene                | 323.15 | 7.37                     |
| 6529-87-9  | 1,2,4,8-tetrachloronaphthalene                | 313.15 | 7.69                     |
| 6529-87-9  | 1,2,4,8-tetrachloronaphthalene                | 303.15 | 8.14                     |
| 6529-87-9  | 1,2,4,8-tetrachloronaphthalene                | 298.15 | 8.41                     |
| 6529-87-9  | 1,2,4,8-tetrachloronaphthalene                | 293.15 | 8.69                     |
| 6529-87-9  | 1,2,4,8-tetrachloronaphthalene                | 283.15 | 9.16                     |
| 65510-44-3 | 2,3,4,4',5-pentachlorobiphenyl<br>(PCB-123)   | 298.15 | 9.36                     |
| 66-25-1    | hexanal                                       | 298.15 | 4.41                     |
| 6733-54-6  | 1,2,4,5-tetrachloronaphthalene                | 323.15 | 7.52                     |
| 6733-54-6  | 1,2,4,5-tetrachloronaphthalene                | 313.15 | 7.88                     |
| 6733-54-6  | 1,2,4,5-tetrachloronaphthalene                | 303.15 | 8.29                     |
| 6733-54-6  | 1,2,4,5-tetrachloronaphthalene                | 298.15 | 8.58                     |
| 6733-54-6  | 1,2,4,5-tetrachloronaphthalene                | 293.15 | 8.87                     |
| 67-56-1    | methanol                                      | 298.15 | 2.84                     |
| 67-63-0    | propan-2-ol                                   | 298.15 | 3.38                     |
| 67-64-1    | propanone                                     | 298.15 | 2.31                     |
| 67-66-3    | trichloromethane                              | 298.15 | 2.8                      |
| 67-68-5    | dimethylsulfoxide                             | 298.15 | 4.96                     |
| 67-72-1    | hexachloroethane                              | 298.15 | 4.47                     |
| 678-39-7   | 1h,1h,2h,2h-pefluorodecan-1-ol<br>(8:2 FTOH)  | 298.15 | 5.56                     |
| 67922-21-8 | 1,2,4,7-tetrachloronaphthalene                | 298.15 | 8.13                     |
| 67922-22-9 | 1,2,5,6-tetrachloronaphthalene                | 298.15 | 8.28                     |
| 67922-25-2 | 1,2,3,4,5-pentachloronaphthalene              | 298.15 | 9.29                     |
| 67922-26-3 | 1,2,3,4,6-pentachloronaphthalene              | 323.15 | 7.75                     |
| 67922-26-3 | 1,2,3,4,6-pentachloronaphthalene              | 313.15 | 8.12                     |
| 67922-26-3 | 1,2,3,4,6-pentachloronaphthalene              | 303.15 | 8.63                     |
| 67922-26-3 | 1,2,3,4,6-pentachloronaphthalene              | 298.15 | 8.91                     |
| 67922-26-3 | 1,2,3,4,6-pentachloronaphthalene              | 293.15 | 9.2                      |

| CAS-RN     | Name                                               | T/K    | logK <sub>OA</sub> (Exp) |
|------------|----------------------------------------------------|--------|--------------------------|
| 67922-26-3 | 1,2,3,4,6-pentachloronaphthalene                   | 283.15 | 9.74                     |
| 67922-27-4 | 1,2,3,4,5,7-hexachloronaphthalene                  | 323.15 | 8.54                     |
| 67922-27-4 | 1,2,3,4,5,7-hexachloronaphthalene                  | 313.15 | 8.95                     |
| 67922-27-4 | 1,2,3,4,5,7-hexachloronaphthalene                  | 303.15 | 9.57                     |
| 67922-27-4 | 1,2,3,4,5,7-hexachloronaphthalene                  | 298.15 | 9.8                      |
| 67922-27-4 | 1,2,3,4,5,7-hexachloronaphthalene                  | 293.15 | 10.07                    |
| 68194-13-8 | 2,2',3,4',5,6-hexachlorobiphenyl<br>(PCB-147)      | 293.15 | 9.67                     |
| 68194-13-8 | 2,2',3,4',5,6-hexachlorobiphenyl<br>(PCB-147)      | 273.15 | 10.79                    |
| 68194-14-9 | 2,2',3,4,5',6-hexachlorobiphenyl<br>(PCB-144)      | 293.15 | 9.62                     |
| 68194-14-9 | 2,2',3,4,5',6-hexachlorobiphenyl<br>(PCB-144)      | 273.15 | 10.73                    |
| 68194-16-1 | 2,2',3,3',4,5,6-heptachlorobiphenyl<br>(PCB-173)   | 293.15 | 10.6                     |
| 68194-16-1 | 2,2',3,3',4,5,6-heptachlorobiphenyl<br>(PCB-173)   | 273.15 | 11.79                    |
| 68194-17-2 | 2,2',3,3',4,5,5',6-octachlorobiphenyl<br>(PCB-198) | 293.15 | 11.05                    |
| 68194-17-2 | 2,2',3,3',4,5,5',6-octachlorobiphenyl<br>(PCB-198) | 273.15 | 12.32                    |
| 693-65-2   | dipentyl ether                                     | 298.15 | 4.8                      |
| 69-72-7    | 2-hydroxybenzoic acid                              | 298.15 | 7.44                     |
| 69782-90-7 | 2,3,3',4,4',5'-hexachlorobiphenyl<br>(PCB-157)     | 293.15 | 11.07                    |
| 69782-90-7 | 2,3,3',4,4',5'-hexachlorobiphenyl<br>(PCB-157)     | 273.15 | 12.28                    |
| 69782-91-8 | 2,3,3',4',5,5',6-heptachlorobiphenyl<br>(PCB-193)  | 293.15 | 10.82                    |
| 69782-91-8 | 2,3,3',4',5,5',6-heptachlorobiphenyl<br>(PCB-193)  | 273.15 | 11.99                    |
| 7012-37-5  | 2,4,4'-trichlorobiphenyl (PCB-28)                  | 316.15 | 7.13                     |
| 7012-37-5  | 2,4,4'-trichlorobiphenyl (PCB-28)                  | 308.15 | 7.48                     |
| 7012-37-5  | 2,4,4'-trichlorobiphenyl (PCB-28)                  | 298.15 | 7.85                     |
| 7012-37-5  | 2,4,4'-trichlorobiphenyl (PCB-28)                  | 297.15 | 7.98                     |
| 7012-37-5  | 2,4,4'-trichlorobiphenyl (PCB-28)                  | 293.15 | 8.4                      |
| 7012-37-5  | 2,4,4'-trichlorobiphenyl (PCB-28)                  | 286.15 | 8.52                     |
| 7012-37-5  | 2,4,4'-trichlorobiphenyl (PCB-28)                  | 283.15 | 8.68                     |
| 7012-37-5  | 2,4,4'-trichlorobiphenyl (PCB-28)                  | 273.15 | 9.43                     |
| 70362-47-9 | 2,2',4,5-tetrachlorobiphenyl (PCB-48)              | 293.15 | 8.5                      |
| 70362-47-9 | 2,2',4,5-tetrachlorobiphenyl (PCB-48)              | 273.15 | 9.49                     |
| 71-23-8    | propan-1-ol                                        | 298.15 | 3.68                     |

