QSAR METHOD REPORTING FORMAT

QMRF FOR ARNOT-GOBAS BCFBAF

CONTENTS

TABLES

FIGURES

1 QSAR IDENTIFIER

1.1 QSAR identifier

Arnot-Gobas screening-level method for the bioconcentration factor (BCF) in BCFBAF

1.2 QSAR related models

BCFBAF is part of EPI Suite (Estimations Programs Interface for Windows). The Arnot-Gobas screening-level BCF and BAF models documented in Costanza et al., 2012 are available in the Exposure And Safety Estimation (EAS-E) Suite on-line platform (www.eas-e-suite.com).

1.3 Software coding

BCFBAF v3.02 in EPI Suite v4.11

2 GENERAL INFORMATION

2.1 Date of QMRF

October 2024

2.2 QMRF authors and contact details

Jon Arnot on behalf of Concawe (https://www.concawe.eu/)

2.3 Date of QMRF updates

Not applicable

2.4 QMRF updates

Not applicable

2.5 Model developer and contact details

The BCFBAF Program is an update and expansion of the previous BCFWIN Program that was part of the EPI Suite version 3.20. The screening-level "Arnot and Gobas" (A-G) bioconcentration factor (BCF) and bioaccumulation factor (BAF) models are based on models originally developed by Jon Arnot and Frank Gobas at Simon Fraser University (Arnot and Gobas, 2003). The original A-G BCF and BAF models (Arnot and Gobas, 2003) were subsequently revised in a Technical Report for Environment Canada (Gobas and Arnot, 2003). The revisions included calibrating the BAF models to three different datasets of measured field BAFs representing three general trophic levels of fish (lower, middle and upper) instead of calibrating the BAF model to the entire BAF dataset as was done initially. Jon Arnot further analysed the measured field BAF data and re-parameterized and re-calibrated the BAF models representing three trophic levels of fish. These equations were provided to the US Environmental Protection Agency (EPA) and Syracuse Research Corporation (SRC) for coding the A-G BCF and BAF models in the BCFBAF v.3.02 module of EPI Suite™ with the model code documented in Costanza et al., 2012.

Jon Arnot is the President of ARC Arnot Research and Consulting: jon@arnotresearch.com

Frank Gobas is a Professor at Simon Fraser University: gobas@sfu.ca

2.6 Date of model development and/or publication

September 2012

2.7 References to main scientific papers and/or software package

ARC Arnot Research and Consulting. 2024. Bioaccumulation Estimation Tool (BET) in the Exposure And Safety Estimation (EAS-E) Suite. Ver.0.973; November 2024. Available from: www.eas-e-suite.com

Arnot JA, Gobas FAPC. 2003. A generic QSAR for assessing the bioaccumulation potential of organic chemicals in aquatic food webs. QSAR and Combinatorial Science 22: 337-345.

Arnot JA, Meylan W, Tunkel J, Howard PH, Mackay D, Bonnell M, Boethling RS. 2009. A QSAR for predicting metabolic biotransformation rates for organic chemicals in fish. Environmental Toxicology & Chemistry. 28(6): 1168-1177.

Costanza J, Lynch DG, Boethling RS, Arnot JA. 2012. Use of the bioaccumulation factor to screen chemicals for bioaccumulation potential. Environmental Toxicology & Chemistry 31: 2261-2268.

U.S. EPA. 2017. Estimation Programs Interface (EPI) Suite for Microsoft® Windows, Ver. 4.11., Released November, 2017 ed. U. S. Environmental Protection Agency, Washington, D.C.

2.8 Availability of information about the model

The "Arnot and Gobas" (A-G) BCF and BAF models are available for free from the EPA Office of Pollution Prevention and Toxics (OPPT) in the BCFBAF module of EPI Suite. Information on the model is available in the 'Help' guide in the BCFBAF program and in Costanza et al., 2012. The A-G BCF and BAF models are also available in the Exposure and Safety Estimation (EAS-E) Suite on-line platform (www.eas-e-suite.com) as part of the Bioaccumulation Estimation Tool (BET) module. The same model equations in EPI Suite and EAS-E Suite will make different BCF and BAF calculations if different values for the octanol-water partition coefficient (K_{OW}) and the whole-body biotransformation rate constant (denoted k_M or k_B) are used to parameterize the models.

2.9 Availability of another QMRF for exactly the same model

A search of the (Q)SAR Model Reporting Format Inventory for 'BCFBAF' returned no results.

3 DEFINING THE ENDPOINT: OECD PRINCIPLE 1

3.1 Species

Fish Genera

3.2 Endpoint

Bioconcentration factor (BCF; L-water/kg-wet weight fish)

3.3 Comment on the endpoint

The bioconcentration factor (BCF) is determined under controlled laboratory conditions in which the fish is only exposed to chemical in the water. The Organization for Economic Cooperation and Development (OECD) provides technical guidance for measuring the BCF in fish (OECD 2012). The BCF can be measured as the ratio of the chemical concentration in the fish (Cfish; µg-chemical/kg-fish) and the water (Cwater; µg-chemical/L-water) as Cfish/Cwater, if steady-state conditions are approximated (OECD 2012). Alternatively, the BCF can be calculated as the ratio of the chemical uptake rate constant from water (k_1; L-water/kg-fish/d) and the total elimination rate constant of the chemical from the fish (k_T; 1/d) as k_1/k_T (OECD 2012). The BCF can be measured and calculated based on the total water concentration (i.e., BCF; L-water total/kg-wet weight fish) or the freely-dissolved (bioavailable) water concentration (i.e., BCF; L-water dissolved/kg-wet weight fish). Only BCF calculations based on total water concentrations are considered in the BCFBAF module in EPI Suite, while both types of BCFs are provided in EAS-E Suite.

3.4 Endpoint units

Log BCF: Unitless

BCF: L-water total/kg-wet weight fish

BCF: L-water dissolved/kg-wet weight fish

3.5 Dependent variables

The A-G BCF models calculate BCFs for neutral organic chemicals using input data (parameters) for the octanol-water partition coefficient (K_{OW}) and the whole-body biotransformation rate constant (denoted k_M in the BCFBAF module). The whole-body biotransformation rate constant is assumed to be first-order and therefore the corresponding whole body biotransformation half-life (HL_N) is $HL_N = \ln 2/k_M$. The "N" associated with the half-life is because the input into the A-G BCF and BAF models is normalized to a fish mass of 10 g and a temperature of 15 °C (see Arnot et al., 2009 for further details). Arnot and colleagues developed and validated a QSAR for predicting HL_N (k_M) from chemical structure using SMILES notations (Arnot et al., 2009) and the HL_N (k_M) QSAR is also included in the BCFBAF module of EPI Suite. If measured values for K_{OW} and k_M are not available, these parameters are predicted by QSARs in EPI Suite, namely KOWWIN for K_{OW} (Meylan et al., 1996) and the QSAR

for predicting HL_N (k_M) (Arnot et al., 2009), respectively, and these data are subsequently used to parameterize the A-G BCF models in EPI Suite. The A-G BCF models in BCFBAF also provide BCF and BAF calculations assuming no biotransformation in fish ($k_M = 0$).

The same general approach is used to obtain input parameters for the A-G BCF models in EAS-E Suite (measured data are selected preferentially over predicted chemical information); however, when using the model in EAS-E Suite the user can also enter preferred values and use in vitro biotransformation rate data and built-in in vitro-in vivo extrapolation models to calculate the whole-body biotransformation rate constant (noted "k_B" in EAS-E Suite).

3.6 Experimental protocol

Arnot and Gobas critically reviewed more than 7,000 measured lab BCFs and field BAFs for autotrophs, aquatic invertebrates and fish reported in approximately 400 published documents (Arnot and Gobas, 2006). In total 4,323 measured fish BCFs for 770 organic chemicals reported in 65 fish species were critically reviewed based on criteria developed from OECD BCF testing guidelines (OECD, 1996). The experimental lab BCF data in the BCFBAF module are values selected by Jon Arnot (ca., 2009) based on the critical review published by Arnot and Gobas (2006). When multiple reliable quality BCFs were available for the same chemical, the median was calculated and used to train and test a new BCF regression model (formerly known as "BCFWIN") in BCFBAF (Costanza et al., 2012). The BCF data used to train and validate the "new BCFWIN" regression QSAR are included in EPI Suite (Appendices G and H in the Help file of the BCFBAF program). Appendices I and J of the Help file in BCFBAF document the empirically-based whole body biotransformation half-lives (HL) used to train and test the HL(k_M) QSAR model (Arnot et al., 2009) that is part of the BCFBAF program and the HL(k_M) QSAR model is used to parameterize the A-G BCF and BAF models in BCFBAF.

3.7 Endpoint data quality

The measured fish BCFs in the dataset were evaluated for reliability using methods and criteria based on OECD BCF testing guidelines (OECD, 1996) as detailed in Arnot and Gobas (2006). **Figure 3.1** (from Arnot and Gobas, 2006) provides an overview of the BCF data quality assessment methods and criteria. **Figure 3.2** (from Arnot and Gobas, 2006) outlines the general BCF data quality assessment workflow.

Criteria	Confidence score		
	1 — High	2 — Moderate	3 — Low
1. Water analysis	Measured	Not reported or uncertain	Not measured or nominal
2. Radio-label	Radio-label not used or corrected for parent compound	N/A	Not corrected for parent compound or analysis not clearly described to ascertain parent compound correction
3. Aqueous solubility	$[C_{WT}] \leq 0.2S_W$	2A — $0.2S_W < [C_{WT}] \leq S_W$; 2B — $S_W < [C_{WT}] \leq 5S_W$; 2C — Not reported or S_W not available	$[C_{WT}] > 5S_W$
4. Exposure duration	Declared "steady state" or sufficient for 80% steady state or k_1/k_2	Not reported	Insufficient for 80% steady state or reported "not at steady state"
5. Tissue analysis	1A — Whole body and lipid content; 1B — Whole body; no lipid content	Tissue or organ with lipid content reported or muscle tissue using k_1/k_2 or tissue analysis not reported	Tissue or organ without lipid content
6. Other factors considered	N/A	N/A	Details provided in the text

Note: N/A, not applicable; $[C_{WT}]$, exposure concentration; S_W, aqueous solubility of the chemical; k_1/k_2, kinetic methods.

Figure 3.1 Criteria for assessing BCF data quality (Arnot and Gobas, 2006)

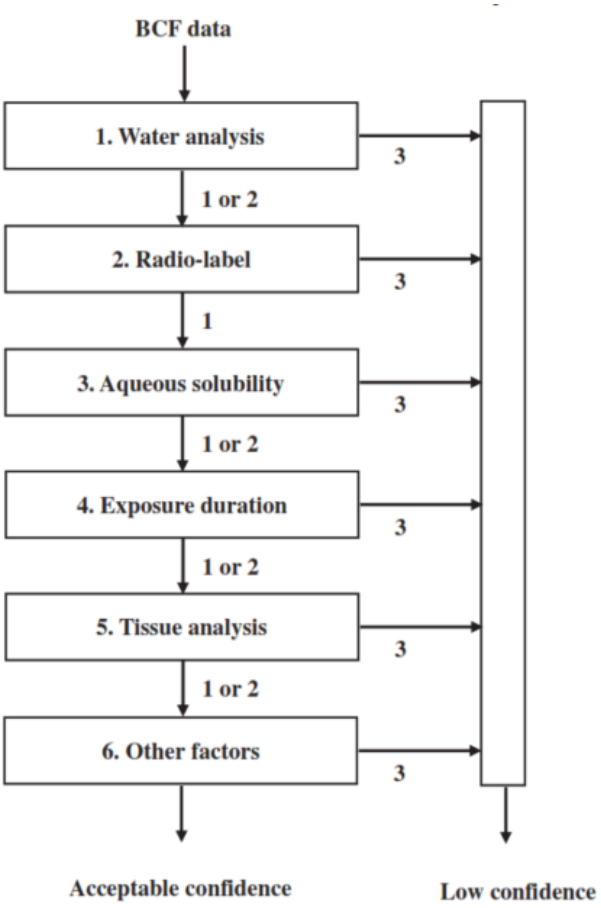

Figure 3.2 General BCF data quality assessment workflow (Arnot and Gobas, 2006)

4 DEFINING THE ALGORITHM: OECD PRINCIPLE 2

4.1 Type of model

The screening-level A-G models are simplified versions of the mass balance bioaccumulation model for fish developed by Frank Gobas (Gobas, 1993). The A-G BCF and BAF models published in 2003 were developed to generate screening-level predictions for field BAFs so that BAFs could be considered in screening-level bioaccumulation assessments for the Government of Canada's Bioaccumulation Categorization of the Domestic Substances List (Gobas and Arnot, 2003). In 2003, there were several BCF models for predicting BCFs in laboratory conditions but readily applicable screening-level BAF models for predicting BAFs in the environment were not available. The primary objective of the original screening-level A-G BCF and BAF models (Arnot and Gobas 2003) and the revised models in Costanza et al., 2012 was to calculate field BAFs for fish, not BCFs. Food web bioaccumulation models are data intensive and are not suited for screening-level bioaccumulation assessments. The A-G BAF model was developed so that thousands of data poor organic chemicals could be screened for bioaccumulation potential in the environment using BAFs without having to develop site-specific food web bioaccumulation models that require several model input parameters (e.g., organism-specific body weights and lipid contents and food web specific feeding preferences, temperatures, etc). The screening-level A-G models (2003) were developed for data poor chemicals so that only chemical-specific K_{OW} and k_M values are required as input parameters. Thus, the model is not a typical QSAR model and this QMRF format is used to provide pertinent details of the model.

The screening-level A-G BCF models were not calibrated to measured BCF data and the BCF model was not trained on a BCF dataset in the same way other BCF QSAR models are typically developed, e.g., Meylan et al., 1999. The A-G BCF models are mass balance models that calculate chemical uptake and elimination rate constants in a fish at a defined system temperature, body mass and lipid content (See Section 4.2 for details). The A-G BCF models consider three representative fish with different body masses and whole-body lipid contents.

In the original publication (Arnot and Gobas, 2003) there was only one calibration of the generalized BAF equation to the measured field BAF data to develop the "BAF-QSAR" model. The BAF-QSAR was calibrated to a large dataset of field BAF measurements to capture the observed bioaccumulation potential of organic chemicals in aquatic food webs. At the request of Environment Canada, the total field BAF data set used in the initial calibration (Arnot and Gobas, 2003) was split into three general trophic levels of fish ("Upper", "Middle", "Lower") (Gobas and Arnot, 2003). The general BAF-QSAR equation was re-parameterized for fish body mass and lipid contents corresponding to the median values of the biological conditions from the measured field BAF data and the model was re-calibrated three times for each of the three trophic levels of BAF data. The field BAF data were further evaluated and three new sets of BAF values and biological parameters were selected by Arnot in the version of the model published in Costanza et al., 2012. The representative upper trophic level fish has an assumed body mass of 1.53 kg and a whole body lipid content of 10.7%. The representative middle trophic level fish has an assumed body mass of 0.184 kg and a whole body lipid content of 6.85%. The representative lower trophic level fish has an assumed body mass of 0.096 kg

(ca., 100 g) and a whole body lipid content of 5.98%. Other relevant parameters are outlined in Costanza et al., 2012 and the Help file of BCFBAF in EPI Suite. Of the three general trophic level fish, the "lower trophic level" fish has body mass and lipid content (ca. 100 g and 6% lipid content) that are most similar to biological parameters from which laboratory BCF data are measured (Arnot and Gobas, 2006). Thus, the lower trophic level BCF is the most suitable model of the three for predicting laboratory BCFs.

4.2 Explicit algorithm

$BCF = (1 - L_B) + (k_1 * \phi / (k_2 + k_E + k_G + k_M))$

Where:

- L_B is the lipid content of an organism (see below) and the term $1 – L_B$ accounts for chemical partitioning into aqueous components of the organism.

- k_1 is the gill uptake rate constant (L/kg/d), which is a function of the octanol-water partition coefficient (K_{OW}) and the organism weight (W, kg): $k_1 = 1 / ((0.01 + 1 / K_{OW}) * W^{0.4})$.