| CAS-RN     | Name                                                | T/K    | logK <sub>OA</sub> (Exp) |
|------------|-----------------------------------------------------|--------|--------------------------|
| 71-36-3    | butan-1-ol                                          | 298.15 | 4.19                     |
| 71-41-0    | pentan-1-ol                                         | 298.15 | 4.69                     |
| 71-43-2    | benzene                                             | 298.15 | 2.8                      |
| 71-55-6    | 1,1,1-trichloroethane                               | 298.15 | 2.7                      |
| 72-20-8    | endrin                                              | 308.15 | 8.29                     |
| 72-20-8    | endrin                                              | 298.15 | 8.13                     |
| 72-20-8    | endrin                                              | 293.15 | 8.65                     |
| 72-20-8    | endrin                                              | 288.15 | 9.37                     |
| 72-20-8    | endrin                                              | 278.15 | 10.28                    |
| 72-54-8    | p,p'-dichlorodiphenyldichloroethane<br>(p,p'-DDD)   | 308.15 | 9.87                     |
| 72-54-8    | p,p'-dichlorodiphenyldichloroethane<br>(p,p'-DDD)   | 298.15 | 10.1                     |
| 72-54-8    | p,p'-dichlorodiphenyldichloroethane<br>(p,p'-DDD)   | 293.15 | 10.29                    |
| 72-54-8    | p,p'-dichlorodiphenyldichloroethane<br>(p,p'-DDD)   | 288.15 | 11.24                    |
| 72-54-8    | p,p'-dichlorodiphenyldichloroethane<br>(p,p'-DDD)   | 278.15 | 11.29                    |
| 72-55-9    | p,p'-dichlorodiphenyldichloroethylene<br>(p,p'-DDE) | 308.15 | 9.2                      |
| 72-55-9    | p,p'-dichlorodiphenyldichloroethylene<br>(p,p'-DDE) | 298.15 | 9.68                     |
| 72-55-9    | p,p'-dichlorodiphenyldichloroethylene<br>(p,p'-DDE) | 293.15 | 9.91                     |
| 72-55-9    | p,p'-dichlorodiphenyldichloroethylene<br>(p,p'-DDE) | 288.15 | 10.36                    |
| 72-55-9    | p,p'-dichlorodiphenyldichloroethylene<br>(p,p'-DDE) | 278.15 | 10.91                    |
| 73575-54-9 | 2,2',3,6,6'-pentachlorobiphenyl<br>(PCB-96)         | 303.15 | 8.3                      |
| 73575-54-9 | 2,2',3,6,6'-pentachlorobiphenyl<br>(PCB-96)         | 298.15 | 8.53                     |
| 73575-54-9 | 2,2',3,6,6'-pentachlorobiphenyl<br>(PCB-96)         | 293.15 | 8.77                     |
| 73575-54-9 | 2,2',3,6,6'-pentachlorobiphenyl<br>(PCB-96)         | 283.15 | 9.22                     |
| 73575-54-9 | 2,2',3,6,6'-pentachlorobiphenyl<br>(PCB-96)         | 273.15 | 9.72                     |
| 73575-54-9 | 2,2',3,6,6'-pentachlorobiphenyl<br>(PCB-96)         | 263.15 | 10.28                    |
| 7439-90-9  | krypton                                             | 298.15 | -0.24                    |
| 7440-37-1  | argon                                               | 298.15 | -0.71                    |

| CAS-RN     | Name                                               | T/K    | logK <sub>OA</sub> (Exp) |
|------------|----------------------------------------------------|--------|--------------------------|
| 7440-59-7  | helium                                             | 298.15 | -1.72                    |
| 7440-63-3  | xenon                                              | 298.15 | 0.38                     |
| 74472-34-7 | 2,3,4',5-tetrachlorobiphenyl<br>(PCB-63)           | 293.15 | 9.06                     |
| 74472-34-7 | 2,3,4',5-tetrachlorobiphenyl<br>(PCB-63)           | 273.15 | 10.15                    |
| 74472-42-7 | 2,3,3',4,4',6-hexachlorobiphenyl<br>(PCB-158)      | 293.15 | 10.14                    |
| 74472-42-7 | 2,3,3',4,4',6-hexachlorobiphenyl<br>(PCB-158)      | 273.15 | 11.25                    |
| 74472-44-9 | 2,3,3',4',5,6-hexachlorobiphenyl<br>(PCB-163)      | 293.15 | 10.16                    |
| 74472-44-9 | 2,3,3',4',5,6-hexachlorobiphenyl<br>(PCB-163)      | 273.15 | 11.26                    |
| 74472-47-2 | 2,2',3,4,4',5,6-heptachlorobiphenyl<br>(PCB-181)   | 298.15 | 10.51                    |
| 74472-50-7 | 2,3,3',4,4',5',6-heptachlorobiphenyl<br>(PCB-191)  | 293.15 | 10.91                    |
| 74472-50-7 | 2,3,3',4,4',5',6-heptachlorobiphenyl<br>(PCB-191)  | 273.15 | 12.07                    |
| 74472-53-0 | 2,3,3',4,4',5,5',6-octachlorobiphenyl<br>(PCB-205) | 293.15 | 11.62                    |
| 74472-53-0 | 2,3,3',4,4',5,5',6-octachlorobiphenyl<br>(PCB-205) | 273.15 | 12.86                    |
| 74-82-8    | methane                                            | 298.15 | -0.38                    |
| 74-84-0    | ethane                                             | 298.15 | 0.42                     |
| 74-85-1    | ethene                                             | 298.15 | 0.28                     |
| 74-87-3    | chloromethane                                      | 298.15 | 1.39                     |
| 74-88-4    | iodomethane                                        | 298.15 | 2.16                     |
| 74-89-5    | methylamine                                        | 298.15 | 1.9                      |
| 74-95-3    | dibromomethane                                     | 298.15 | 3.07                     |
| 74-96-4    | bromoethane                                        | 298.15 | 2.11                     |
| 74-98-6    | propane                                            | 298.15 | 0.97                     |
| 75-15-0    | carbon disulfide                                   | 298.15 | 2.28                     |
| 75-34-3    | 1,1-dichloroethane                                 | 298.15 | 2.41                     |
| 75-50-3    | trimethylamine                                     | 298.15 | 1.94                     |
| 75-52-5    | nitromethane                                       | 298.15 | 2.52                     |
| 75-65-0    | 2-methylpropan-2-ol                                | 298.15 | 3.5                      |
| 75-73-0    | tetrafluoromethane                                 | 298.15 | -0.95                    |
| 76-44-8    | heptachlor                                         | 298.15 | 7.76                     |
| 771-56-2   | pentafluorotoluene                                 | 298.15 | 3.19                     |
| 7727-37-9  | nitrogen                                           | 298.15 | -1.02                    |
| 7782-44-7  | oxygen                                             | 298.15 | -0.76                    |

| CAS-RN     | Name                                             | T/K    | logK <sub>OA</sub> (Exp) |
|------------|--------------------------------------------------|--------|--------------------------|
| 78-79-5    | 2-methyl-1,3-butadiene                           | 298.15 | 2.06                     |
| 78-82-0    | 2-cyanopropane                                   | 298.15 | 2.87                     |
| 78-83-1    | 2-methylpropan-1-ol                              | 298.15 | 3.93                     |
| 78-87-5    | 1,2-dichloropropane                              | 298.15 | 2.96                     |
| 78-92-2    | 2-butanol                                        | 298.15 | 3.8                      |
| 78-93-3    | butanone                                         | 298.15 | 2.77                     |
| 79-00-5    | 1,1,2-trichloroethane                            | 298.15 | 3.4                      |
| 79-20-9    | methyl acetate                                   | 298.15 | 2.31                     |
| 79-24-3    | nitroethane                                      | 298.15 | 2.88                     |
| 83-32-9    | acenaphthene                                     | 298.15 | 6.31                     |
| 84-66-2    | diethyl phthalate                                | 298.15 | 7.48                     |
| 84-74-2    | dibutyl phthalate                                | 298.15 | 8.66                     |
| 865-86-1   | 1h,1h,2h,2h-perfluorododecan-1-ol<br>(10:2 FTOH) | 298.15 | 5.71                     |
| 86-73-7    | fluorene                                         | 313.15 | 6.09                     |
| 86-73-7    | fluorene                                         | 303.15 | 6.52                     |
| 86-73-7    | fluorene                                         | 298.15 | 6.79                     |
| 86-73-7    | fluorene                                         | 293.15 | 7.13                     |
| 86-73-7    | fluorene                                         | 283.15 | 7.5                      |
| 86-73-7    | fluorene                                         | 273.15 | 8.13                     |
| 87-61-6    | 1,2,3-trichlorobenzene                           | 298.15 | 5.19                     |
| 87-61-6    | 1,2,3-trichlorobenzene                           | 293.15 | 5.37                     |
| 87-61-6    | 1,2,3-trichlorobenzene                           | 283.15 | 5.7                      |
| 87-61-6    | 1,2,3-trichlorobenzene                           | 273.15 | 6.07                     |
| 87-61-6    | 1,2,3-trichlorobenzene                           | 263.15 | 6.49                     |
| 87-85-4    | hexamethylbenzene                                | 298.15 | 6.31                     |
| 90-13-1    | 1-chloronaphthalene                              | 298.15 | 5.8                      |
| 90948-28-0 | 1,2,4,5,6,8-hexachloronaphthalene                | 323.15 | 8.61                     |
| 90948-28-0 | 1,2,4,5,6,8-hexachloronaphthalene                | 313.15 | 9.05                     |
| 90948-28-0 | 1,2,4,5,6,8-hexachloronaphthalene                | 303.15 | 9.67                     |
| 90948-28-0 | 1,2,4,5,6,8-hexachloronaphthalene                | 298.15 | 9.89                     |
| 90948-28-0 | 1,2,4,5,6,8-hexachloronaphthalene                | 293.15 | 10.14                    |
| 91-20-3    | naphthalene                                      | 298.15 | 5.19                     |
| 91-58-7    | 2-chloronaphthalene                              | 298.15 | 5.8                      |
| 92-52-4    | biphenyl                                         | 298.15 | 6.15                     |
| 92-52-4    | biphenyl                                         | 293.15 | 6.09                     |
| 92-52-4    | biphenyl                                         | 273.15 | 6.92                     |
| 95-47-6    | o-xylene                                         | 298.15 | 3.91                     |
| 95-50-1    | 1,2-dichlorobenzene                              | 298.15 | 4.36                     |
| 95-50-1    | 1,2-dichlorobenzene                              | 293.15 | 4.51                     |
| 95-50-1    | 1,2-dichlorobenzene                              | 283.15 | 4.82                     |
| 95-50-1    | 1,2-dichlorobenzene                              | 273.15 | 5.16                     |
| 95-50-1    | 1,2-dichlorobenzene                              | 263.15 | 5.51                     |

| CAS-RN   | Name                       | T/K    | logK <sub>OA</sub> (Exp) |
|----------|----------------------------|--------|--------------------------|
| 95-94-3  | 1,2,4,5-tetrachlorobenzene | 298.15 | 5.63                     |
| 95-94-3  | 1,2,4,5-tetrachlorobenzene | 293.15 | 5.83                     |
| 95-94-3  | 1,2,4,5-tetrachlorobenzene | 283.15 | 6.2                      |
| 95-94-3  | 1,2,4,5-tetrachlorobenzene | 273.15 | 6.62                     |
| 95-94-3  | 1,2,4,5-tetrachlorobenzene | 263.15 | 7.06                     |
| 959-98-8 | $\alpha$ -endosulfan       | 298.15 | 8.64                     |
| 959-98-8 | $\alpha$ -endosulfan       | 293.15 | 8.83                     |
| 959-98-8 | $\alpha$ -endosulfan       | 288.15 | 9.17                     |
| 959-98-8 | $\alpha$ -endosulfan       | 283.15 | 9.36                     |
| 959-98-8 | $\alpha$ -endosulfan       | 278.15 | 9.72                     |
| 96-22-0  | pentan-3-one               | 298.15 | 3.2                      |
| 98-82-8  | isopropylbenzene           | 298.15 | 3.98                     |
| 99-76-3  | methyl 4-hydroxybenzoate   | 298.15 | 8.57                     |
| 99-96-7  | 4-hydroxybenzoic acid      | 298.15 | 8.08                     |