- ϕ is the concentration of freely dissolved chemical in the water (i.e. the ratio of the bioavailable concentration of the chemical in water (C_{WD}) to the concentration of the chemical in water (C_W). For non-ionising, hydrophobic organic substances this is estimated from K_{OW}, and assumed concentrations of particulate organic matter (X_{POC}) and dissolved organic matter (X_{DOC}) in the water: $\phi = C_{WD} / C_W = 1 / (1 + X_{POC} * 0.35 * K_{OW} + X_{DOC} * 0.08 * 0.35 * K_{OW})$.

- k_2 is the elimination rate constant (d^{-1}), the rate at which chemicals are eliminated via the respiratory surface, which is estimated from the gill uptake rate constant (k_1), the organism lipid content (L_B) and the K_{OW}: $k_2 = k_1 / L_B * K_{OW}$.

- k_E is the faecal egestion (i.e. elimination) rate constant (1/d), which is dependent on K_{OW} and the feeding rate and is generalised as one eighth of the ingestion rate constant (k_D): $k_E = 0.125 * k_D$, where k_D is the dietary uptake rate constant (kg/kg/d), which is dependent on the bioenergetics of the weight of the organism (W, kg), the temperature (T, °C) and the rate of diffusion of the chemical across the intestinal wall, which is dependent on the K_{OW}: $k_D = 0.02 * W^{-0.15} * e^{(0.06 * T)} / (5.1 * 10^{-8} * K_{OW} + 2)$.

- k_G is the growth rate constant (1/d), which is dependent on the organism weight (W, kg) and the environmental temperature (assumed to be 10°C): $k_G = 0.0005 * W^{-0.2}$.

- k_M is the chemical-specific whole-body biotransformation rate constant (1/d).

The following code is used by the BCFBAF program to calculate the Arnot-Gobas BCF values.

```
static double Lbup = 0.107;
static double Lbmid = 0.0685;
static double Lblow = 0.0598;
```

```
static double Kow, phi, k1up, kDup, k2up, kEup, kGup, k1mid, kDmid, k2mid, kEmid, kGmid, k1low, kDlow, k2low, kElow, kGlow;
static double kMup, kMmid, kMlow;
static double Wup = 1.53;   // upper trophic level – kg
static double Wmid = 0.184;   // middle trophic level - kg
static double Wlow = 0.096;   // lower trophic level - kg
static double T = 10;  // deg C
static double Xpoc = 0.0000005;
static double Xdoc = 0.0000005;
double ArnotLogBCFup;
double ArnotBCFup;
double ArnotLogBCFmid;
double ArnotBCFmid;
double ArnotLogBCFlow;
double ArnotBCFlow;
double HLN; half-life corresponding to kM as HLN = ln(2)/kM for 10 g fish at 15 ° C
pow(x,y) function is x raised to the power y
Kow = pow(10,UseLogKow);
phi = 1 / (1 + (0.35 * Xpoc * Kow) + (0.08 * Xdoc * Kow));
k1up = 1 / ((0.01 + 1/Kow) * pow(Wup,0.4) );
kDup = (0.02 * pow(Wup,-0.15) * exp(0.06*T)) / (0.00000005 * Kow + 2);
k2up = k1up / (Lbup * Kow);
kEup = 0.125 * kDup;
kGup = 0.000502 * pow(Wup, -0.2);
kMup = 0.693/ HLN * pow(Wup/0.01, -0.25);
ArnotLogBCFup = log10((1-Lbup) + ((k1up*phi) / (k2up+kEup+kGup+kMup)));
ArnotBCFup = pow(10,ArnotLogBCFup);
k1mid = 1 / ((0.01 + 1/Kow) * pow(Wmid,0.4) );
kDmid = (0.02 * pow(Wmid,-0.15) * exp(0.06*T)) / (0.00000005 * Kow + 2);
k2mid = k1mid / (Lbmid * Kow);
kEmid = 0.125 * kDmid;
kGmid = 0.000502 * pow(Wmid, -0.2);
kMmid = 0.693/HLN * pow(Wmid/0.01, -0.25);
ArnotLogBCFmid = log10((1-Lbmid) + ((k1mid*phi) / (k2mid+kEmid+kGmid+kMmid)));
ArnotBCFmid = pow(10,ArnotLogBCFmid);
k1low = 1 / ((0.01 + 1/Kow) * pow(Wlow,0.4) );
kDlow = (0.02 * pow(Wlow,-0.15) * exp(0.06*T)) / (0.00000005 * Kow + 2);
k2low = k1low / (Lblow * Kow);
kElow = 0.125 * kDlow;
kGlow = 0.000502 * pow(Wlow, -0.2);
kMlow = 0.693/HLN * pow(Wlow/0.01, -0.25);
ArnotLogBCFlow = log10((1-Lblow) + ((k1low*phi) / (k2low+kElow+kGlow+kMlow)));
ArnotBCFlow = pow(10,ArnotLogBCFlow)
```

4.3 Descriptors in the model

The parameters describing the model and its default parameterization are provided in Section 4.2 and outlined in Costanza et al., 2012 and in the Help file of the BCFBAF module of EPI Suite. The biological and system parameters are fixed in the model and cannot be changed by the user. The screening-level A-G BCF models require chemical-specific K_{OW} and biotransformation HL(k_M) values and this parameterization is automated in EPI Suite and EAS-E Suite.

4.4 Descriptor selection

BCFBAF is designed to search the database of experimental BCF (Appendix G and H) and k_M (half-Life) values (Appendix I and J) and display values if found. BCFBAF generates a "structure-representation" for each SMILES entry and then searches the database for a matching "structure-representation". If a match is found, the experimental value is shown in the Results Window. A "structure-representation" will produce a database match if there is an exact atom-to-atom connection match. If more than one match is found, all exact matches are presented in a selection box for user selection.

The A-G BCF and BAF models in EAS-E Suite are also readily parameterized using built in databases of measured and predicted K_{OW} and biotransformation HL values following a chemical query using chemical name, CAS or SMILES notation. When using the A-G models in EAS-E Suite the user can also enter preferred values for K_{OW} and biotransformation HL and use in vitro biotransformation rate data and built in in vitro-in vivo extrapolation (IVIVE) models to calculate the whole-body biotransformation rate constant and corresponding half-life (noted "k_B" and "HL_B" in EAS-E Suite).

4.5 Algorithm and descriptor generation

A general mass balance model for calculating BAFs for fish in aquatic food webs was obtained by modification of an existing bioaccumulation model (Gobas 1993). When dietary exposure is ignored (as is the case in laboratory BCF studies), dietary uptake can be ignored in the model and the equations simplified to calculate the BCF rather than the BAF as shown in Section 4.2.

4.6 Software name and version for descriptor generation

See the "Help" guide in the BCFBAF program, Arnot and Gobas (2003) and Costanza et al., (2012) for further information on the methods.

4.7 Descriptors/Chemicals ratio

See the Help guide in the BCFBAF program and Arnot and Gobas (2003) and Costanza et al., (2012) for further information on the methods.

5 DEFINING THE APPLICABILITY DOMAIN: OECD PRINCIPLE 3

5.1 Description of the applicability domain of the model

Currently there is no universally accepted definition of model domain and EPI Suite does not include an explicit method for determining uncertainty or the applicability domain of any QSAR predictions in EPI Suite. Methods for better characterizing the Applicability Domain (AD) of EPI Suite fragment models were developed for the US EPA by ARC Arnot Research and Consulting (Sangion et al., 2018), and while these methods are not implemented in EPI Suite ver.4.11, the methods are included to characterize the AD of EPI Suite QSAR predictions included in EAS-E Suite. The general recommendations provided by US EPA and SRC for EPI Suite AD is that users may wish to consider the possibility that BCF estimates are less accurate for compounds outside the molecular weight and log K_{OW} ranges for the chemicals used to evaluate the BCF models described in this QMRF.

EAS-E Suite includes AD information for both K_{OW} and biotransformation HL inputs into the A-G BCF and BAF models.

5.2 Method used to assess the applicability domain assessment

Appendices G and H of the Help guide in BCFBAF provide the evaluated measured fish BCF data used to train and validate the BCF regression model "formerly known as BCFWIN" (not the subject of this QMRF). Appendices I and J of the Help guide in BCFBAF provide the biotransformation half-life QSAR training and validation datasets (not the subject of this QMRF), respectively, which are taken from the in vivo k_M database (Arnot et al., 2008). The details of the biotransformation half-life model training and validation are documented in Arnot et al., 2009.

In this QMRF we use the BCF data for organic chemicals that are not appreciably dissociated at pH 7 (i.e., acid pKa > 5 or base pKa < 9) listed in Appendices G and H of the BCFBAF Help guide to evaluate the A-G BCF models described in Costanza et al., 2012. **Table 5.1** summarizes the minimum and maximum values for molecular weight, log K_{OW} and experimental log BCF for the 572 organic chemicals used to evaluate the A-G BCF models.

Table 5.1 Range of molecular weights, log K_{OW} and log BCF for the structures in the BCFBAF training and validation sets

Parameter	Evaluation Set (non-ionic)
Minimum molecular weight	68.08
Maximum molecular weight	959.2
Minimum Log K_{OW}	-1.69
Maximum Log K_{OW}	11.59
Minimum Log BCF	-0.35
Maximum Log BCF	5.43

5.3 Software name and version for applicability of domain assessment

BCFBAF v.3.02

5.4 Limits of applicability

The A-G BCF model estimates the BCF for non-ionic organic chemicals (Arnot and Gobas, 2003). The model predictions may be highly uncertain for chemicals that have estimated log K_{OW} values above 9 and the model is not recommended for chemicals that appreciably ionise, for pigments and dyes, or for perfluorinated substances because these chemicals are outside of the model domain (Arnot and Gobas, 2003).

6 DEFINING GOODNESS OF FIT AND ROBUSTNESS: OECD PRINCIPLE 4

6.1 Availability of the training set

The A-G model was not trained on laboratory BCF data. The equations used in the screening-level A-G models are simplifications and re-arrangement of the equations used in the Gobas food web model for Lake Ontario (Gobas 1993). Those equations for chemical uptake and elimination rate constants (see Section 4.2) were derived from experimental data predominantly from 1980s (see Gobas 1993 for details). The A-G BCF models ignore dietary uptake because the BCF calculation is for a laboratory endpoint in which there is no dietary exposure of the chemical to the fish, i.e., the BCF.

6.2 Available information for the training set

The A-G BCF model is not trained on a specific dataset of chemicals to predict the BCF like other BCF QSAR models (e.g., Meylan et al., 1999), but rather includes various sub-models quantifying mechanistic processes of chemical uptake and elimination in a laboratory setting based on several empirical and theoretical relationships (See Section 4.2 and Arnot and Gobas, 2003 and Costanza et al., 2012). The evolution of the A-G BCF model coded in BCFBAF is documented in the following publications:

- Gobas 1993 documents the initial chemical uptake and elimination rate constants used to develop the screening-level A-G BCF and BAF models.
- Arnot and Gobas 2003 documents the re-arrangement of the Gobas 1993 equations and calibrating a generic BAF equation to available measured field BAF data for fish.
- Gobas and Arnot 2003 refines the BAF model calibrations from one set of field BAFs (for all fish) to three separate calibrations for three general trophic levels of fish.
- Costanza et al., 2012 details another set of biological parameters for three general trophic levels of fish and a recalibration of the general BAF equation published in Arnot and Gobas 2003 providing the "Upper", "Middle" and "Lower" trophic level BAF models provided to SRC and EPA for inclusion in BCFBAF and EPI Suite.

6.3 Data for each descriptor variable for the training set

Not Applicable

6.4 Data for the dependent variable (response) for the training set

Not Applicable

6.5 Robustness – statistics

Not Applicable

7 DEFINING PREDICTABILITY: OECD PRINCIPLE 4

7.1 Availability of external validation set

The external validation set used in this QMRF are the critically evaluated laboratory BCF data summarized in Appendices G and H of the BCFBAF Help file and are data published by Arnot and Gobas (2006). Details of the collected and critically evaluated laboratory BCF data for fish are available in the publication by Arnot and Gobas (2006) that includes an Excel spreadsheet with the study details as part of the Supporting Information. The spreadsheet (database) is also available for free download at https://arnotresearch.com/databases/.

7.2 Available information for the external validation set

CAS number, chemical name, molecular weight and SMILES notation are available for the fish BCF data in EPI Suite. The Arnot and Gobas (2006) database includes information on the chemical, the organism, the exposure conditions and other pertinent experimental data if it was reported in the original publications. The A-G experimental BCF database compiled measured BCF values for aquatic organisms, predominantly fish, from databases and literature, namely the US EPA's ECOTOX database, SRC's BCFWIN, Japan's Chemicals Evaluation and Research Institute (CERI) and National Institute of Technology and Evaluation (NITE) datasets, the Physical-Chemical Properties and Environmental Fate Handbook, National Library of Medicines (NLM's) Hazardous Substances Database (HSBD), and Devillers et al., (1998). The data are taken from 380 sources, which were published between 1966 and 2005, with approximately 70% of the data having been generated between 1995 and 2005.

The BCF database was refined to remove repeated values (i.e. the same measurement cited in different sources). Chemical congeners, i.e., polychlorinated biphenyls (PCBs), and chemical isomers with separate CAS numbers and distinct physical–chemical properties that influence their bioaccumulation behaviour (e.g., K_{OW}) were considered as separate chemicals. The BCF data were critically evaluated for their reliability for applications in bioaccumulation assessment and for model development and testing as summarized in Section 3.7 and detailed in Arnot and Gobas 2006.

7.3 Data for each descriptor variable for the external validation set

Table 9.1 lists the CAS, SMILES, log K_{OW} and $k_{M,N}$ values (originally in Arnot et al., 2009) for the 572 chemicals used as input to the A-G BCF models in this evaluation.

7.4 Data for the dependent variable for the external validation set

Table 9.2 lists the CAS, Names and log BCF values for the 572 chemicals used to evaluate the performance of the A-G BCF models as coded in BCFBAF in EPI Suite. These data are from Appendices G and H of the Help file in BCFBAF and as described in Costanza et al., (2012) were originally from the critical review of fish BCF data conducted by Arnot and Gobas (2006).

7.5 Other information about the external validation set

7.6 Experimental design of test set

See Section 3 and Arnot and Gobas 2006 for details.

7.7 Predictivity – statistics obtained by external validation

Figures 7.1 to **7.3** show the A-G BCF model predictions for three sets of biological conditions (body mass and lipid content) against the critically evaluated measured BCF data listed in **Table 9.2**. The "lower trophic level" fish has biological conditions (about 100 g and 6% lipid content) that are most similar to most laboratory BCF biological conditions (Arnot and Gobas, 2006) compared to the conditions of the "middle trophic level" fish (about 180 g and 7% lipid content) and the "upper trophic level" fish (about 1,500 g and 11% lipid content). This explains the slightly better evaluation of the "lower trophic level" fish model with the measured data. All the A-G BCF models show root mean square errors (RMSE) of about 0.51 to 0.54 which corresponds to an average prediction error for BCFs of a factor of about 3.2 to 3.4. The r^2 (q^2) value for the lower trophic BCF model is also the highest of the three and the slope is closest to 1. The x-intercept is highest for the "upper trophic level" BCF model because this model assumes the highest whole-body lipid content. In these BCF model evaluations, if the BCFBAF database has an empirical value for K_{OW} or k_M those data are selected and used preferentially to parameterize the A-G BCF models rather than QSAR predictions for K_{OW} or k_M.