**Table S3. *VIF*, *p* values for the pp-LFER model.**

|                   |            | <i>L</i> | <i>S</i> | <i>A</i> | <i>B</i> | <i>E</i> | <i>c</i> |
|-------------------|------------|----------|----------|----------|----------|----------|----------|
| pp-LFER model (5) | <i>VIF</i> | 4.7      | 5.1      | 1.2      | 1.2      | 7.2      |          |
|                   | <i>p</i>   | 0.000    | 0.000    | 0.000    | 0.000    | 0.001    | 0.002    |
| pp-LFER model (6) | <i>VIF</i> | 4.8      | 5.3      | 1.2      | 1.2      | 7.5      |          |
|                   | <i>p</i>   | 0.000    | 0.000    | 0.000    | 0.000    | 0.000    | 0.000    |

**Table S4. Number of compounds used in the pp-LFER models developed by this study and Abraham and Acree (2008) respectively.**

| Compounds | This study | Abraham and Acree (2008) |
|-----------|------------|--------------------------|
| PCBs      | 34         | 16                       |
| PAHs      | 16         | 7                        |
| PCNs      | 52         | 0                        |
| PFCs      | 6          | 2                        |
| OSCs      | 6          | 0                        |

**Table S5. *VIF*, *p* values for the pp-LFER-*T* model.**

|                              |            | <i>L/T</i> | <i>S/T</i> | <i>A/T</i> | <i>B/T</i> | <i>E/T</i> | <i>1/T</i> | <i>c</i> |
|------------------------------|------------|------------|------------|------------|------------|------------|------------|----------|
| pp-LFER- <i>T</i> model (10) | <i>VIF</i> | 7.1        | 6.1        | 1.4        | 1.3        | 9.3        | 1.2        |          |
|                              | <i>p</i>   | 0.000      | 0.000      | 0.000      | 0.000      | 0.000      | 0.000      | 0.000    |
| pp-LFER- <i>T</i> model (11) | <i>VIF</i> | 7.1        | 6.2        | 1.4        | 1.3        | 9.3        | 1.2        |          |
|                              | <i>p</i>   | 0.000      | 0.000      | 0.000      | 0.000      | 0.000      | 0.000      | 0.000    |

**Table S6. Comparison of external predictive abilities between models in this study and by Mintz *et al.* (2007).**

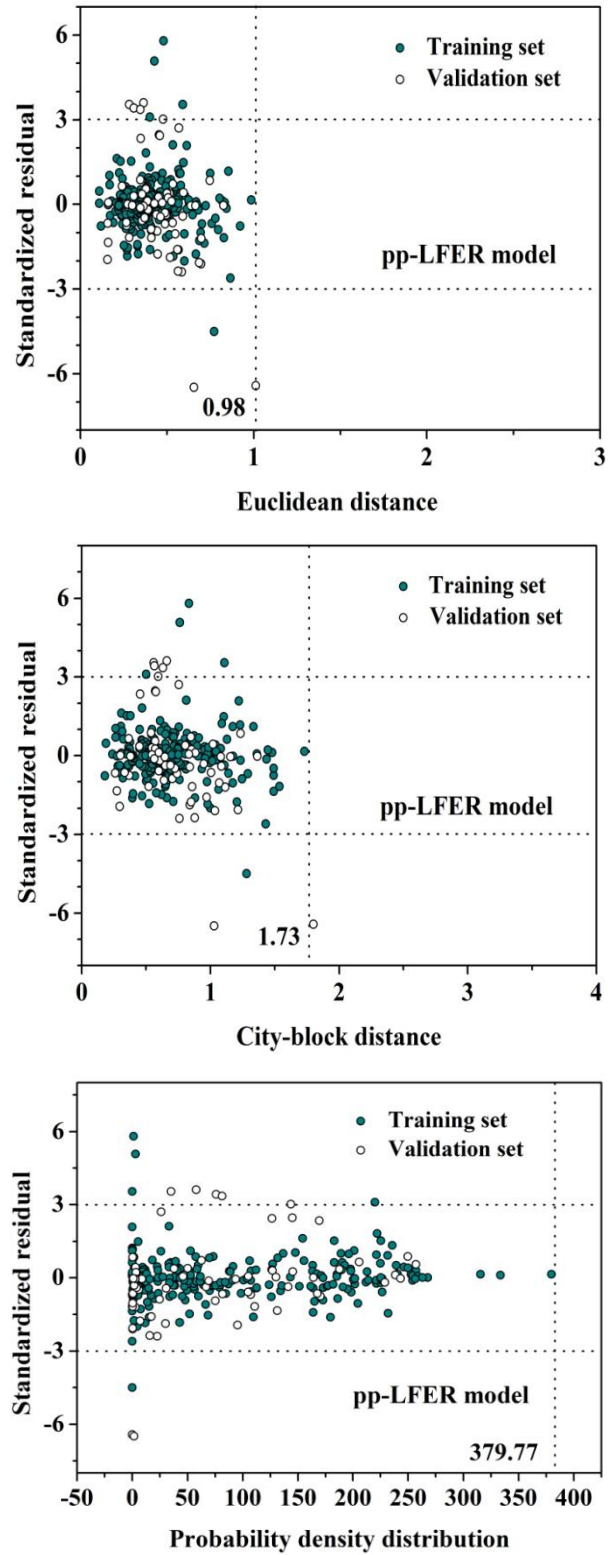
| CAS-RN      | Name                                                  | <i>T/K</i> | log $K_{OA}$ (Exp) | log $K_{OA}$ (Pre <sub>1</sub> ) <sup>a</sup> | log $K_{OA}$ (Pre <sub>2</sub> ) <sup>b</sup> |
|-------------|-------------------------------------------------------|------------|--------------------|-----------------------------------------------|-----------------------------------------------|
| 103426-93-3 | 1,2,3,4,5,8-hexachloronaphthalene                     | 303.15     | 10.21              | 10.07                                         | 9.72                                          |
| 103426-94-4 | 1,2,3,5,7,8-hexachloronaphthalene                     | 303.15     | 9.62               | 9.69                                          | 9.20                                          |
| 103426-96-6 | 1,2,3,4,6,7-hexachloronaphthalene                     | 303.15     | 9.46               | 9.51                                          | 9.09                                          |
| 118-74-1    | hexachlorobenzene (HCB)                               | 293.15     | 7.56               | 7.33                                          | 7.38                                          |
| 118-74-1    | hexachlorobenzene (HCB)                               | 283.15     | 7.89               | 7.81                                          | 8.40                                          |
| 149864-80-2 | 1,2,5,8-tetrachloronaphthalene                        | 283.15     | 9.14               | 9.35                                          | 10.15                                         |
| 150224-18-3 | 1,2,3,5,6-pentachloronaphthalene                      | 293.15     | 9.48               | 9.26                                          | 9.74                                          |
| 150224-22-9 | 1,2,4,6,8-pentachloronaphthalene                      | 323.15     | 7.67               | 7.81                                          | 6.10                                          |
| 150224-24-1 | 1,2,3,5,8-pentachloronaphthalene                      | 293.15     | 9.44               | 9.52                                          | 9.73                                          |
| 16606-02-3  | 2,4',5-trichlorobiphenyl (PCB-31)                     | 316.15     | 7.13               | 7.05                                          | 6.22                                          |
| 16606-02-3  | 2,4',5-trichlorobiphenyl (PCB-31)                     | 308.15     | 7.48               | 7.40                                          | 6.95                                          |
| 16606-02-3  | 2,4',5-trichlorobiphenyl (PCB-31)                     | 297.15     | 7.98               | 7.91                                          | 8.02                                          |
| 16606-02-3  | 2,4',5-trichlorobiphenyl (PCB-31)                     | 293.15     | 8.4                | 8.10                                          | 8.43                                          |
| 16606-02-3  | 2,4',5-trichlorobiphenyl (PCB-31)                     | 286.15     | 8.52               | 8.46                                          | 9.17                                          |
| 16606-02-3  | 2,4',5-trichlorobiphenyl (PCB-31)                     | 283.15     | 8.68               | 8.62                                          | 9.50                                          |
| 16606-02-3  | 2,4',5-trichlorobiphenyl (PCB-31)                     | 273.15     | 9.43               | 9.17                                          | 10.65                                         |
| 1746-01-6   | 2,3,7,8-tetrachlorodibenzo-p-dioxin<br>(2,3,7,8-TCDD) | 293.15     | 10.32              | 10.01                                         | 10.66                                         |
| 1825-31-6   | 1,4-dichloronaphthalene                               | 293.15     | 7.13               | 6.84                                          | 7.38                                          |
| 2050-68-2   | 4,4'-dichlorobiphenyl (PCB-15)                        | 263.15     | 9.36               | 9.37                                          | 11.56                                         |
| 2051-61-8   | 3-chlorobiphenyl                                      | 303.15     | 6.63               | 6.39                                          | 6.39                                          |
| 2051-61-8   | 3-chlorobiphenyl                                      | 293.15     | 7                  | 6.83                                          | 7.27                                          |
| 2051-61-8   | 3-chlorobiphenyl                                      | 283.15     | 7.43               | 7.29                                          | 8.20                                          |
| 2051-61-8   | 3-chlorobiphenyl                                      | 273.15     | 7.9                | 8.00                                          | 9.23                                          |
| 2051-61-8   | 3-chlorobiphenyl                                      | 263.15     | 8.37               | 8.34                                          | 10.29                                         |
| 2437-54-9   | 1,4,6-trichloronaphthalene                            | 283.15     | 7.91               | 8.13                                          | 8.81                                          |
| 2437-55-0   | 1,4,5-trichloronaphthalene                            | 283.15     | 8.24               | 8.54                                          | 9.18                                          |
| 31508-00-6  | 2',3,4,4',5'-pentachlorobiphenyl<br>(PCB-118)         | 263.15     | 11.93              | 11.50                                         | 14.46                                         |
| 319-84-6    | $\alpha$ -hexachlorocyclohexane ( $\alpha$ -HCH)      | 293.15     | 7.81               | 7.59                                          | 8.14                                          |
| 319-84-6    | $\alpha$ -hexachlorocyclohexane ( $\alpha$ -HCH)      | 283.15     | 8.18               | 8.09                                          | 9.26                                          |