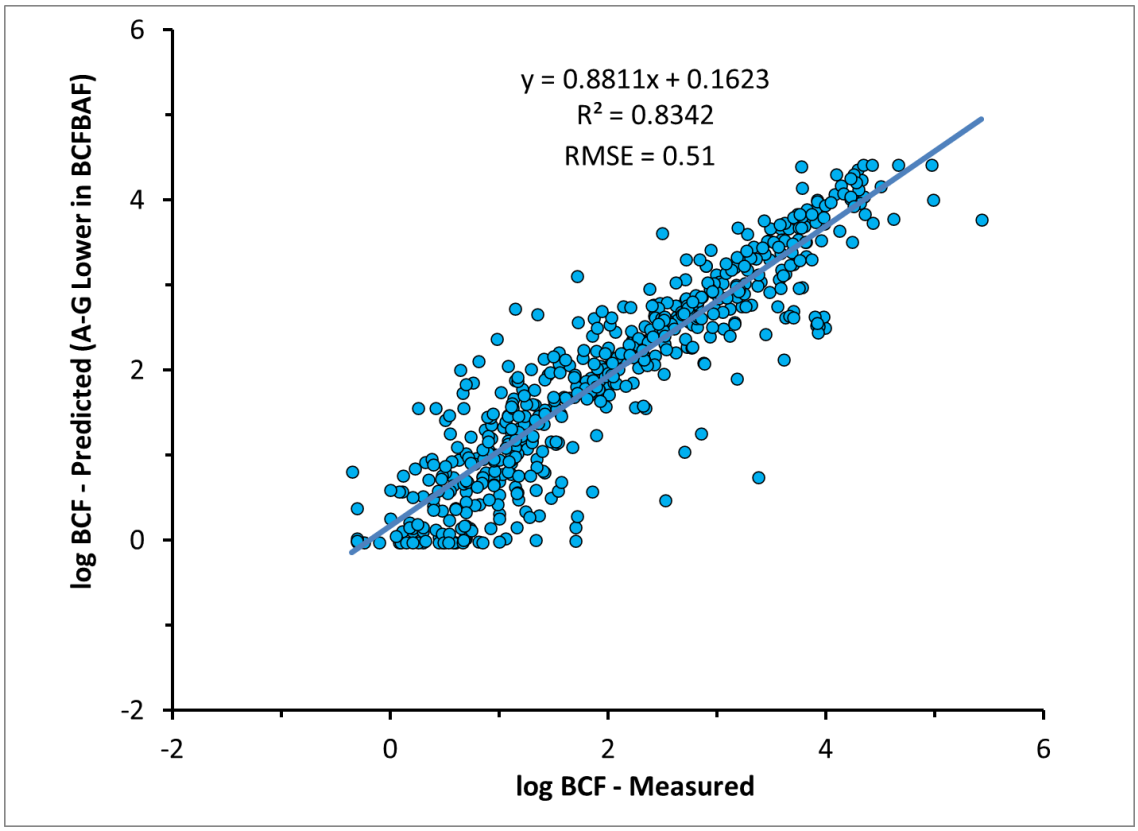

Figure 7.1 **A-G "lower trophic level" fish laboratory BCF predictions against critically evaluated measured lab BCF data.**

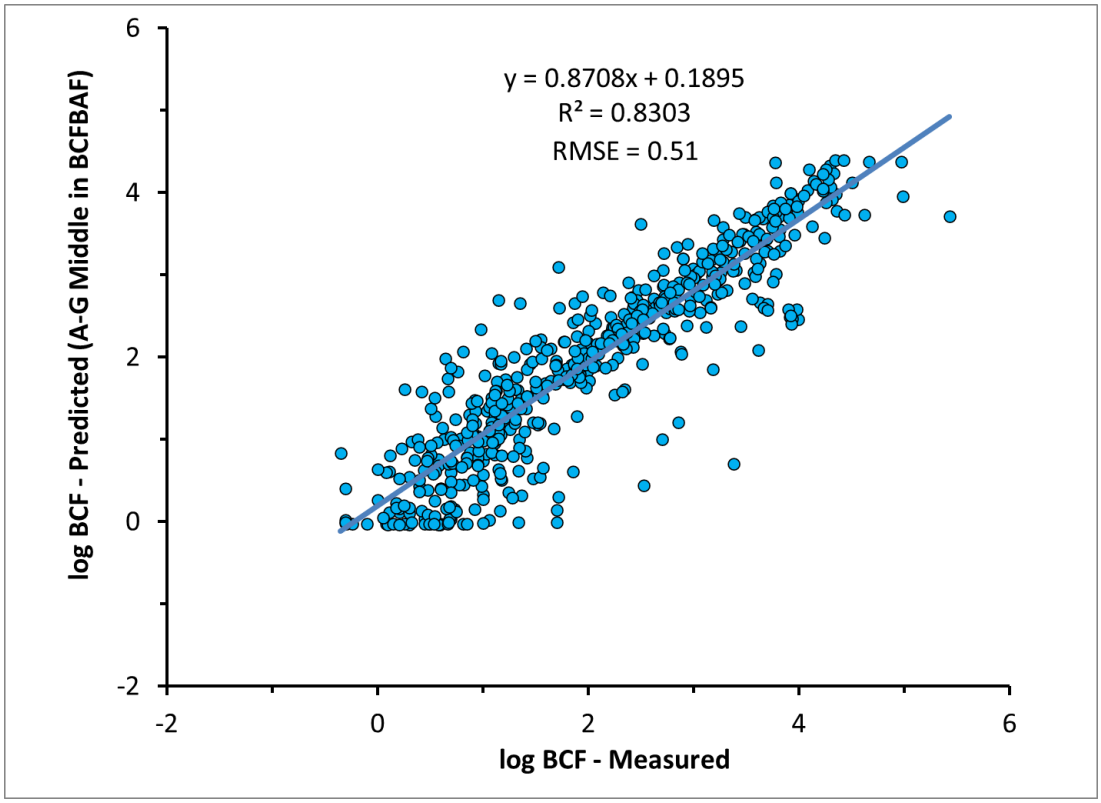

Figure 7.2 **A-G "middle trophic level" fish laboratory BCF predictions against critically evaluated measured lab BCF data.**

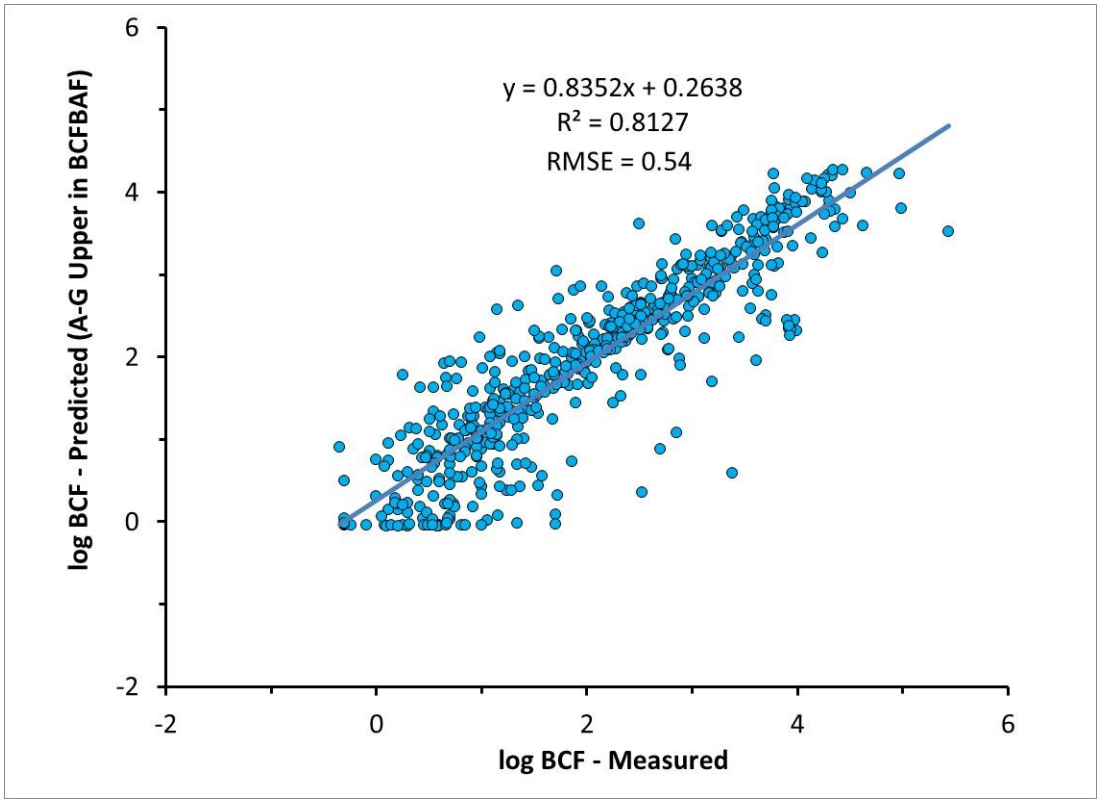

Figure 7.3 **A-G "upper trophic level" fish laboratory BCF predictions against critically evaluated measured lab BCF data.**

7.8 Predictivity – assessment of the external validation set

As discussed in Sections 3.7 and 7.6 and detailed in Arnot and Gobas (2006) the BCF data were evaluated against six assessment criteria, and only 55% of the BCF values were of acceptable reliability for model development and evaluation.

7.9 Comments on the external validation of the models

The statistical evaluations of the BCF models conducted here are unpublished and were prepared for this QMRF document.

8 PROVIDING A MECHANISTIC APPROACH – OECD PRINCIPLE 5

8.1 Mechanistic basis of the models

The screening-level A-G BCF models include mechanistic processes for bioconcentration such as chemical uptake from the water at the gill surface and chemical elimination at the gill surface, faecal egestion, growth dilution and biotransformation. Other processes included in the calculations are bioavailability in the water column (only the freely dissolved fraction can permeate epithelial boundaries) and chemical absorption efficiencies at the gill.

The model requires the K_{OW} of the chemical and the normalized whole-body metabolic biotransformation rate constant ($k_{M,N}$; 1/day) as input parameters to predict BCFs. The required $k_{M,N}$ value is normalized to a fish mass of 10 g at 15 °C (See Arnot et al., 2008 and Arnot et al., 2009).

8.2 *A priori* or *a posteriori* mechanistic interpretation

Mechanistic mass-balance equations describing the uptake and elimination of organic chemicals in fish and aquatic organisms were developed *a priori* to the development of the EPI Suite BCFBAF model. As described in this QMRF, the equations used in the screening-level A-G models are simplifications and re-arrangement of the equations used in the Gobas food web model for Lake Ontario (Gobas 1993). Those equations for chemical uptake and elimination rate constants (see Section 4.2) were derived from experimental data (see Gobas 1993 for details).

Arnot and Gobas (2003) describe an *a posteriori* evaluation of the model and make comparisons of model predictions relative to empirical BCF data.

9 MISCELLANEOUS INFORMATION

9.1 Comments

See the peer-reviewed publications Arnot and Gobas (2003), Costanza et al., (2012) and the Help guide in the BCFBAF program for further information.

9.2 Bibliography

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9.3 List of Chemicals used in the External Validation

Table 9.1 lists the SMILES, log K_{OW} and log HLN ($k_{M,N}$) values for 572 chemicals from BCFBAF used to parameterize the A-G BCF models for the model evaluations in this QMRF.

Table 9.2 lists the CAS, name and log BCF values for 572 chemicals used to evaluate the A-G BCF models in BCFBAF in this QMRF.

Table 9.1 SMILES, log K_{OW} and log HL_N ($k_{M,N}$) values for 572 chemicals from BCFBAF used to parameterize the A-G BCF models for the model evaluations in this QMRF.

CAS	SMILES	log K_{OW}	log HLN
2-35-5	S=P(OC)(OC)Oc1c(C#N)cc([Cl])cc1	3.41	0.65
50-29-3	c1(ccc(cc1)[Cl])C(c1ccc(cc1)[Cl])C([Cl])([Cl])[Cl]	6.91	1.93
55-38-9	COP(=S)(OC)Oc1ccc(SC)c(C)c1	4.09	-0.36
56-23-5	C([Cl])([Cl])([Cl])[Cl]	2.83	-1.19
56-38-2	CCOP(=S)(OCC)Oc1ccc(cc1)[N+]([O-])=O	3.83	-0.41
56-55-3	c13c(c2c(cc1)cccc2)cc1c(cccc1)c3	5.76	0.02
57-15-8	OC(C([Cl])([Cl])[Cl])(C)C	2.03	-0.39
57-74-9	[Cl]C1CC2C(C1[Cl])C1([Cl])C(=C([Cl])C2([Cl])C1([Cl])[Cl])[Cl]	6.16	2.37
58-89-9	C1(C(C(C(C([Cl])C1[Cl])[Cl])[Cl])[Cl])[Cl]	3.72	1.60
59-50-7	Oc1ccc(c(C)c1)[Cl]	3.10	-1.28
60-29-7	O(CC)CC	0.89	-0.70
60-51-5	O=C(NC)CSP(OC)(OC)=S	0.78	-1.01
60-57-1	[Cl]C4=C([Cl])C5([Cl])C3C1CC(C2OC12)C3C4([Cl])C5([Cl])[Cl]	5.40	1.72
61-82-5	[nH]1nc(N)nc1	-0.97	-1.75
62-44-2	CC(=O)Nc1ccc(OCC)cc1	1.58	-0.55
62-53-3	Nc1ccccc1	0.90	-0.78
62-56-6	NC(=S)N	-1.08	-2.66
62-73-7	O=P(OC)(OC)O\C=C(\[Cl])[Cl]	1.43	-0.96
63-25-2	O=C(Oc2c1c(cccc1)ccc2)NC	2.36	-1.18
66-81-9	CC1CC(C)C(=O)C(C1)C(O)CC1CC(=O)NC(=O)C1	0.55	-1.57
67-66-3	C([Cl])([Cl])[Cl]	1.97	-0.76
67-68-5	O=S(C)C	-1.35	-1.66
67-72-1	C(C([Cl])([Cl])[Cl])([Cl])([Cl])[Cl]	4.14	0.76
68-12-2	O=CN(C)C	-1.01	-2.14
70-30-4	Oc1c(c(c(cc1[Cl])[Cl])[Cl])Cc1c(c(cc([Cl])c1O)[Cl])[Cl]	7.54	0.58
71-43-2	c1ccccc1	2.13	0.19
71-55-6	C([Cl])([Cl])([Cl])C	2.49	-1.39
72-20-8	[Cl]C4=C([Cl])C5([Cl])C3C1CC(C2OC12)C3C4([Cl])C5([Cl])[Cl]	5.20	1.57
72-43-5	COc1ccc(cc1)C(c1ccc(OC)cc1)C([Cl])([Cl])[Cl]	5.08	1.26

CAS	SMILES	log Kow	log HLN
72-55-9	[Cl]\C([Cl])=C(/c1ccc([Cl])cc1)c1ccc([Cl])cc1	6.51	1.71
74-31-7	N(c2ccc(Nc1ccccc1)cc2)c1ccccc1	4.93	-0.03
74-97-5	[Br]C[Cl]	1.41	-0.74
75-09-2	[Cl]C[Cl]	1.25	-0.51
75-25-2	[Br]C([Br])[Br]	2.40	-0.70
75-35-4	C(=C)([Cl])[Cl]	2.13	-0.72
75-65-0	OC(C)(C)C	0.35	-1.13
75-71-8	FC(F)([Cl])[Cl]	2.16	-0.21
76-12-0	FC(C(F)([Cl])[Cl])([Cl])[Cl]	3.41	0.39
76-13-1	FC(F)(C(F)([Cl])[Cl])[Cl]	3.16	0.27
76-44-8	[Cl]C1C=CC2C1C1([Cl])C(=C([Cl])C2([Cl])C1([Cl])[Cl])[Cl]	5.47	1.45
76-83-5	c1(ccccc1)C(c1ccccc1)(c1ccccc1)[Cl]	5.25	-0.15
77-73-6	C23C1C=CC(C1)C2C=CC3	2.78	0.26
78-30-8	O=P(Oc1c(cccc1)C)(Oc1c(cccc1)C)Oc1c(cccc1)C	5.11	0.55
78-40-0	O=P(OCC)(OCC)OCC	0.80	-1.09
78-42-2	O=P(OCC(CCCC)CC)(OCC(CCCC)CC)OCC(CCCC)CC	9.49	-0.29
78-51-3	O=P(OCCOCCCC)(OCCOCCCC)OCCOCCCC	3.75	-0.86
78-59-1	O=C1C=C(CC(C)(C)C1)C	1.70	-1.29
78-63-7	O(OC(C)(C)C)C(CCC(OOC(C)(C)C)(C)C)(C)C	6.55	0.77
78-79-5	C(C=C)(=C)C	2.42	-0.61
78-87-5	[Cl]CC([Cl])C	1.98	-1.06
79-00-5	[Cl]CC([Cl])[Cl]	1.89	-1.01
79-01-6	C(=C\[Cl])(/[Cl])[Cl]	2.42	-0.41
79-27-6	[Br]C([Br])C([Br])[Br]	2.55	-0.93
79-34-5	C(C([Cl])[Cl])([Cl])[Cl]	2.39	-0.67
79-46-9	[N+]([O-])(=O)C(C)C	0.93	-1.20
79-92-5	C2(C1CC(CC1)C2(C)C)=C	4.22	0.96
79-94-7	Oc1c(cc(cc1[Br])C(c1cc(c(O)c([Br])c1)[Br])(C)C)[Br]	6.53	0.12
80-05-7	Oc1ccc(cc1)C(c1ccc(O)cc1)(C)C	3.32	0.27
80-43-3	O(OC(c1ccccc1)(C)C)C(c1ccccc1)(C)C	5.50	-0.01
81-15-2	[N+]([O-])(=O)c1c(c([N+]([O-])=O)c(c([N+]([O-])=O)c1C)C(C)(C)C)C	4.90	-0.67
82-05-3	O=C1c4c(c3c2c(cccc12)ccc3)cccc4	4.81	-0.69
82-44-0	O=C2c1c(c(ccc1)[Cl])C(=O)c1ccccc21	3.98	-0.23

CAS	SMILES	log K_{ow}	log HLN
82-45-1	O=C2c1c(c(N)ccc1)C(=O)c1ccccc21	3.74	-0.59
82-68-8	[O-][N+](=O)c1c(c(c(c([Cl])c1[Cl])[Cl])[Cl])[Cl]	4.64	-0.17
83-32-9	c12c3cccc1CCc2ccc3	3.92	-0.60
83-42-1	[N+]([O-])(=O)c1c(c(ccc1)[Cl])C	3.09	-0.21
83-79-4	COc5cc4OCC3Oc2c1CC(Oc1ccc2C(=O)C3c4cc5OC)C(C)=C	4.10	-0.59
84-15-1	c2(c(c1ccccc1)cccc2)c1ccccc1	5.52	0.86
84-51-5	O=C1c3c(C(=O)c2ccccc12)ccc(CC)c3	4.37	-0.36
84-74-2	O=C(OCCCC)c1c(cccc1)C(=O)OCCCC	4.50	-0.40
85-01-8	c13c(c2c(cc1)cccc2)cccc3	4.46	0.70
85-22-3	c1(c(c(c(c([Br])c1[Br])[Br])[Br])[Br])CC	7.48	0.02
85-68-7	O=C(OCc1ccccc1)c1c(cccc1)C(=O)OCCCC	4.73	-1.03
86-30-6	O=NN(c1ccccc1)c1ccccc1	3.13	-0.91
86-73-7	c23c(c1c(cccc1)C2)cccc3	4.18	0.70
86-74-8	[nH]1c3c(c2ccccc12)cccc3	3.72	0.06
87-40-1	c1c([Cl])c(OC)c([Cl])cc1[Cl]	4.11	1.38
87-61-6	c1(c(c(ccc1)[Cl])[Cl])[Cl]	4.05	0.92
87-65-0	Oc1c(cccc1[Cl])[Cl]	2.75	-0.46
87-68-3	C(=C(\C(=C(\[Cl])[Cl])[Cl])/[Cl])(\[Cl])[Cl]	4.78	2.07
87-82-1	c1(c(c(c(c([Br])c1[Br])[Br])[Br])[Br])[Br]	6.07	0.43
87-83-2	c1(c(c(c(c([Br])c1[Br])[Br])[Br])[Br])C	5.43	-0.13
87-84-3	[Br]C1C(C([Br])C([Br])C([Br])C1[Br])[Cl]	4.72	-0.31
88-06-2	Oc1c(cc(cc1[Cl])[Cl])[Cl]	3.69	-0.57
88-19-7	O=S(=O)(N)c1c(cccc1)C	0.84	-0.89
88-72-2	[N+]([O-])(=O)c1c(cccc1)C	2.30	-0.48
88-73-3	[O-][N+](=O)c1c(cccc1)[Cl]	2.24	-0.58
88-74-4	[N+]([O-])(=O)c1c(N)cccc1	1.85	-0.46
88-75-5	[N+]([O-])(=O)c1c(O)cccc1	1.79	-1.20
89-59-8	[N+]([O-])(=O)c1c(ccc([Cl])c1)C	3.05	-0.22
89-61-2	[O-][N+](=O)c1c(ccc([Cl])c1)[Cl]	3.09	0.56
89-63-4	[N+]([O-])(=O)c1c(N)ccc([Cl])c1	2.72	-0.96
89-69-0	[O-][N+](=O)c1c(cc(c([Cl])c1)[Cl])[Cl]	3.48	-0.64
90-12-0	c12c(c(ccc1)C)cccc2	3.87	0.52
90-30-2	N(c2c1c(cccc1)ccc2)c1ccccc1	4.20	0.34

CAS	SMILES	log K_{ow}	log HLN
90-41-5	Nc2c(c1ccccc1)cccc2	2.84	-1.06
90-94-8	O=C(c1ccc(N(C)C)cc1)c1ccc(N(C)C)cc1	3.87	-0.77
91-15-6	C(#N)c1c(C#N)cccc1	0.99	-0.67
91-20-3	c12c(cccc1)cccc2	3.30	0.41
91-22-5	n2c1c(cccc1)ccc2	2.03	-1.33
91-23-6	[O-][N+](=O)c1c(OC)cccc1	1.73	-1.04
91-57-6	c12c(ccc(C)c1)cccc2	3.86	1.02
91-58-7	c12c(ccc([Cl])c1)cccc2	3.90	0.76
91-66-7	N(c1ccccc1)(CC)CC	3.31	-0.84
91-94-1	Nc2c(cc(c1ccc(N)c([Cl])c1)cc2)[Cl]	3.51	-0.13
91-96-3	O=C(Nc2c(cc(c1ccc(NC(=O)CC(=O)C)c(C)c1)cc2)C)CC(=O)C	1.75	-1.50
92-52-4	c2(c1ccccc1)ccccc2	4.01	0.23
92-69-3	Oc2ccc(c1ccccc1)cc2	3.20	-0.81
92-77-3	O=C(Nc1ccccc1)c2c(O)cc1c(cccc1)c2	4.62	-0.68
92-84-2	N1c3c(Sc2ccccc12)cccc3	4.15	0.04
92-86-4	c2(ccc(c1ccc(cc1)[Br])cc2)[Br]	5.72	1.57
94-52-0	[N+]([O-])(=O)c2ccc1nc[nH]c1c2	1.50	-1.15
95-16-9	c2ccc1ncsc1c2	2.01	-0.86
95-47-6	c1(c(cccc1)C)C	3.16	-0.02
95-48-7	Oc1c(cccc1)C	1.95	-0.52
95-49-8	c1(c(cccc1)[Cl])C	3.42	-0.72
95-50-1	c1(c(cccc1)[Cl])[Cl]	3.43	0.50
95-51-2	Nc1c(cccc1)[Cl]	1.90	-0.61
95-56-7	Oc1c(cccc1)[Br]	2.35	-0.24
95-57-8	Oc1c(cccc1)[Cl]	2.15	-0.38
95-63-6	c1(ccc(c(C)c1)C)C	3.63	-0.31
95-64-7	Nc1ccc(c(C)c1)C	1.84	-0.99
95-69-2	Nc1c(cc(cc1)[Cl])C	2.40	-0.61
95-76-1	Nc1ccc(c([Cl])c1)[Cl]	2.69	-1.09
95-77-2	Oc1ccc([Cl])c([Cl])c1	3.33	-0.92
95-78-3	Nc1c(ccc(C)c1)C	1.83	-0.99
95-80-7	Nc1c(ccc(N)c1)C	0.14	-1.92
95-82-9	Nc1c(ccc([Cl])c1)[Cl]	2.75	-1.13

CAS	SMILES	log K_{ow}	log HLN
95-94-3	c1(c(cc(c([Cl])c1)[Cl])[Cl])[Cl]	4.64	1.79
95-95-4	Oc1c(cc(c([Cl])c1)[Cl])[Cl]	3.72	-0.13
96-12-8	[Br]CC([Br])C[Cl]	2.96	-1.14
96-18-4	[Cl]CC([Cl])C[Cl]	2.27	-0.53
96-29-7	N(/O)=C(\CC)C	0.63	-1.33
96-45-7	N1C(=S)NCC1	-0.66	-2.40
96-76-4	Oc1c(cc(cc1)C(C)(C)C)C(C)(C)C	5.19	-0.37
96-96-8	[N+]([O-])(=O)c1c(N)ccc(OC)c1	1.94	-0.87
97-23-4	Oc1c(cc(cc1)[Cl])Cc1c(O)ccc([Cl])c1	4.26	-0.51
98-08-8	FC(F)(F)c1ccccc1	3.01	-0.48
98-10-2	O=S(=O)(N)c1ccccc1	0.31	-0.71
98-15-7	FC(F)(F)c1cccc([Cl])c1	3.60	0.64
98-54-4	Oc1ccc(cc1)C(C)(C)C	3.31	-0.87
98-82-8	c1(ccccc1)C(C)C	3.66	-0.21
98-83-9	c1(C(=C)C)ccccc1	3.48	-0.71
98-84-0	CC(N)c1ccccc1	1.49	-0.90
98-95-3	[N+]([O-])(=O)c1ccccc1	1.85	-0.93
99-08-1	[N+]([O-])(=O)c1cccc(C)c1	2.45	-0.79
99-09-2	[N+]([O-])(=O)c1cccc(N)c1	1.37	-0.77
99-54-7	[N+]([O-])(=O)c1ccc(c([Cl])c1)[Cl]	3.12	-0.27
99-62-7	c1(cccc(C(C)C)c1)C(C)C	4.90	0.56
99-65-0	[N+]([O-])(=O)c1cccc([N+]([O-])=O)c1	1.49	-0.92
99-71-8	Oc1ccc(cc1)C(CC)C	3.08	-0.84
99-99-0	[N+]([O-])(=O)c1ccc(cc1)C	2.37	-1.01
100-00-5	[N+]([O-])(=O)c1ccc(cc1)[Cl]	2.39	-0.48
100-01-6	[N+]([O-])(=O)c1ccc(N)cc1	1.39	-0.51
100-02-7	[N+]([O-])(=O)c1ccc(O)cc1	1.91	-1.16
100-17-4	[O-][N+](=O)c1ccc(OC)cc1	2.03	-0.95
100-18-5	c1(ccc(cc1)C(C)C)C(C)C	5.23	0.60
100-40-3	C1=CCCC(C=C)C1	3.93	-0.41
100-42-5	c1(ccccc1)C=C	2.95	-0.30
100-43-6	n1ccc(cc1)C=C	1.71	-0.82
100-61-8	N(c1ccccc1)C	1.66	-0.88

CAS	SMILES	log K_{ow}	log HLN
100-80-1	c1(cccc(C=C)c1)C	3.35	0.21
101-14-4	Nc1c(cc(cc1)Cc1ccc(N)c([Cl])c1)[Cl]	3.91	-0.15
101-53-1	Oc1ccc(cc1)Cc1ccccc1	3.47	-0.86
101-77-9	Nc1ccc(cc1)Cc1ccc(N)cc1	1.59	-1.02
101-81-5	c1(ccccc1)Cc1ccccc1	4.14	-0.25
101-84-8	O(c1ccccc1)c1ccccc1	4.21	-0.09
102-70-5	N(CC=C)(CC=C)CC=C	2.59	-0.91
102-71-6	OCCN(CCO)CCO	-1.00	-3.05
103-44-6	O(CC(CCCC)CC)C=C	3.79	0.95
103-50-4	O(Cc1ccccc1)Cc1ccccc1	3.31	0.63
103-69-5	N(c1ccccc1)CC	2.16	-0.65
103-83-3	N(Cc1ccccc1)(C)C	1.98	-1.60
104-40-5	Oc1ccc(cc1)CCCCCCCCC	5.76	-0.23
104-88-1	O=Cc1ccc(cc1)[Cl]	2.10	0.01
105-05-5	c1(ccc(cc1)CC)CC	4.58	-0.01
105-06-6	c1(ccc(cc1)C=C)C=C	4.18	0.50
106-37-6	c1(ccc(cc1)[Br])[Br]	3.79	0.31
106-41-2	Oc1ccc(cc1)[Br]	2.59	-0.62
106-42-3	c1(ccc(cc1)C)C	3.15	-0.02
106-43-4	c1(ccc(cc1)[Cl])C	3.33	-0.83
106-46-7	c1(ccc(cc1)[Cl])[Cl]	3.44	1.10
106-47-8	Nc1ccc(cc1)[Cl]	1.83	-0.61
106-48-9	Oc1ccc(cc1)[Cl]	2.39	-0.41
106-93-4	[Br]CC[Br]	1.96	-0.83
107-05-1	C(=C)C[Cl]	1.55	-0.93
107-39-1	C(=C)(CC(C)(C)C)C	4.55	0.12
108-36-1	c1(cccc([Br])c1)[Br]	3.75	1.16
108-38-3	c1(cccc(C)c1)C	3.20	-0.01
108-42-9	Nc1cccc([Cl])c1	1.88	-0.71
108-43-0	Oc1cccc([Cl])c1	2.50	-0.68
108-45-2	Nc1cccc(N)c1	-0.33	-1.86
108-57-6	c1(cccc(C=C)c1)C=C	4.15	0.59
108-60-1	O(C(C[Cl])C)C(C[Cl])C	2.48	-1.07

CAS	SMILES	log K_{ow}	log HLN
108-67-8	c1(cc(cc(C)c1)C)C	3.42	0.40
108-70-3	c1(cc(cc([Cl])c1)[Cl])[Cl]	4.19	1.19
108-78-1	n1c(nc(nc1N)N)N	-1.37	-3.16
108-80-5	N1C(=O)NC(=O)NC1=O	1.95	-5.03
108-86-1	c1(ccccc1)[Br]	2.99	-1.19
108-87-2	C1(CCCCC1)C	3.61	0.57
108-88-3	c1(ccccc1)C	2.73	-0.54
108-90-7	c1(ccccc1)[Cl]	2.84	-1.02
108-95-2	Oc1ccccc1	1.46	-1.50
109-09-1	n1c(cccc1)[Cl]	1.22	-0.85
109-69-3	[Cl]CCCC	2.64	-0.45
110-00-9	o1cccc1	1.34	-0.84
110-02-1	s1cccc1	1.81	-0.82
110-82-7	C1CCCCC1	3.44	-0.66
110-91-8	O1CCNCC1	-0.86	-1.26
110-98-5	O(CC(O)C)CC(O)C	-0.64	-2.07
111-44-4	O(CC[Cl])CC[Cl]	1.29	-0.81
111-94-4	C(#N)CCNCCC#N	-1.34	-1.45
112-40-3	C(CCCCCCCCCC)C	6.10	0.26
115-32-2	OC(c1ccc([Cl])cc1)(c1ccc([Cl])cc1)C([Cl])([Cl])[Cl]	5.02	1.99
115-77-5	OCC(CO)(CO)CO	-1.69	-2.85
115-86-6	O=P(Oc1ccccc1)(Oc1ccccc1)Oc1ccccc1	4.59	-0.76
115-96-8	O=P(OCC[Cl])(OCC[Cl])OCC[Cl]	1.70	-0.66
117-18-0	[Cl]c1cc([Cl])c([Cl])c([N+]([O-])=O)c1[Cl]	4.38	0.49
117-79-3	O=C1c3c(C(=O)c2ccccc12)ccc(N)c3	3.31	-1.06
117-81-7	O=C(OCC(CCCC)CC)c1c(cccc1)C(=O)OCC(CCCC)CC	7.60	0.44
118-44-5	N(c2c1c(cccc1)ccc2)CC	3.45	0.43
118-74-1	c1(c(c(c(c([Cl])c1[Cl])[Cl])[Cl])[Cl])[Cl]	5.73	2.44
118-79-6	Oc1c(cc(cc1[Br])[Br])[Br]	4.13	-0.29
118-83-2	C(F)(F)(F)c1cc([Cl])ccc1[N+]([O-])=O	3.20	-0.36
118-96-7	[O-][N+](=O)c1cc([N+]([O-])=O)c(c([N+]([O-])=O)c1)C	1.60	-1.50
119-12-0	S=P(OCC)(OCC)OC2=NN(c1ccccc1)C(=O)C=C2	3.20	-0.70
119-33-5	[O-][N+](=O)c1c(O)ccc(C)c1	2.37	-1.23