|            |                                             |        |       |       |       |
|------------|---------------------------------------------|--------|-------|-------|-------|
| 32598-10-0 | 2,3',4,4'-tetrachlorobiphenyl (PCB-66)      | 273.15 | 10.21 | 10.09 | 12.01 |
| 3432-57-3  | 1,4,5,8-tetrachloronaphthalene              | 313.15 | 7.72  | 8.07  | 6.80  |
| 3432-57-3  | 1,4,5,8-tetrachloronaphthalene              | 283.15 | 9.19  | 9.60  | 10.27 |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 316.15 | 6.67  | 6.42  | 5.82  |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 308.15 | 6.99  | 6.75  | 6.50  |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 297.15 | 7.45  | 7.24  | 7.49  |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 293.15 | 7.61  | 7.43  | 7.87  |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 286.15 | 7.94  | 7.76  | 8.56  |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 283.15 | 8.08  | 7.91  | 8.87  |
| 34883-43-7 | 2,4'-dichlorobiphenyl (PCB-8)               | 273.15 | 8.58  | 8.44  | 9.94  |
| 35065-28-2 | 2,3,4,2',4',5'-hexachlorobiphenyl (PCB-138) | 316.15 | 8.68  | 8.91  | 7.46  |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)      | 316.15 | 7.39  | 7.38  | 6.48  |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)      | 308.15 | 7.74  | 7.74  | 7.23  |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)      | 297.15 | 8.27  | 8.26  | 8.32  |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)      | 293.15 | 8.49  | 8.46  | 8.74  |
| 35693-99-3 | 2,2',5,5'-tetrachlorobiphenyl (PCB-52)      | 283.15 | 8.99  | 8.99  | 9.84  |
| 37680-65-2 | 2,2',5-trichlorobiphenyl (PCB-18)           | 293.15 | 7.79  | 7.78  | 8.09  |
| 37680-65-2 | 2,2',5-trichlorobiphenyl (PCB-18)           | 273.15 | 8.7   | 8.82  | 10.21 |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)    | 303.15 | 8.55  | 8.48  | 8.18  |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)    | 293.15 | 9.06  | 8.99  | 9.26  |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)    | 283.15 | 9.51  | 9.53  | 10.41 |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)    | 273.15 | 10.02 | 10.11 | 11.65 |
| 38379-99-6 | 2,2',3,5',6-pentachlorobiphenyl (PCB-95)    | 263.15 | 10.51 | 10.74 | 12.98 |
| 38380-03-9 | 2,3,3',4',6-pentachlorobiphenyl (PCB-110)   | 293.15 | 9.58  | 9.48  | 9.64  |
| 38380-03-9 | 2,3,3',4',6-pentachlorobiphenyl (PCB-110)   | 273.15 | 10.61 | 10.64 | 12.18 |
| 38380-04-0 | 2,2',3,4',5',6-hexachlorobiphenyl (PCB-149) | 293.15 | 9.74  | 9.72  | 9.86  |
| 38380-04-0 | 2,2',3,4',5',6-hexachlorobiphenyl (PCB-149) | 273.15 | 10.83 | 10.91 | 12.42 |
| 38444-77-8 | 2,4',6-trichlorobiphenyl (PCB-32)           | 293.15 | 7.97  | 7.96  | 8.22  |
| 38444-77-8 | 2,4',6-trichlorobiphenyl (PCB-32)           | 273.15 | 8.89  | 9.01  | 10.39 |
| 41464-39-5 | 2,2',3,5'-tetrachlorobiphenyl (PCB-44)      | 293.15 | 8.71  | 8.62  | 8.89  |
| 41464-39-5 | 2,2',3,5'-tetrachlorobiphenyl (PCB-44)      | 273.15 | 9.67  | 9.72  | 11.22 |
| 5103-71-9  | cis-chlordane                               | 293.15 | 9.09  | 9.18  | 9.50  |
| 5103-71-9  | cis-chlordane                               | 283.15 | 9.8   | 9.73  | 10.72 |
| 51570-45-7 | 1,2,4,6-tetrachloronaphthalene              | 283.15 | 8.79  | 8.81  | 9.73  |