CAS	SMILES	log Kow	log HLN
119-47-1	Oc1c(cc(cc1C(C)(C)C)C)Cc1c(O)c(cc(C)c1)C(C)(C)C	6.25	0.03
119-56-2	OC(c1ccccc1)c1ccc(cc1)[Cl]	3.61	-0.89
119-61-9	O=C(c1ccccc1)c1ccccc1	3.18	-1.17
119-64-2	c12c(cccc1)CCCC2	3.49	0.75
119-93-7	Nc2c(cc(c1ccc(N)c(C)c1)cc2)C	2.34	-0.69
120-12-7	c12c(cccc1)cc1c(cccc1)c2	4.45	0.65
120-54-7	N2(C(=S)SSSSC(N1CCCCC1)=S)CCCCC2	2.80	-0.70
120-71-8	O(c1c(N)cc(cc1)C)C	1.74	-1.00
120-78-5	n1c3c(sc1SSc2nc1c(cccc1)s2)cccc3	4.66	-0.91
120-82-1	c1(ccc(c([Cl])c1)[Cl])[Cl]	4.02	1.20
120-83-2	Oc1c(cc(cc1)[Cl])[Cl]	3.06	-0.94
121-14-2	[N+]([O-])(=O)c1ccc(c([N+]([O-])=O)c1)C	1.98	-0.22
121-69-7	N(c1ccccc1)(C)C	2.31	-0.96
121-73-3	[O-][N+](=O)c1cccc([Cl])c1	2.46	-0.19
121-75-5	CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC	2.36	0.29
121-82-4	[N+]([O-])(=O)N1CN([N+]([O-])=O)CN([N+]([O-])=O)C1	0.87	-1.55
122-14-5	COP(=S)(OC)Oc1ccc([N+]([O-])=O)c(C)c1	3.30	0.03
122-20-3	OC(C)CN(CC(O)C)CC(O)C	-0.02	-2.77
122-34-9	n1c(nc(nc1[Cl])NCC)NCC	2.18	-0.94
122-39-4	N(c1ccccc1)c1ccccc1	3.50	0.35
123-63-7	O1C(OC(OC1C)C)C	0.67	-0.94
123-91-1	O1CCOCC1	-0.27	-1.51
124-11-8	C(=C)CCCCCCC	5.15	0.52
126-30-7	OCC(CO)(C)C	0.12	-1.65
126-33-0	O=S1(=O)CCCC1	-0.77	-1.70
126-72-7	O=P(OCC([Br])C[Br])(OCC([Br])C[Br])OCC([Br])C[Br]	4.29	-1.40
126-73-8	O=P(OCCCC)(OCCCC)OCCCC	4.00	-0.76
127-18-4	C(=C(\[Cl])[Cl])(/[Cl])[Cl]	3.40	-0.88
127-90-2	C([Cl])([Cl])([Cl])C([Cl])COCC([Cl])C([Cl])([Cl])[Cl]	5.30	1.04
128-37-0	Oc1c(cc(cc1C(C)(C)C)C)C(C)(C)C	5.10	0.32
129-00-0	c12c3c4ccc1cccc2ccc3ccc4	4.88	0.32
129-43-1	O=C2c1c(c(O)ccc1)C(=O)c1ccccc21	3.52	-1.15
131-09-9	O=C1c3c(C(=O)c2ccccc12)ccc([Cl])c3	4.46	-0.36

CAS	SMILES	log K_{ow}	log HLN
131-57-7	O=C(c1ccccc1)c1c(O)cc(OC)cc1	3.79	-0.76
132-64-9	o1c3c(c2ccccc12)cccc3	4.12	1.35
132-65-0	s1c3c(c2ccccc12)cccc3	4.38	0.83
133-06-2	O=C1N(SC([Cl])([Cl])[Cl])C(=O)C2CC=CCC12	2.80	0.40
134-32-7	c12c(c(N)ccc1)cccc2	2.25	-0.24
134-62-3	O=C(N(CC)CC)c1cccc(C)c1	2.18	-0.69
135-88-6	N(c2ccc1c(cccc1)c2)c1ccccc1	4.38	-0.41
137-26-8	N(C(=S)SSC(N(C)C)=S)(C)C	1.73	-1.18
140-66-9	Oc1ccc(cc1)C(CC(C)(C)C)(C)C	5.28	-0.04
141-93-5	c1(cccc(CC)c1)CC	4.57	0.09
142-96-1	O(CCCC)CCCC	3.21	-0.25
143-50-0	[Cl]C2([Cl])C4([Cl])C1([Cl])C5([Cl])C(=O)C3([Cl])C1([Cl])C2([Cl])C3([Cl])C45[Cl]	5.41	1.12
144-19-4	OCC(C(O)C(C)C)(C)C	1.24	-1.34
156-43-4	O(c1ccc(N)cc1)CC	1.24	-1.24
206-44-0	c12c3cccc1c1c(cccc1)c2ccc3	5.16	-0.02
208-96-8	c2ccc1cccc3c1c2C=C3	3.94	0.52
225-11-6	c4ccc3nc2ccc1ccccc1c2cc3c4	4.48	-0.18
226-36-8	c1ccc3c(c1)ccc4nc1c(ccc2ccccc12)cc34	5.73	-0.14
260-49-6	n2c1c(cccc1)cc1ccccc21	3.40	-0.29
294-62-2	C1CCCCCCCCCCC1	6.12	1.33
298-00-0	COP(=S)(OC)Oc1ccc(cc1)[N+]([O-])=O	2.86	0.55
298-04-4	CCOP(=S)(OCC)SCCSCC	4.02	0.03
299-84-3	COP(=S)(OC)Oc1cc([Cl])c([Cl])cc1[Cl]	4.88	0.95
309-00-2	[Cl]C3=C([Cl])C4([Cl])C2C1CC(C=C1)C2C3([Cl])C4([Cl])[Cl]	6.50	1.37
314-40-9	N1C(=O)N(C(C)CC)C(=O)C([Br])=C1C	2.11	-1.33
315-18-4	CNC(=O)Oc1cc(C)c(N(C)C)c(C)c1	2.56	-1.86
319-84-6	C1(C(C(C(C([Cl])C1[Cl])[Cl])[Cl])[Cl])[Cl]	3.80	1.23
319-85-7	C1(C(C(C(C([Cl])C1[Cl])[Cl])[Cl])[Cl])[Cl]	3.78	1.44
319-86-8	C1(C(C(C(C([Cl])C1[Cl])[Cl])[Cl])[Cl])[Cl]	4.14	1.70
320-60-5	FC(F)(F)c1c(cc(cc1)[Cl])[Cl]	4.24	1.81
328-84-7	FC(F)(F)c1ccc(c([Cl])c1)[Cl]	4.24	1.52
330-54-1	O=C(N(C)C)Nc1ccc(c([Cl])c1)[Cl]	2.68	-1.45
330-55-2	O=C(N(OC)C)Nc1ccc(c([Cl])c1)[Cl]	3.20	-0.97

CAS	SMILES	log Kow	log HLN
333-41-5	O(P(OCC)(Oc1nc(nc(C)c1)C(C)C)=S)CC	3.81	0.07
461-58-5	N\C(=N/C#N)N	-1.15	-2.11
462-08-8	n1cccc(N)c1	0.11	-1.87
479-27-6	c12c(c(N)ccc1)c(N)ccc2	1.78	-0.73
493-01-6	C12C(CCCC1)CCCC2	4.20	1.41
493-02-7	C12C(CCCC1)CCCC2	4.70	1.50
500-28-7	COP(=S)(OC)Oc1ccc([N+]([O-])=O)c([Cl])c1	3.45	-0.47
504-29-0	n1c(N)cccc1	0.48	-1.76
510-15-6	O=C(OCC)C(O)(c1ccc(cc1)[Cl])c1ccc(cc1)[Cl]	4.74	-0.08
512-56-1	O=P(OC)(OC)OC	-0.65	-1.96
526-73-8	c1(c(c(ccc1)C)C)C	3.66	-0.22
527-20-8	Nc1c([Cl])c([Cl])c([Cl])c([Cl])c1[Cl]	4.82	0.44
527-60-6	Oc1c(cc(cc1C)C)C	2.73	-1.30
535-77-3	c1(cccc(C(C)C)c1)C	4.50	0.07
541-73-1	c1(cccc([Cl])c1)[Cl]	3.53	-0.21
542-18-7	C1(CCCCC1)[Cl]	3.36	0.41
544-01-4	O(CCC(C)C)CCC(C)C	4.25	-0.45
544-76-3	C(CCCCCCCCCCCCCC)C	8.20	1.47
554-00-7	Nc1c(cc(cc1)[Cl])[Cl]	2.78	-0.65
554-84-7	[N+]([O-])(=O)c1cccc(O)c1	2.00	-0.49
555-03-3	[O-][N+](=O)c1cccc(OC)c1	2.16	-1.04
576-24-9	Oc1c(c(ccc1)[Cl])[Cl]	2.84	-0.43
577-55-9	c1(c(cccc1)C(C)C)C(C)C	4.10	0.57
579-10-2	O=C(N(c1ccccc1)C)C	1.12	-1.12
583-78-8	Oc1c(ccc([Cl])c1)[Cl]	3.06	-0.36
591-20-8	Oc1cccc([Br])c1	2.63	-0.95
591-27-5	Oc1cccc(N)c1	0.21	-1.88
591-35-5	Oc1cc([Cl])cc([Cl])c1	3.62	-0.91
606-20-2	[N+]([O-])(=O)c1c(c([N+]([O-])=O)ccc1)C	2.10	-0.94
606-28-0	O=C(OC)c1c(cccc1)C(=O)c1ccccc1	2.70	-1.30
608-93-5	c1(c(c(c(c([Cl])c1)[Cl])[Cl])[Cl])[Cl]	5.18	1.87
610-39-9	[O-][N+](=O)c1c([N+]([O-])=O)ccc(C)c1	2.08	-1.40
611-06-3	[O-][N+](=O)c1c(cc(cc1)[Cl])[Cl]	3.07	0.83

CAS	SMILES	log Kow	log HLN
611-21-2	N(c1c(cccc1)C)C	2.16	-0.74
612-22-6	CCc1ccccc1[N+]([O-])=O	2.58	-0.56
615-54-3	c1(ccc(c([Br])c1)[Br])[Br]	4.66	0.65
615-74-7	Oc1c(ccc(C)c1)[Cl]	2.90	-0.64
616-44-4	c1(C)cscc1	2.34	-1.27
618-62-2	[O-][N+](=O)c1cc(cc([Cl])c1)[Cl]	3.09	0.57
622-57-1	N(c1ccc(cc1)C)CC	2.32	-0.46
622-97-9	c1(ccc(cc1)C=C)C	3.44	0.24
623-26-7	N#Cc1ccc(C#N)cc1	0.93	-0.81
626-17-5	N#Cc1cccc(C#N)c1	0.80	-0.62
626-39-1	c1(cc(cc([Br])c1)[Br])[Br]	4.51	1.65
634-66-2	c1(c(c(c(cc1)[Cl])[Cl])[Cl])[Cl]	4.60	0.69
634-67-3	Nc1ccc([Cl])c([Cl])c1[Cl]	3.33	-0.27
634-83-3	Nc1cc([Cl])c([Cl])c([Cl])c1[Cl]	4.27	0.24
634-90-2	c1(cc(c(c([Cl])c1)[Cl])[Cl])[Cl]	4.56	0.93
634-91-3	Nc1cc([Cl])c([Cl])c([Cl])c1	3.32	0.28
634-93-5	Nc1c(cc(cc1[Cl])[Cl])[Cl]	3.52	0.67
636-28-2	c1(c(cc(c([Br])c1)[Br])[Br])[Br]	5.13	1.35
636-30-6	Nc1c(cc(c([Cl])c1)[Cl])[Cl]	3.45	-0.01
680-31-9	O=P(N(C)C)(N(C)C)N(C)C	0.28	-0.44
696-44-6	N(c1cccc(C)c1)C	2.19	-0.79
709-98-8	CCC(=O)Nc1ccc([Cl])c([Cl])c1	3.07	-0.35
732-11-6	COP(=S)(OC)SCN2C(=O)c1ccccc1C2=O	2.78	0.35
732-26-3	Oc1c(cc(cc1C(C)(C)C)C(C)(C)C)C(C)(C)C	6.06	1.81
760-23-6	C(C([Cl])C[Cl])=C	2.37	-1.28
764-13-6	C(=C\C=C(\C)C)(\C)C	3.50	0.49
767-00-0	C(#N)c1ccc(O)cc1	1.60	-1.03
782-74-1	N(Nc1c(cccc1)[Cl])c1c(cccc1)[Cl]	5.10	1.41
839-90-7	O=C1N(C(=O)N(C(=O)N1CCO)CCO)CCO	0.07	-5.99
873-63-2	OCc1cc([Cl])ccc1	1.94	-0.69
877-10-1	[Cl]c1c(C)c([Cl])c([Cl])c(C)c1[Cl]	5.67	1.12
877-11-2	Cc1c([Cl])c([Cl])c([Cl])c([Cl])c1[Cl]	5.62	1.40
879-39-0	[Cl]c1cc([N+]([O-])=O)c([Cl])c([Cl])c1[Cl]	3.93	-0.69

CAS	SMILES	log K_{ow}	log HLN
920-66-1	FC(F)(F)C(O)C(F)(F)F	1.66	-1.32
938-22-7	c1c([Cl])c(OC)c([Cl])c([Cl])c1[Cl]	4.75	1.60
938-86-3	c1c([Cl])c([Cl])c([Cl])c([Cl])c1OC	4.51	1.53
947-04-6	O=C1NCCCCCCCCCCC1	2.92	-0.68
947-72-8	[Cl]c2cc1ccccc1c1c2cccc1	4.99	1.80
950-37-8	S=P(OC)(OC)SCN1C(=O)SC(OC)=N1	2.20	-1.15
961-11-5	COP(=O)(OC)O\C(=C\[Cl])c1cc([Cl])c([Cl])cc1[Cl]	3.53	-1.02
962-58-3	CCOP(=O)(OCC)Oc1cc(C)nc(n1)C(C)C	2.07	-1.14
1163-19-5	O(c1c(c(c(c([Br])c1[Br])[Br])[Br])[Br])c1c(c(c(c([Br])c1[Br])[Br])[Br])[Br]	9.97	1.16
1212-29-9	N(C(=S)NC1CCCCC1)C1CCCCC1	3.69	-0.63
1241-94-7	O=P(Oc1ccccc1)(Oc1ccccc1)OCC(CC)CCCC	5.73	-0.15
1321-74-0	C=Cc1ccccc1C=C	3.80	0.53
1330-78-5	O=P(Oc1ccccc1C)(Oc1ccccc1C)Oc1ccccc1C	5.11	0.55
1460-02-2	c1c(cc(C(C)(C)C)cc1C(C)(C)C)C(C)(C)C	7.72	2.70
1490-04-6	OC1C(CCC(C)C1)C(C)C	3.19	-1.19
1502-22-3	O=C2C(C1=CCCCC1)CCCC2	3.17	-0.32
1544-19-0	FC(F)C(F)(F)Oc2ccc(C(C)(C)c1ccc(OC(F)(F)C(F)F)cc1)cc2	7.41	2.79
1570-64-5	Oc1c(cc(cc1)[Cl])C	2.78	-0.83
1582-09-8	CCCN(CCC)c1c(cc(cc1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O	5.34	0.62
1623-19-4	O=P(OCC=C)(OCC=C)OCC=C	1.76	-1.20
1631-58-9	CN(C)C1CSSC1	1.38	-1.58
1634-04-4	O(C(C)(C)C)C	0.94	-0.88
1634-78-2	CCOC(=O)CC(SP(=O)(OC)OC)C(=O)OCC	0.52	-1.04
1712-70-5	c1cc([Cl])ccc1C(C)=C	4.62	1.30
1746-01-6	[Cl]c3cc2Oc1cc([Cl])c([Cl])cc1Oc2cc3[Cl]	6.80	1.78
1746-81-2	O=C(N(OC)C)Nc1ccc(cc1)[Cl]	2.30	-1.13
1805-32-9	c1c([Cl])c([Cl])ccc1CO	2.74	-0.42
1825-21-4	COc1c([Cl])c([Cl])c([Cl])c([Cl])c1[Cl]	5.45	2.67
1825-31-6	c12c(c(ccc1[Cl])[Cl])cccc2	4.80	2.37
1836-77-7	[Cl]c2cc([Cl])c(Oc1ccc(cc1)[N+]([O-])=O)c([Cl])c2	4.97	0.75
1843-05-6	O=C(c1ccccc1)c1c(O)cc(OCCCCCCCC)cc1	6.96	0.16
1897-45-6	N#Cc1c(c(c(c(C#N)c1[Cl])[Cl])[Cl])[Cl]	2.90	0.27
1912-24-9	n1c(nc(nc1[Cl])NC(C)C)NCC	2.61	-1.05

CAS	SMILES	log Kow	log HLN
2042-14-0	c1c(O)ccc(C)c1[N+]([O-])=O	2.18	-0.80
2050-74-0	c12c(c(ccc1)[Cl])c(ccc2)[Cl]	4.30	0.91
2050-76-2	Oc1c2c(c(cc1[Cl])[Cl])cccc2	4.23	0.11
2051-24-3	[Cl]c1c([Cl])c([Cl])c(c([Cl])c1[Cl])c1c([Cl])c([Cl])c([Cl])c([Cl])c1[Cl]	8.27	2.86
2104-64-5	CCOP(=S)(Oc1ccc(cc1)[N+]([O-])=O)c1ccccc1	4.78	0.02
2104-96-3	COP(=S)(OC)Oc1cc([Cl])c([Br])cc1[Cl]	5.21	0.97
2122-19-2	S=C1NC(C)CN1	-0.07	-2.10
2173-57-1	O(c2ccc1c(cccc1)c2)CC(C)C	4.65	0.23
2212-67-1	CCSC(=O)N1CCCCCC1	3.21	-1.08
2216-51-5	OC1C(CCC(C)C1)C(C)C	3.19	-1.19
2216-69-5	O(c2c1c(cccc1)ccc2)C	3.45	0.39
2234-13-1	c12c(c(c(c([Cl])c1[Cl])[Cl])[Cl])c(c(c([Cl])c2[Cl])[Cl])[Cl]	8.50	1.62
2243-62-1	Nc1cccc2c(N)cccc12	0.89	-0.52
2255-17-6	O=P(OC)(OC)Oc1cc(C)c([N+]([O-])=O)cc1	1.69	0.01
2385-85-5	[Cl]C2([Cl])C4([Cl])C1([Cl])C5([Cl])C([Cl])([Cl])C3([Cl])C1([Cl])C2([Cl])C3([Cl])C45[Cl]	6.89	1.80
2460-49-3	COc1cc([Cl])c([Cl])cc1O	3.26	-0.15
2463-84-5	COP(=S)(OC)Oc1ccc(cc1[Cl])[N+]([O-])=O	3.58	0.01
2497-06-5	CCOP(=S)(OCC)SCCS(=O)(=O)CC	1.87	-0.67
2497-07-6	CCOP(=S)(OCC)SCCS(=O)CC	1.73	-0.70
2498-66-0	O=C3c1c(c2c(cc1)cccc2)C(=O)c1ccccc31	4.40	-0.84
2531-84-2	c3cc2c1ccc(C)cc1ccc2cc3	4.86	0.22
2539-17-5	COc1c(O)c([Cl])c([Cl])c([Cl])c1[Cl]	4.59	0.77
2581-34-2	[O-][N+](=O)c1c(cc(O)cc1)C	2.48	-1.20
2597-03-7	CCOC(=O)C(SP(=S)(OC)OC)c1ccccc1	3.69	-0.75
2631-40-5	O=C(Oc1c(cccc1)C(C)C)NC	2.31	-1.25
2636-26-2	COP(=S)(OC)Oc1ccc(C#N)cc1	2.71	0.23
2655-14-3	CNC(=O)Oc1cc(C)cc(C)c1	2.23	-1.29
2668-24-8	COc1cc([Cl])c([Cl])c([Cl])c1O	3.72	-0.30
2668-47-5	Oc2c(cc(c1ccccc1)cc2C(C)(C)C)C(C)(C)C	6.25	1.16
2691-41-0	[O-][N+](=O)N1CN([N+]([O-])=O)CN([N+]([O-])=O)CN([N+]([O-])=O)C1	0.16	-1.86
2921-88-2	CCOP(=S)(OCC)Oc1nc([Cl])c([Cl])cc1[Cl]	4.96	0.77
3089-11-0	O(CN(c1nc(nc(N(COC)COC)n1)N(COC)COC)COC)C	1.61	-2.84
3209-22-1	[O-][N+](=O)c1c(c(ccc1)[Cl])[Cl]	3.05	0.54

CAS	SMILES	log Kow	log HLN
3229-00-3	[Br]CC(C[Br])(C[Br])C[Br]	3.99	0.76
3268-87-9	[Cl]c3c([Cl])c([Cl])c2Oc1c([Cl])c([Cl])c([Cl])c([Cl])c1Oc2c3[Cl]	8.20	1.16
3296-90-0	OCC(C[Br])(C[Br])CO	1.06	-1.40
3319-31-1	O=C(OCC(CCCC)CC)c1ccc(c(C(=O)OCC(CCCC)CC)c1)C(=O)OCC(CCCC)CC	8.00	-1.03
3380-34-5	O(c1c(O)cc(cc1)[Cl])c1c(cc(cc1)[Cl])[Cl]	4.76	0.52
3389-71-7	C1(=C(C2(C([Cl])([Cl])C1(C=C2)[Cl])[Cl])[Cl])[Cl]	5.15	1.40
3481-20-7	Nc1c([Cl])c([Cl])cc([Cl])c1[Cl]	4.10	0.19
3761-41-9	COP(=S)(OC)Oc1ccc(S(C)=O)c(C)c1	1.92	-0.38
3761-42-0	S(=O)(=O)(C)c1c(C)cc(OP(=S)(OC)OC)cc1	2.05	-0.03
3766-81-2	O=C(Oc1c(cccc1)C(CC)C)NC	2.78	-0.52
3811-49-2	c2ccc1COP(=S)(OC)Oc1c2	2.67	-1.15
3846-71-7	Oc1c(cc(cc1n2nc1c(cccc1)n2)C(C)(C)C)C(C)(C)C	6.27	0.89
3864-99-1	Oc1c(cc(cc1n2nc1c(cc(cc1)[Cl])n2)C(C)(C)C)C(C)(C)C	6.91	0.72
4101-68-2	[Br]CCCCCCCCCC[Br]	6.12	-0.47
4130-42-1	Oc1c(cc(cc1C(C)(C)C)CC)C(C)(C)C	5.52	0.86
4390-04-9	C(CC(CC(CC(C)(C)C)C)(C)C)(C)(C)C	7.79	1.81
4821-19-6	C3(c2c(O)c(C1CCCCC1)ccc2)CCCCC3	6.30	0.20
4883-72-1	O=NN(C1CCCCC1)O	1.40	-0.90
4904-61-4	C/1=C/CC\C=C/CC\C=C/CC1	5.50	1.74
5103-71-9	[Cl]C1CC2C(C1[Cl])C1([Cl])C(=C([Cl])C2([Cl])C1([Cl])[Cl])[Cl]	6.22	2.74
5124-25-4	O=S(=O)(Nc1ccccc1)c2ccc(Nc1ccccc1)c([N+]([O-])=O)c2	4.60	-0.66
5428-54-6	[O-][N+](=O)c1ccc(c(O)c1)C	2.47	-1.24
5510-99-6	CCC(C)c1cccc(C(C)CC)c1O	4.36	-0.22
5566-34-7	[Cl]C13C([Cl])([Cl])C(C2C1CC([Cl])([Cl])C2)([Cl])C([Cl])=C3[Cl]	7.00	2.23
5707-44-8	CCc1ccc(cc1)c1ccccc1	5.08	0.06
6130-75-2	O(c1c(cc(c([Cl])c1)[Cl])[Cl])C	3.85	1.30
6165-51-1	c1(ccccc1)C(c1c(ccc(C)c1)C)C	5.39	0.10
6639-30-1	c1(c(cc(c([Cl])c1)[Cl])[Cl])C	4.56	2.01
6731-36-8	O(OC(C)(C)C)C1(OOC(C)(C)C)CC(CC(C)(C)C1)C	6.53	1.01
6842-15-5	CC(C)CC(C)CC(C)\C=C/C	5.80	0.51
6936-40-9	c1c([Cl])c([Cl])c(OC)c([Cl])c1[Cl]	4.68	1.58
7756-94-7	CC(C)CCC(C)CCC(C)=C	6.01	0.77
10315-98-7	C1COCCN1CC(C)C	1.17	-1.64

CAS	SMILES	log Kow	log HLN
10605-21-7	c2ccc1nc(NC(=O)OC)[nH]c1c2	1.52	-1.60
12002-48-1	[Cl]c1cc(cc(c1)[Cl])[Cl]	4.19	1.19
12789-03-6	[Cl]C1C([Cl])CC2C1C1([Cl])C(=C(C2([Cl])C1([Cl])[Cl])[Cl])[Cl]	6.22	2.74
13116-53-5	C(C[Cl])(C[Cl])([Cl])[Cl]	2.72	-0.28
13358-11-7	C2=CC1(C(C)C)CCC2(C2C(N(C(C12)=O)CC(CC)CCCC)=O)C	5.96	0.31
13475-82-6	C(CC(CC(C)(C)C)C)(C)(C)C	5.94	0.72
13540-50-6	c1ccccc1Cc1cc(C)ccc1C	5.65	0.45
13674-84-5	O=P(OC(C[Cl])C)(OC(C[Cl])C)OC(C[Cl])C	2.68	-1.31
13674-87-8	O=P(OC(C[Cl])C[Cl])(OC(C[Cl])C[Cl])OC(C[Cl])C[Cl]	3.65	-0.52
13936-21-5	O=C1c3c(C(=O)c2ccccc12)ccc(CCCCC)c3	5.59	0.20
14816-18-3	CCOP(=S)(OCC)O\N=C(\C#N)c1ccccc1	4.39	0.84
15087-24-8	O=C1\C(C2C(C)(C)C1(CC2)C)=C\c1ccccc1	5.37	-0.21
15258-73-8	c1c([Cl])c(CO)c([Cl])cc1	2.02	-1.37
15862-07-4	[Cl]c1cc([Cl])c(cc1[Cl])c1ccccc1	5.81	1.84
15972-60-8	CCc1cccc(CC)c1N(COC)C(=O)C[Cl]	3.52	-1.10
16219-75-3	C\2(C1C=CC(C1)C2)=C\C	3.82	-0.56
16605-91-7	[Cl]c2cccc(c1ccccc1)c2[Cl]	5.02	2.15
17109-49-8	c1ccccc1SP(=O)(OCC)Sc1ccccc1	3.48	-1.04
17700-09-3	[Cl]c1ccc([N+]([O-])=O)c([Cl])c1[Cl]	3.61	-0.19
18181-70-9	COP(=S)(OC)Oc1cc([Cl])c(I)cc1[Cl]	5.51	0.86
18708-70-8	[O-][N+](=O)c1c(cc(cc1[Cl])[Cl])[Cl]	3.69	0.71
18854-01-8	S=P(OCC)(OCC)Oc2noc(c1ccccc1)c2	3.73	1.05
19408-74-3	[Cl]c3c2c(Oc1c(c([Cl])c(c([Cl])c1)[Cl])O2)cc(c3[Cl])[Cl]	8.21	1.30
19666-30-9	CC(C)Oc1cc(c([Cl])cc1[Cl])N1N=C(OC1=O)C(C)(C)C	4.80	0.77
20020-02-4	c2ccc1c([Cl])c([Cl])c([Cl])c([Cl])c1c2	5.75	1.20
21564-17-0	c2ccc1nc(SCSC#N)sc1c2	3.23	-1.01
21609-90-5	COP(=S)(Oc1cc([Cl])c([Br])cc1[Cl])c1ccccc1	6.31	1.26
24019-05-4	OS(=O)(=O)c1cc([Cl])ccc1Oc1ccc([Cl])cc1NC(=O)Nc1ccc([Cl])c([Cl])c1	3.61	-0.44
25154-52-3	Oc1ccc(cc1)C(C)CC(C)CC(C)C	5.77	-0.45
25154-54-5	[O-][N+](=O)c1ccccc1[N+]([O-])=O	1.69	-0.85
25265-71-8	CC(O)COCC(O)C	-0.64	-2.07
25311-71-1	CCOP(=S)(NC(C)C)Oc1ccccc1C(=O)OC(C)C	4.12	-0.51
25321-09-9	c1ccc(C(C)C)c(c1)C(C)C	4.10	0.57

CAS	SMILES	log Kow	log HLN
25321-14-6	Cc1cccc([N+]([O-])=O)c1[N+]([O-])=O	2.18	-0.92
25323-68-6	[Cl]c1c(cc(cc1)[Cl])c1c(cccc1)[Cl]	5.48	1.87
25512-42-9	[Cl]c1c(cccc1)c1c(cccc1)[Cl]	5.00	1.78
26087-47-8	CC(C)OP(=O)(OC(C)C)SCc1ccccc1	3.34	-1.20
26444-49-5	O=P(Oc1ccccc1)(Oc1ccccc1)Oc1ccccc1C	4.51	-0.27
26601-64-9	[Cl]c1c(cc(c(c1)[Cl])[Cl])c1c(cc(c(c1)[Cl])[Cl])[Cl]	6.34	2.55
26603-23-6	CCCCCCCCc1ccc(cc1)Nc1ccc(cc1)CCCCCCCC	11.26	2.43
26761-40-0	CC(C)CCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCC(C)C	10.36	0.55
26898-17-9	Cc1cc(ccc1Cc1ccccc1)Cc1ccccc1	6.59	1.55
26914-33-0	[Cl]c1c(cc(cc1)[Cl])c1c(ccc(c1)[Cl])[Cl]	6.09	2.16
28106-30-1	C=Cc1ccc(cc1)CC	4.19	0.16
28249-77-6	CCN(CC)C(=O)SCc1ccc([Cl])cc1	3.40	0.66
28575-17-9	CCc1cc(ccc1)c1cc(ccc1)CC	5.83	1.24
28680-45-7	[Cl]C1(C(C2(C(C1([Cl])C=C2)[Cl])[Cl])([Cl])[Cl])[Cl]	5.67	1.53
29082-74-4	[Cl]c1c([Cl])c([Cl])c(\C([Cl])=C(\[Cl])[Cl])c(c1[Cl])[Cl]	7.46	2.04
29253-36-9	CC(c1cccc2c1cccc2)C	4.63	0.13
29761-21-5	O=P(Oc1ccccc1)(Oc1ccccc1)OCCCCCCCC(C)C	5.44	-0.14
30171-80-3	[Br]c1c(c(cc(c1)OCC1OC1)C)[Br]	3.94	-1.21
32598-13-3	[Cl]c1ccc(cc1[Cl])c1ccc([Cl])c([Cl])c1	6.63	1.35
32669-06-0	c1ccccc1C(OCC[Cl])c1ccccc1	4.38	-0.07
32861-85-1	c1cc([Cl])cc([Cl])c1Oc1cc(OC)c([N+]([O-])=O)cc1	4.40	0.59
33423-92-6	c3c([Cl])cc2Oc1cc([Cl])cc([Cl])c1Oc2c3[Cl]	7.10	1.10
33576-92-0	S=P(OC)(OC)Oc1ccccc1	3.03	0.75
34883-39-1	[Cl]c1ccc([Cl])c(c1)c1ccccc1	5.10	2.38
34883-41-5	c1ccccc1c1cc([Cl])cc([Cl])c1	5.41	1.11
35065-27-1	[Cl]c1cc([Cl])c(cc1[Cl])c1cc([Cl])c([Cl])cc1[Cl]	7.75	2.55
35367-38-5	O=C(NC(=O)c1c(F)cccc1F)Nc1ccc(cc1)[Cl]	3.89	-0.45
35693-99-3	c1c([Cl])ccc([Cl])c1c1c([Cl])ccc([Cl])c1	6.09	2.16
35822-46-9	[Cl]c3c([Cl])c([Cl])c2Oc1cc([Cl])c([Cl])c([Cl])c1Oc2c3[Cl]	8.00	1.21
35860-37-8	CC(c1cc(cc2c1cccc2C(C)C)C(C)C)C	7.54	1.75
36065-30-2	[Br]CC([Br])(C)COc1c([Br])cc([Br])cc1[Br]	6.79	2.21
36335-67-8	S=P(OCC)(NC(C)CC)Oc1c([N+]([O-])=O)ccc(C)c1	4.62	-0.20
36734-19-7	c1c([Cl])cc([Cl])cc1N1C(=O)CN(C(=O)NC(C)C)C1=O	3.00	-2.45