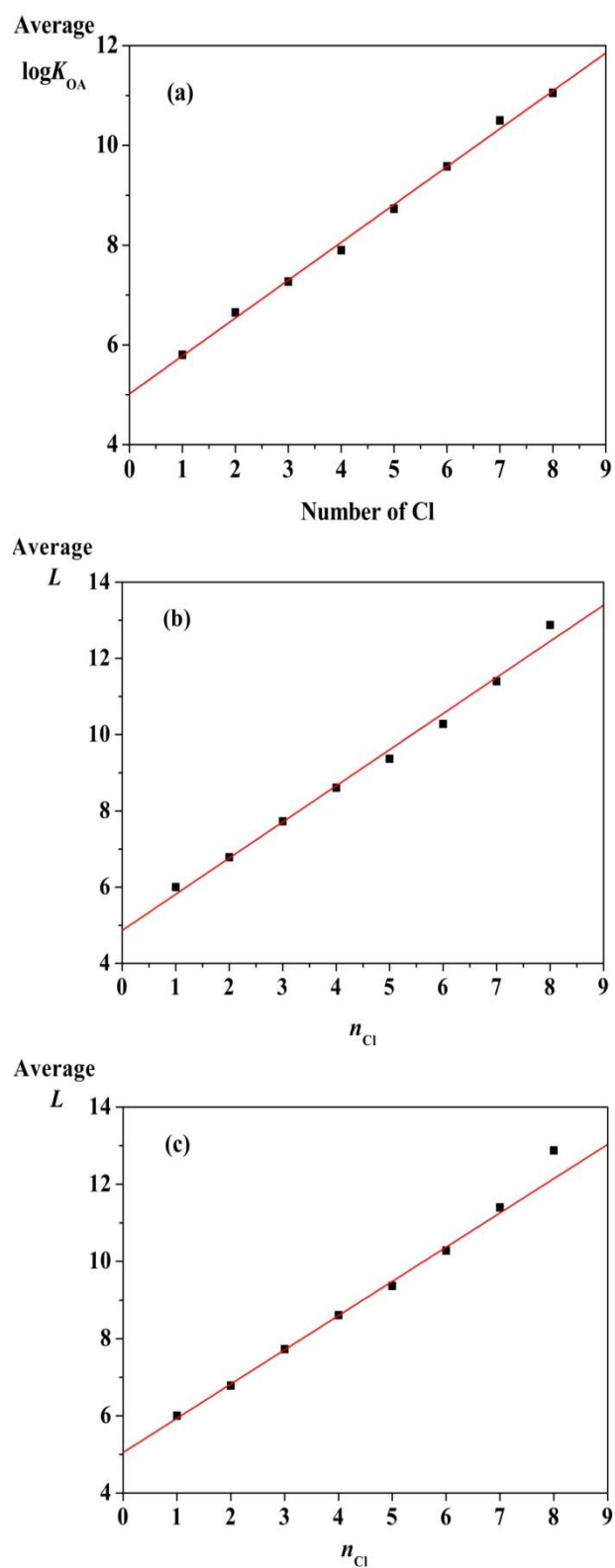
|            |                                                  |        |       |       |       |
|------------|--------------------------------------------------|--------|-------|-------|-------|
| 52663-58-8 | 2,3,4',6-tetrachlorobiphenyl (PCB-64)            | 293.15 | 8.63  | 8.66  | 8.94  |
| 52663-58-8 | 2,3,4',6-tetrachlorobiphenyl (PCB-64)            | 273.15 | 9.62  | 9.76  | 11.28 |
| 52663-60-2 | 2,2',3,3',6-pentachlorobiphenyl (PCB-84)         | 293.15 | 9.28  | 9.14  | 9.36  |
| 52663-60-2 | 2,2',3,3',6-pentachlorobiphenyl (PCB-84)         | 273.15 | 10.28 | 10.28 | 11.79 |
| 52663-68-0 | 2,2',3,4',5,5',6-heptachlorobiphenyl (PCB-187)   | 293.15 | 10.22 | 10.26 | 10.48 |
| 52663-68-0 | 2,2',3,4',5,5',6-heptachlorobiphenyl (PCB-187)   | 273.15 | 11.38 | 11.49 | 13.16 |
| 53555-65-0 | 1,2,3,5,7-pentachloronaphthalene                 | 293.15 | 9.04  | 9.03  | 9.30  |
| 55720-43-9 | 1,4,6,7-tetrachloronaphthalene                   | 293.15 | 8.42  | 8.49  | 8.68  |
| 58863-15-3 | 1,2,3,4,5,6,8-heptachloronaphthalene             | 323.15 | 9.261 | 9.72  | 7.41  |
| 58-89-9    | $\gamma$ -hexachlorocyclohexane ( $\gamma$ -HCH) | 293.15 | 8.06  | 7.86  | 8.38  |
| 58-89-9    | $\gamma$ -hexachlorocyclohexane ( $\gamma$ -HCH) | 283.15 | 8.45  | 8.36  | 9.50  |
| 60-57-1    | dieldrin                                         | 318.15 | 8.08  | 8.42  | 6.83  |
| 608-93-5   | pentachlorobenzene                               | 293.15 | 6.54  | 6.80  | 6.73  |
| 608-93-5   | pentachlorobenzene                               | 283.15 | 6.93  | 7.27  | 7.69  |
| 608-93-5   | pentachlorobenzene                               | 273.15 | 7.42  | 7.77  | 8.73  |
| 608-93-5   | pentachlorobenzene                               | 263.15 | 7.93  | 8.31  | 9.84  |
| 634-66-2   | 1,2,3,4-tetrachlorobenzene                       | 293.15 | 5.82  | 6.20  | 6.05  |
| 634-66-2   | 1,2,3,4-tetrachlorobenzene                       | 283.15 | 6.21  | 6.64  | 6.90  |
| 634-66-2   | 1,2,3,4-tetrachlorobenzene                       | 273.15 | 6.64  | 7.12  | 7.82  |
| 6529-87-9  | 1,2,4,8-tetrachloronaphthalene                   | 283.15 | 9.16  | 9.26  | 10.15 |
| 67922-26-3 | 1,2,3,4,6-pentachloronaphthalene                 | 293.15 | 9.2   | 9.23  | 9.49  |
| 67922-27-4 | 1,2,3,4,5,7-hexachloronaphthalene                | 303.15 | 9.57  | 9.64  | 9.18  |
| 87-61-6    | 1,2,3-trichlorobenzene                           | 293.15 | 5.37  | 5.47  | 5.55  |
| 87-61-6    | 1,2,3-trichlorobenzene                           | 283.15 | 5.7   | 5.89  | 6.31  |
| 87-61-6    | 1,2,3-trichlorobenzene                           | 273.15 | 6.07  | 6.34  | 7.12  |
| 90948-28-0 | 1,2,4,5,6,8-hexachloronaphthalene                | 303.15 | 9.67  | 9.74  | 9.26  |
| 92-52-4    | biphenyl                                         | 293.15 | 6.09  | 6.27  | 6.56  |
| 92-52-4    | biphenyl                                         | 273.15 | 6.92  | 7.19  | 8.35  |
| 95-50-1    | 1,2-dichlorobenzene                              | 293.15 | 4.51  | 4.63  | 4.67  |
| 95-50-1    | 1,2-dichlorobenzene                              | 283.15 | 4.82  | 5.02  | 5.31  |
| 95-50-1    | 1,2-dichlorobenzene                              | 273.15 | 5.16  | 5.44  | 6.01  |
| 95-94-3    | 1,2,4,5-tetrachlorobenzene                       | 293.15 | 5.83  | 5.92  | 6.02  |
| 95-94-3    | 1,2,4,5-tetrachlorobenzene                       | 283.15 | 6.2   | 6.36  | 6.85  |
| 95-94-3    | 1,2,4,5-tetrachlorobenzene                       | 273.15 | 6.62  | 6.82  | 7.74  |
| 95-94-3    | 1,2,4,5-tetrachlorobenzene                       | 263.15 | 7.06  | 7.33  | 8.69  |