CAS	SMILES	log Kow	log HLN
37680-65-2	[Cl]c1ccc([Cl])c(c1)c1ccccc1[Cl]	5.55	1.87
38444-93-8	[Cl]c1cccc(c1[Cl])c1cccc([Cl])c1[Cl]	6.18	2.00
38640-62-9	CC(c2c1cc(ccc1ccc2)C(C)C)C	6.08	0.73
39001-02-0	[Cl]c3c([Cl])c([Cl])c1c(oc2c([Cl])c([Cl])c([Cl])c([Cl])c12)c3[Cl]	8.60	1.22
39227-28-6	[Cl]c3c([Cl])c([Cl])c2Oc1ccc([Cl])c([Cl])c1Oc2c3[Cl]	8.21	1.27
40321-76-4	[Cl]c3c2c(Oc1cc([Cl])c(cc1O2)[Cl])cc(c3[Cl])[Cl]	6.64	1.56
41122-70-7	N#Cc2ccc(c1ccc(cc1)CCCCCC)cc2	6.09	0.85
42240-73-3	[Cl]c1c(ccc(c1[Cl])c1ccc(c(c1[Cl])[Cl])N)N	5.39	1.28
50375-10-5	c1c([Cl])c(OC)c([Cl])c([Cl])c1	3.64	1.24
50512-35-1	CC(C)OC(=O)\C(C(=O)OC(C)C)=C/1SCCS1	2.88	-2.13
51207-31-9	[Cl]c3cc2oc1cc([Cl])c([Cl])cc1c2cc3[Cl]	6.53	0.56
52315-07-8	[Cl]\C([Cl])=C/C1C(C)(C)C1C(=O)OC(C#N)c2cccc(Oc1ccccc1)c2	6.94	0.70
54135-80-7	c1c(OC)c([Cl])c([Cl])c([Cl])c1	3.74	1.40
54135-81-8	c1c([Cl])c([Cl])c(OC)cc1[Cl]	3.93	1.33
54135-82-9	c1c(OC)cc([Cl])c([Cl])c1[Cl]	4.22	0.63
55720-37-1	[Cl]c2ccc1cc([Cl])cc([Cl])c1c2	5.35	1.26
56348-72-2	[Cl]c1c(ccc(c1)Oc1cc(c(cc1)[Cl])[Cl])[Cl]	6.36	1.81
57018-04-9	S=P(OC)(OC)Oc1c([Cl])cc(C)cc1[Cl]	4.56	-0.11
57057-83-7	COc1c(O)cc([Cl])c([Cl])c1[Cl]	3.77	0.11
57117-31-4	c3([Cl])cc2c1cc([Cl])c([Cl])cc1oc2c([Cl])c3[Cl]	6.92	1.36
57117-39-2	c3([Cl])cc2c1ccc([Cl])c([Cl])c1oc2cc3[Cl]	6.23	0.66
57117-41-6	c3([Cl])c([Cl])c2c1cc([Cl])c([Cl])cc1oc2cc3[Cl]	6.79	1.36
57117-43-8	[Cl]c1c(c(cc2c1oc1c2ccc(c1[Cl])[Cl])[Cl])[Cl]	6.47	0.90
57117-44-9	[Cl]c3c([Cl])c2c1cc([Cl])c([Cl])c([Cl])c1oc2cc3[Cl]	7.92	1.00
57653-85-7	[Cl]c2cc1Oc3c(Oc1c([Cl])c2[Cl])cc([Cl])c([Cl])c3[Cl]	8.21	1.21
59080-33-0	[Br]c1c(c(cc(c1)[Br])[Br])c1ccccc1	6.03	1.25
59080-37-4	[Br]c1c(c(ccc1)[Br])c1c(cccc1[Br])[Br]	6.50	2.76
59261-08-4	[Br]c1c(c(cc(c1)[Br])[Br])c1c(cc(cc1[Br])[Br])[Br]	6.39	2.66
59365-60-5	[Cl]c1ccccc1C(O)CO	1.17	-1.13
59722-76-8	O=C2c4c(C(=O)c3c(N)c(Oc1ccc(cc1)[Br])cc(O)c23)cccc4	5.58	-0.85
60782-58-3	O[Si](CCCCCC)(CCCCCC)CCCCCC	8.51	0.04
60851-34-5	[Cl]c3cc2c1cc([Cl])c([Cl])c([Cl])c1oc2c([Cl])c3[Cl]	7.92	1.12
66332-96-5	C(F)(F)(F)c1ccccc1C(=O)Nc1cccc(OC(C)C)c1	3.70	-0.61

CAS	SMILES	log K_{ow}	log HLN
67562-39-4	c3([Cl])c([Cl])c2c1cc([Cl])c([Cl])c([Cl])c1oc2c([Cl])c3[Cl]	7.92	0.90
69806-40-2	[Cl]c1cc(C(F)(F)F)cnc1Oc1ccc(OC(C)C(=O)OC)cc1	4.05	-1.08
70648-26-9	[Cl]c3c([Cl])c2c1cc([Cl])c([Cl])cc1oc2c([Cl])c3[Cl]	7.92	1.12
75627-02-0	[Cl]c1c(cc(c2c1oc1c2c(c(cc1[Cl])[Cl])[Cl])[Cl])[Cl]	7.58	1.12
79060-60-9	[Cl]c1c(c(c(c2c1c1c(o2)c(c(cc1)[Cl])[Cl])[Cl])[Cl])[Cl]	7.58	0.43
84852-15-3	Oc1ccc(cc1)CCCCCCC(C)C	5.92	0.03
92341-06-5	[Cl]c1c(c(cc2c1c1c(o2)c(c(cc1[Cl])[Cl])[Cl])[Cl])[Cl]	7.58	1.12
119168-77-3	[Cl]c1c(CC)nn(C)c1C(=O)NCc1ccc(C(C)(C)C)cc1	4.93	-0.03
NA - 1	OCCOCCOCCOCCOCCOCCOCCOCCOCCCCCCCCCCCCC	3.07	-0.61
NA - 2	FC(F)(Oc1ccc(cc1)CCCCCCC)C(F)F	6.89	0.29
NA - 3	FC(F)(Oc1ccc(cc1)C(C)(C)C(C)C(C)C)C(F)F	7.12	0.40
NA - 4	FC(F)(Oc1ccc(cc1)C(C)(C)CC(C)(C)C)C(F)F	7.16	0.36
NA - 5	FC(F)(Oc1ccc(cc1)C(C)(CC(C)C)c1ccc(OC(F)(F)C(F)F)cc1)C(F)F	8.81	2.61
NA - 6	FC(F)(Oc1ccc(cc1)C(c1ccc(OC(F)(F)C(F)F)cc1)C(CC)CCCC)C(F)F	9.83	2.44
NA - 7	FC(F)(Oc1ccc(cc1)C(C)(CCCCCC)c1ccc(OC(F)(F)C(F)F)cc1)C(F)F	9.87	1.66

Table 9.2 CAS, name and log BCF values for 572 chemicals used to evaluate the A-G BCF models in BCFBAF in this QMRF.

CAS	NAME	log BCF
2-35-5	Methylisocyanothion	2.33
50-29-3	1,1-(2,2,2-Trichloroethylidene)bis(4-chlorobenzene)	4.29
55-38-9	O,O-Dimethyl O-[3-Methyl-4-(methylthio)phenyl]ester phosphorothioic acid	2.52
56-23-5	Methane, tetrachloro-	0.87
56-38-2	Phosphorothioic acid, O,O-diethyl-O-(4-nitrophenyl)ester	1.99
56-55-3	Benzo[a]anthracene	2.41
57-15-8	2-Propanol, 1,1,1-trichloro-2-methyl-	0.23
57-74-9	1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene	4.29
58-89-9	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	3.06
59-50-7	Phenol, 4-chloro-3-methyl-	0.93
60-29-7	Ethane, 1,1 -oxybis-	0.73
60-51-5	DIMETHOATE	0.20
60-57-1	DIELDRIN	3.95
61-82-5	1H-1,2,4-Triazol-3-amine	0.49
62-44-2	Acetamide, N-(4-ethoxyphenyl)-	1.48
62-53-3	Benzenamine	0.21
62-56-6	Thiourea	0.30
62-73-7	Phosphoric acid, 2,2-dichloroethenyl dimethyl ester	-0.30
63-25-2	1-Naphthalenol, Methylcarbamate	0.95
66-81-9	CYCLOHEXIMIDE	0.45
67-66-3	Methane, trichloro-	1.11
67-68-5	Methane, sulfinylbis-	0.60
67-72-1	Ethane, hexachloro-	2.71
68-12-2	Formamide, N,N-dimethyl-	-0.10
70-30-4	Phenol, 2,2-methylenebis[3,4,6-trichloro-	2.07
71-43-2	Benzene	0.63
71-55-6	Ethane, 1,1,1-trichloro-	0.70
72-20-8	ENDRIN	3.87
72-43-5	Benzene, 1,1-(2,2,2-trichloroethylidene)bis[4-methoxy-	2.50
72-55-9	1,1'-(Dichloroethenylidene)bis(4-chlorobenzene)	4.08
74-31-7	1,4-Benzenediamine, N,N -diphenyl-	3.12

CAS	NAME	log BCF
74-97-5	Methane, bromochloro-	0.60
75-09-2	Methane, dichloro-	1.36
75-25-2	Methane, tribromo-	1.13
75-35-4	Ethene, 1,1-dichloro-	1.11
75-65-0	2-Propanol, 2-methyl-	0.70
75-71-8	Methane, dichlorodifluoro-	0.79
76-12-0	1,1,2,2,-TETRACHLORODIFLUOROETHANE	1.77
76-13-1	Ethane, 1,1,2-trichloro-1,2,2-trifluoro-	1.70
76-44-8	HEPTACHLOR	3.94
76-83-5	Benzene, 1,1,1-(chloromethylidyne)tris-	2.63
77-73-6	4,7-Methano-1H-indene, 3a,4,7,7a-tetrahydro-	2.34
78-30-8	Phosphoric acid, tris(2-methylphenyl) ester	2.90
78-40-0	Phosphoric acid, triethyl ester	0.11
78-42-2	Phosphoric acid, tris(2-ethylhexyl) ester	1.70
78-51-3	Ethanol, 2-butoxy-, phosphate (3:1)	0.76
78-59-1	2-Cyclohexen-1-one, 3,5,5-trimethyl-	0.30
78-63-7	2,5-dimethyl-2,5-bis(tert-butylperoxy)hexane	3.48
78-79-5	1,3-Butadiene, 2-methyl-	1.30
78-87-5	Propane, 1,2-dichloro-	0.85
79-00-5	Ethane, 1,1,2-trichloro-	0.70
79-01-6	Ethene, trichloro-	1.20
79-27-6	Ethane, 1,1,2,2-tetrabromo-	0.74
79-34-5	Ethane, 1,1,2,2-tetrachloro-	1.11
79-46-9	Propane, 2-nitro-	0.92
79-92-5	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-	2.98
79-94-7	Phenol, 4,4 -(1-methylethylidene)bis[2,6-dibromo-	2.43
80-05-7	Phenol, 4,4 -(1-methylethylidene)bis-	1.64
80-43-3	Peroxide, bis(1-methyl-1-phenylethyl)	2.62
81-15-2	Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitro-	3.61
82-05-3	BENZANTHRONE	2.09
82-44-0	1-CHLOROANTHRAQUINONE	2.30
82-45-1	9,10-Anthracenedione, 1-amino-	1.98
82-68-8	Pentachloronitrobenzene	2.74

CAS	NAME	log BCF
83-32-9	Acenaphthylene, 1,2-dihydro-	2.88
83-42-1	Benzene, 1-chloro-2-methyl-3-nitro-	1.99
83-79-4	[1]Benzopyrano[3,4-b]furo[2,3-h][1]benzopyran-6(6aH)-one,1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-, [2R-(2à,6aà,12aà)]- (Rotenone)	1.41
84-15-1	1,1 :2 ,1 -Terphenyl	3.48
84-51-5	9,10-Anthracenedione, 2-ethyl-	0.98
84-74-2	1,2-Benzenedicarboxylic acid, dibutyl ester	2.22
85-01-8	Phenanthrene	3.40
85-22-3	Pentabromoethylbenzene	2.52
85-68-7	1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	1.21
86-30-6	Benzenamine, N-nitroso-N-phenyl-	1.33
86-73-7	9H-Fluorene	2.72
86-74-8	9H-Carbazole	2.23
87-40-1	Benzene, 1,3,5-trichloro-2-methoxy-	2.86
87-61-6	Benzene, 1,2,3-trichloro-	2.82
87-65-0	2,6-DICHLOROPHENOL	1.08
87-68-3	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-	3.82
87-82-1	Hexabromobenzene	3.00
87-83-2	Pentabromomethylbenzene	2.43
87-84-3	Cyclohexane, 1,2,3,4,5-pentabromo-6-chloro-	2.41
88-06-2	2,4,6-Trichlorophenol	1.94
88-19-7	Benzenesulfonamide, 2-methyl-	0.41
88-72-2	Benzene, 1-methyl-2-nitro-	1.26
88-73-3	1-Chloro-2-nitrobenzene	1.17
88-74-4	Benzenamine, 2-nitro-	1.00
88-75-5	Phenol, 2-nitro-	1.34
89-59-8	Benzene, 4-chloro-1-methyl-2-nitro-	1.92
89-61-2	1,4-Dichloro-2-nitrobenzene	2.05
89-63-4	Benzenamine, 4-chloro-2-nitro-	1.04
89-69-0	1,2,4,-Trichloro-5-nitrobenzene	1.84
90-12-0	Naphthalene, 1-methyl-	1.73
90-30-2	1-Naphthalenamine, N-phenyl-	3.23
90-41-5	O-AMINOBIPHENYL	1.41