<sup>a</sup> Predicted log $K_{OA}$  from pp-LFER- $T$  model (11).

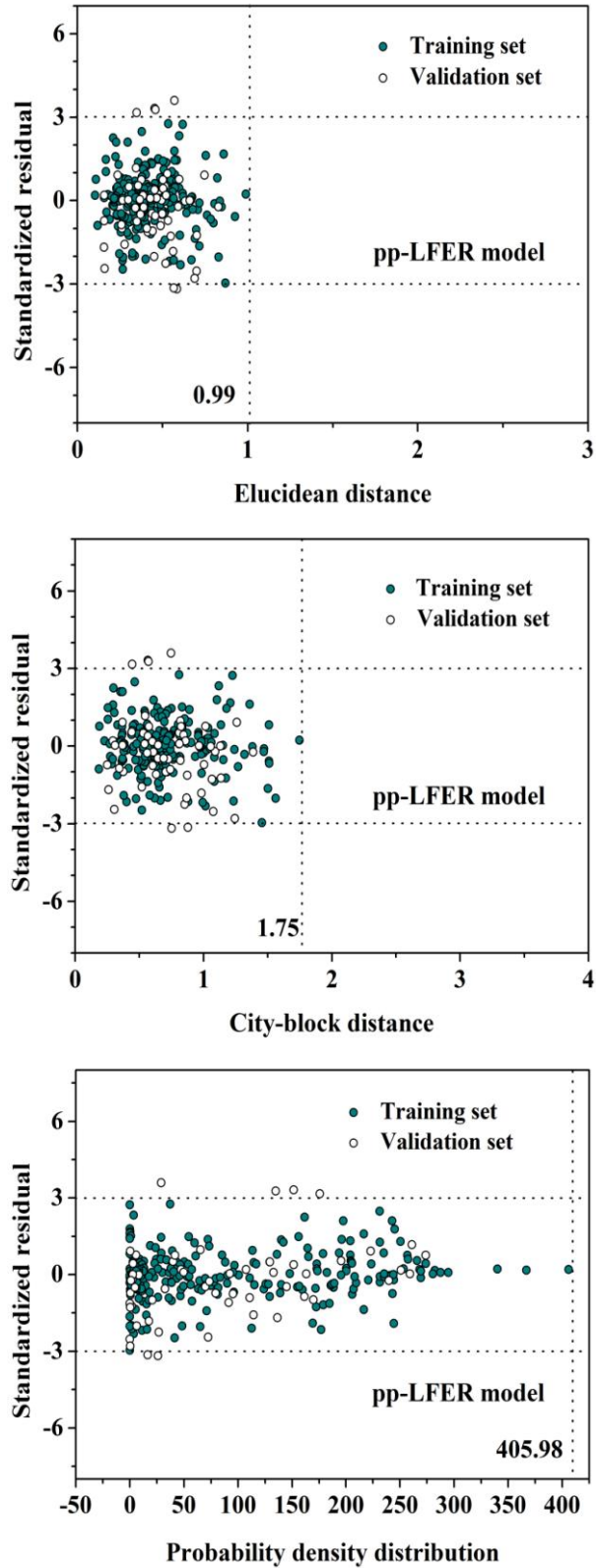
<sup>b</sup> Predicted log $K_{OA}$  from the method established by Mintz *et al.* (2007).



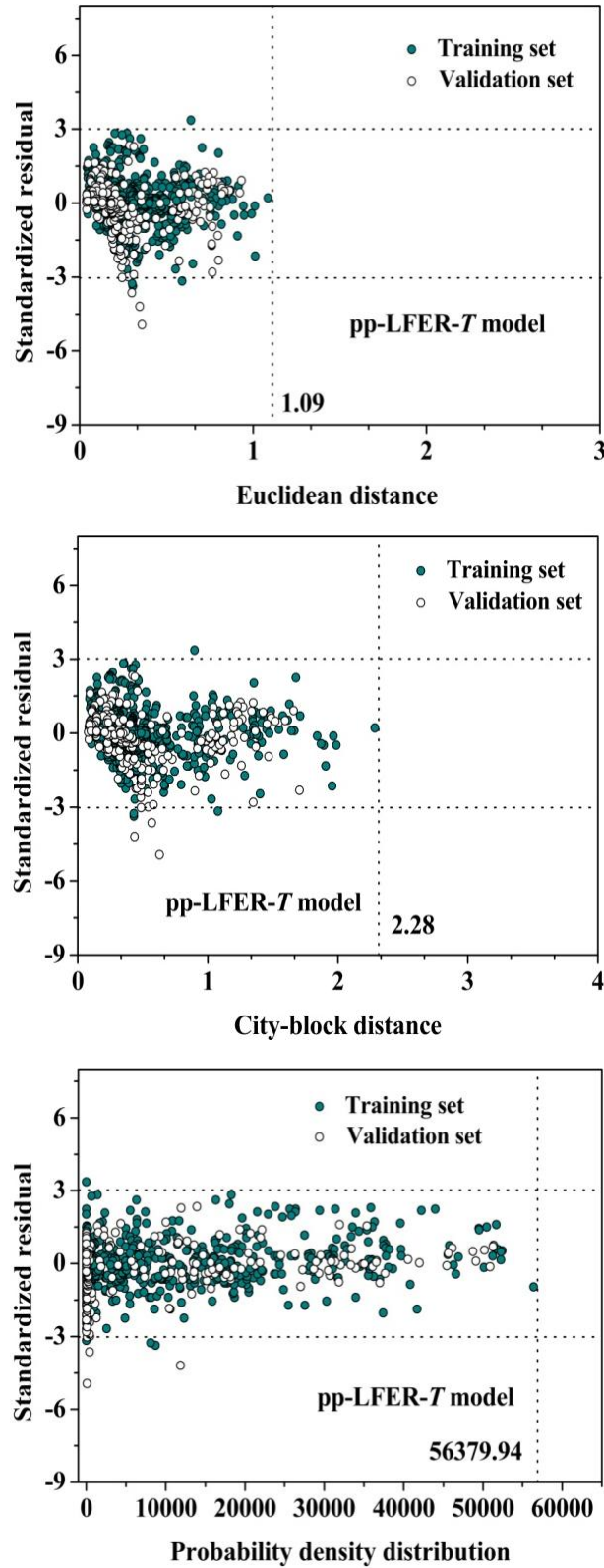
**Fig. S1.** Scatter plot for AD definition of the pp-LFER model (5) by the Euclidean distances, the city-block distances and the probability density distribution method, respectively.



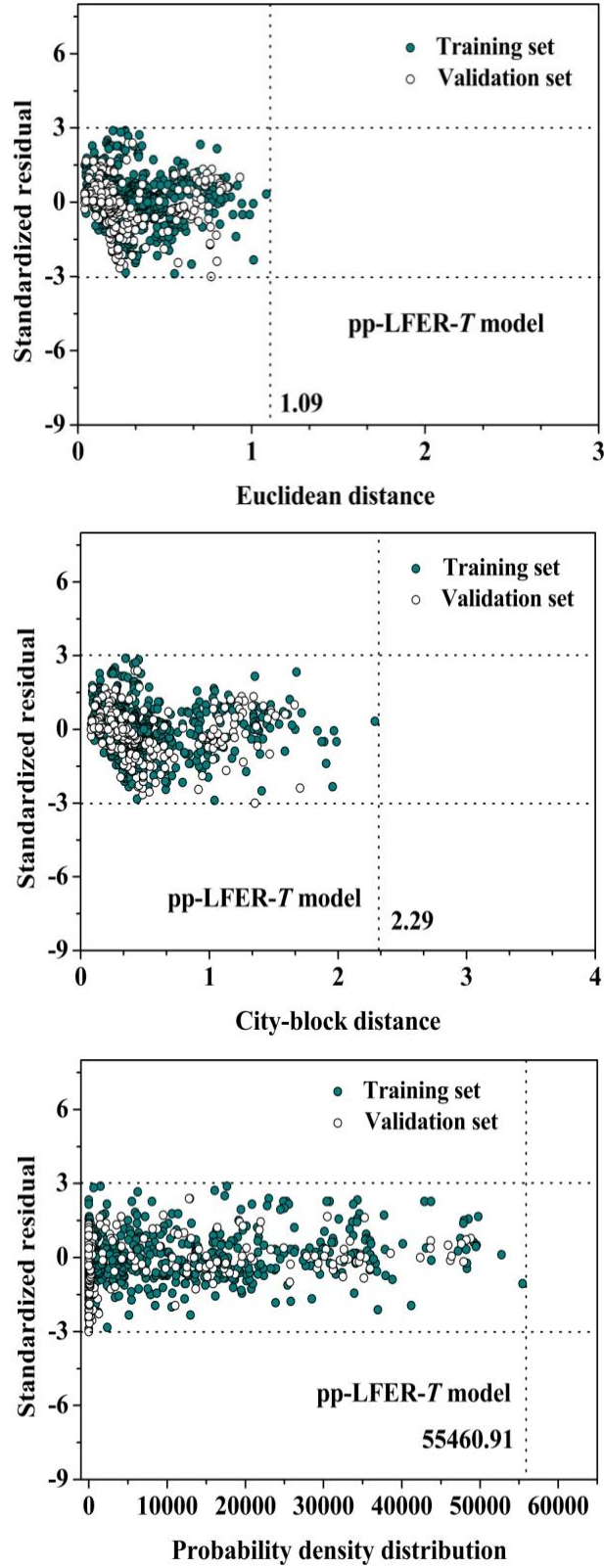
**Fig. S2. Plots of (a) average observed  $\log K_{OA}$  values, (b) average reported  $L$  values and (c) average reported  $L$  values (excluding octaCN) versus number of Cl atoms ( $n_{Cl}$ ) respectively.**



**Fig. S3. Scatter plot for AD definition of the pp-LFER model (6) by the Euclidean distances, the city-block distances and the probability density distribution method, respectively.**



**Fig. S4.** Scatter plot for AD definition of the pp-LFER-*T* model (10) by the Euclidean distances, the city-block distances and the probability density distribution method, respectively.



**Fig. S5.** Scatter plot for AD definition of the pp-LFER-*T* model (11) by the Euclidean distances, the city-block distances and the probability density distribution method, respectively.