CAS	NAME	log BCF
90-94-8	Methanone, bis[4-(dimethylamino)phenyl]-	1.45
91-15-6	1,2-Benzenedicarbonitrile	0.70
91-20-3	Naphthalene	1.93
91-22-5	Quinoline	0.58
91-23-6	2-Nitroanisole	0.70
91-57-6	Naphthalene, 2-methyl-	1.87
91-58-7	2-monochloronaphthalene	3.63
91-66-7	Benzenamine, N,N-diethyl-	2.01
91-94-1	3,3'-DICHLOROBENZIDINE	2.16
91-96-3	Butanamide, N,N-(3,3-dimethyl[1,1-biphenyl]-4,4-diyl)bis[3-oxo-	0.20
92-52-4	1,1 -Biphenyl	2.64
92-69-3	[1,1 -Biphenyl]-4-ol	1.59
92-77-3	2-Naphthalenecarboxamide, 3-hydroxy-N-phenyl-	0.81
92-84-2	10H-Phenothiazine	2.55
92-86-4	4,4'-dibromobiphenyl	3.92
94-52-0	1H-Benzimidazole, 5-nitro-	0.40
95-16-9	Benzothiazole	0.88
95-47-6	Benzene, 1,2-dimethyl	1.15
95-48-7	Phenol, 2-methyl-	1.03
95-49-8	Benzene, 1-chloro-2-methyl-	1.82
95-50-1	Benzene, 1,2-dichloro-	2.43
95-51-2	Benzenamine, 2-chloro-	0.95
95-56-7	O-BROMOPHENOL	1.52
95-57-8	Phenol, 2-chloro-	1.35
95-63-6	Benzene, 1,2,4-trimethyl-	2.08
95-64-7	3,4-DIMETHYLANILINE	0.95
95-69-2	2-METHYL-4-CHLOROANILINE	1.54
95-76-1	Benzenamine, 3,4-dichloro-	1.11
95-77-2	3,4-DICHLOROPHENOL	1.69
95-78-3	2,5-DIMETHYLANILINE	0.58
95-80-7	1,3-Benzenediamine, 4-methyl-	1.70
95-82-9	2,5-DICHLOROANILINE	1.18
95-94-3	Benzene, 1,2,4,5-tetrachloro-	3.44

CAS	NAME	log BCF
95-95-4	2,4,5-TRICHLOROPHENOL	2.73
96-12-8	1,2-DIBROMO-3-CHLOROPROPANE	1.06
96-18-4	Propane, 1,2,3-trichloro-	1.11
96-29-7	2-Butanone, oxime	0.70
96-45-7	2-Imidazolidinethione	0.26
96-76-4	Phenol, 2,4-bis(1,1-dimethylethyl)-	2.40
96-96-8	Benzenamine, 4-methoxy-2-nitro-	0.85
97-23-4	Phenol, 2,2-methylenebis[4-chloro-	2.28
98-08-8	BENZOTRIFLUORIDE	1.65
98-10-2	Benzenesulfonamide	0.68
98-15-7	Benzene, 1-chloro-3-(trifluoromethyl)-	2.35
98-54-4	Phenol, 4-(1,1-dimethylethyl)-	1.83
98-82-8	Benzene, (1-methylethyl)-	1.55
98-83-9	Benzene, (1-methylethenyl)-	1.80
98-84-0	1-Phenyl ethylamine	0.82
98-95-3	Benzene, nitro-	0.67
99-08-1	Benzene, 1-methyl-3-nitro-	1.08
99-09-2	Benzenamine, 3-nitro-	0.48
99-54-7	Benzene, 1,2-dichloro-4-nitro-	1.71
99-62-7	Benzene, 1,3-bis(1-methylethyl)-	3.28
99-65-0	Benzene, 1,3-dinitro-	0.77
99-71-8	4-(1-Methylpropyl)phenol	1.31
99-99-0	Benzene, 1-methyl-4-nitro-	0.90
100-00-5	Benzene, 1-chloro-4-nitro-	1.30
100-01-6	Benzenamine, 4-nitro-	0.60
100-02-7	Phenol, 4-nitro-	0.71
100-17-4	P-NITROANISOLE	1.08
100-18-5	Benzene, 1,4-bis(1-methylethyl)-	3.24
100-40-3	Cyclohexene, 4-ethenyl-	2.22
100-42-5	Benzene, ethenyl-	1.13
100-43-6	Pyridine, 4-ethenyl-	1.86
100-61-8	Benzenamine, N-methyl-	1.00
100-80-1	Benzene, 1-ethenyl-3-methyl-	1.55

CAS	NAME	log BCF
101-14-4	Benzenamine, 4,4-methylenebis[2-chloro-	2.24
101-53-1	4-HYDROXYDIPHENYLMETHANE	1.33
101-77-9	Benzenamine, 4,4 -methylenebis-	1.18
101-81-5	Benzene, 1,1 -methylenebis-	2.94
101-84-8	Benzene, 1,1 -oxybis-	2.50
102-70-5	2-PROPEN-1-AMINE, N,N-DI-2-PROPENYL-	0.55
102-71-6	Ethanol, 2,2 ,2 -nitrilotris-	0.59
103-44-6	2-ETHYLHEXYLVINYLETHER	2.78
103-50-4	Benzene, 1,1 -[oxybis(methylene)]bis-	2.43
103-69-5	N-ETHYLANILINE	1.11
103-83-3	Benzenemethanamine, N,N-dimethyl-	1.15
104-40-5	Phenol, 4-nonyl-	2.58
104-88-1	4-Chlorobenzaldehyde	0.32
105-05-5	P-DIETHYLBENZENE	2.68
105-06-6	Benzene, 1,4-diethenyl-	2.48
106-37-6	Benzene, 1,4-dibromo-	2.21
106-41-2	P-BROMOPHENOL	1.17
106-42-3	Benzene, 1,4-dimethyl	1.17
106-43-4	P-CHLOROTOLUENE	1.76
106-46-7	Benzene, 1,4-dichloro-	2.62
106-47-8	Benzenamine, 4-chloro-	0.84
106-48-9	Phenol, 4-chloro-	1.48
106-93-4	Ethane, 1,2-dibromo-	1.18
107-05-1	1-Propene, 3-chloro-	0.70
107-39-1	1-Pentene, 2,4,4-trimethyl-	2.78
108-36-1	Benzene, 1,3-dibromo-	2.82
108-38-3	Benzene, 1,3-dimethyl	1.17
108-42-9	Benzenamine, 3-chloro-	0.35
108-43-0	Phenol, 3-chloro-	1.20
108-45-2	1,3-Benzenediamine	0.81
108-57-6	Benzene, 1,3-diethenyl-	2.54
108-60-1	DCIP (2,2'-OXYBIS-1-CHLOROPROPANE)	1.08
108-67-8	Benzene, 1,3,5-trimethyl-	2.27

CAS	NAME	log BCF
108-70-3	Benzene, 1,3,5-trichloro-	2.97
108-78-1	1,3,5-Triazine-2,4,6-triamine	0.58
108-80-5	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione	-0.30
108-86-1	Benzene, bromo-	1.36
108-87-2	Cyclohexane, methyl-	2.27
108-88-3	Benzene, methyl-	0.92
108-90-7	Benzene, chloro-	1.25
108-95-2	Phenol	1.24
109-09-1	2-CHLOROPYRIDINE	1.28
109-69-3	Butane, 1-chloro-	1.23
110-00-9	Furan	0.70
110-02-1	Thiophene	0.95
110-82-7	Cyclohexane	1.92
110-91-8	Morpholine	0.45
110-98-5	2-Propanol, 1,1'-oxybis-	0.66
111-44-4	BIS(2-CHLOROETHYL) ETHER	1.00
111-94-4	Propanenitrile, 3,3 -iminobis-	0.08
112-40-3	Dodecane	2.38
115-32-2	DICOFOL	3.79
115-77-5	1,3-Propanediol, 2,2-bis(hydroxymethyl)-	0.10
115-86-6	Phosphoric acid, triphenyl ester	2.28
115-96-8	Ethanol, 2-chloro-, phosphate (3:1)	0.11
117-18-0	1,2,4,5-Tetrachloro-3-nitrobenzene	3.23
117-79-3	2-AMINOANTHRAQUINONE	1.51
117-81-7	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	2.77
118-44-5	1-NAPHTHALENAMINE, N-ETHYL-	2.32
118-74-1	Benzene, hexachloro-	4.33
118-79-6	Phenol, 2,4,6-tribromo-	2.71
118-83-2	4-CHLORO-1-NITRO-2(TRIFLUOROMETHYL)BENZENE	1.87
118-96-7	Benzene, 2-methyl-1,3,5-trinitro-	0.99
119-12-0	Phosphorothioic acid, O-(1,6-Dihydro-6-oxo-1-phenyl-3-pyridazinyl) O,O-diethyl ester	0.67
119-33-5	4-METHYL-2-NITROPHENOL	0.95
119-47-1	Phenol, 2,2 -methylenebis[6-(1,1-dimethylethyl)-4-methyl-	2.74

CAS	NAME	log BCF
119-56-2	BENZENEMETHANOL, 4-CHLORO-.ALPHA.-PHENYL-	1.79
119-61-9	Methanone, diphenyl-	1.08
119-64-2	Naphthalene, 1,2,3,4-tetrahydro-	2.53
119-93-7	[1,1-Biphenyl]-4,4-diamine, 3,3-dimethyl-	1.67
120-12-7	Anthracene	3.26
120-54-7	Piperidine, 1,1 -(tetrathiodicarbonothioyl)bis-	1.23
120-71-8	2-METHOXY-5-METHYLBENZENAMINE	0.55
120-78-5	Benzothiazole, 2,2 -dithiobis-	1.42
120-82-1	Benzene, 1,2,4-trichloro-	3.32
120-83-2	Phenol, 2,4-dichloro-	1.53
121-14-2	Benzene, 1-methyl-2,4-dinitro-	0.96
121-69-7	Benzenamine, N,N-dimethyl-	0.90
121-73-3	1-Chloro-3-nitrobenzene	1.89
121-75-5	Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethylester	1.52
121-82-4	1,3,5-Triazine, hexahydro-1,3,5-trinitro- (RDX)	0.30
122-14-5	O,O-Dimethyl O-(3-methyl-4-nitrophenyl)ester phosphorothioic acid (Fenitrothion)	1.95
122-20-3	2-Propanol, 1,1 ,1 -nitrilotris-	-0.24
122-34-9	SIMAZINE	0.56
122-39-4	Benzenamine, N-phenyl-	2.18
123-63-7	1,3,5-Trioxane, 2,4,6-trimethyl-	0.48
123-91-1	1,4-Dioxane	-0.30
124-11-8	Isononene	3.17
126-30-7	1,3-Propanediol, 2,2-dimethyl-	0.67
126-33-0	Thiophene, tetrahydro-, 1,1-dioxide	0.85
126-72-7	TRIS(2,3-DIBROMOPROPYL) PHOSPHATE	0.51
126-73-8	Phosphoric acid tributyl ester	1.47
127-18-4	Ethene, tetrachloro-	1.72
127-90-2	2,3,3,3,2',3',3',3'-OCTACHLORODIPROPYLETHER	3.28
128-37-0	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	3.03
129-00-0	Pyrene	3.18
129-43-1	1-HYDROXYANTHRAQUINONE	2.25
131-09-9	9,10-Anthracenedione, 2-chloro-	2.28
131-57-7	Methanone, (2-hydroxy-4-methoxyphenyl)phenyl-	1.97

CAS	NAME	log BCF
132-64-9	Dibenzofuran	3.18
132-65-0	Dibenzothiophene	3.05
133-06-2	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]-	1.98
134-32-7	1-Naphthylamine	1.40
134-62-3	Benzamide, N,N-diethyl-3-methyl-	0.38
135-88-6	N-Phenyl-2-naphthylamine	2.37
137-26-8	Thioperoxydicarbonic diamide ([(H2N)C(S)]2S2), tetramethyl-	0.53
140-66-9	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	2.46
141-93-5	M-DIETHYLBENZENE	2.73
142-96-1	Butane, 1,1 -oxybis-	1.86
143-50-0	Kepone	3.19
144-19-4	1,3-Pentanediol, 2,2,4-trimethyl-	0.00
156-43-4	Benzenamine, 4-ethoxy-	1.00
206-44-0	Fluoranthene	3.56
208-96-8	ACENAPHTHYLENE	2.43
225-11-6	BENZ(A)ACRIDINE	2.02
226-36-8	Dibenz(a,h)acridine	2.03
260-49-6	Acridine	2.10
294-62-2	CYCLODODECANE	3.91
298-00-0	Phosphorothioic acid, O,O-Dimethyl O-(4-nitrophenyl)ester	1.93
298-04-4	O,O-Diethyl-S-[2-(ethylthio)ethyl]ester, Phosphorothioic acid	2.34
299-84-3	Phosphorothioic acid, O,O-Dimethyl O-(2,4,5-trichlorophenyl)ester	3.58
309-00-2	1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-(1a,4a,4ab,5a,8a,8ab)-1,4:5,8-dimethanonaphthalene	3.74
314-40-9	2,4(1H,3H)-Pyrimidinedione, 5-bromo-6-methyl-3-(1-methylpropyl)-	0.51
315-18-4	Mexacarbate	1.42
319-84-6	(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.16
319-85-7	(1alpha,2beta,3alpha,4beta,5alpha,6beta)-1,2,3,4,5,6-Hexachloro-cyclohexane	3.16
319-86-8	(1alpha,2alpha,3alpha,4beta,5alpha,6beta)-1,2,3,4,5,6-hexachlorocyclohexane	3.25
320-60-5	2,4-Dichloro-1-(trifluoromethyl)benzene	3.37
328-84-7	3,4-dichlorobenzotrifluoride	3.18
330-54-1	Urea, N-(3,4-dichlorophenyl)-N,N-dimethyl-	1.15
330-55-2	LINURON	1.25
333-41-5	Phosphorothioic acid, o,o-diethyl o-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester	1.85

CAS	NAME	log BCF
461-58-5	Guanidine, cyano-	0.49
462-08-8	3-Pyridinamine	0.32
479-27-6	1,8-Naphthalenediamine	0.80
493-01-6	Naphthalene, decahydro- (cis)	3.21
493-02-7	Naphthalene, decahydro- (trans)	3.28
500-28-7	Phosphorothioic acid, O-(3-Chloro-4-nitrophenyl) O,O-dimethyl ester	1.55
504-29-0	2-Pyridinamine	1.06
510-15-6	CHLOROBENZILATE	2.68
512-56-1	Phosphoric acid, trimethyl ester	0.15
526-73-8	Benzene, 1,2,3-trimethyl-	2.29
527-20-8	Pentachloroaniline	2.71
527-60-6	2,4,6-Trimethylphenol	0.93
535-77-3	M-CYMENE	2.73
541-73-1	Benzene, 1,3-dichloro-	2.33
542-18-7	Cyclohexane, chloro-	2.34
544-01-4	DIISOPENTYL ETHER	2.23
544-76-3	Hexadecane	3.70
554-00-7	Benzenamine, 2,4-dichloro-	1.36
554-84-7	Phenol, 3-nitro-	1.40
555-03-3	M-NITROANISOLE	0.78
576-24-9	2,3-DICHLOROPHENOL	1.13
577-55-9	Benzene, 1,2-bis(1-methylethyl)-	2.14
579-10-2	N-METHYLACETANILIDE	0.18
583-78-8	Phenol, 2,5-dichloro-	1.01
591-20-8	M-BROMOPHENOL	1.18
591-27-5	Phenol, 3-amino-	1.34
591-35-5	3,5-DICHLOROPHENOL	1.91
606-20-2	Benzene, 2-methyl-1,3-dinitro-	1.34
606-28-0	BENZOIC ACID, 2-BENZOYL-, METHYL ESTER	1.15
608-93-5	Benzene, pentachloro-	3.75
610-39-9	1,2-DINO2 4-METHYL BENZENE	0.48
611-06-3	2,4-Dichloro-1-nitrobenzene	2.07
611-21-2	N-METHYL-O-TOLUIDINE	0.95

CAS	NAME	log BCF
612-22-6	2-ETHYLNITROBENZENE	1.11
615-54-3	Benzene, 1,2,4-tribromo-	3.63
615-74-7	PHENOL, 2-CHLORO-5-METHYL-	0.67
616-44-4	Thiophene, 3-methyl-	0.72
618-62-2	1,3-Dichloro-5-nitrobenzene	2.23
622-57-1	N-ETHYL-P-TOLUIDINE	0.61
622-97-9	Benzene, 1-ethenyl-4-methyl-	1.50
623-26-7	1,4-BENZENEDICARBONITRILE	0.30
626-17-5	1,3-DICYANOBENZENE	0.75
626-39-1	Benzene, 1,3,5-tribromo-	3.70
634-66-2	Benzene, 1,2,3,4-tetrachloro-	3.38
634-67-3	2,3,4-Trichloroaniline	2.00
634-83-3	2,3,4,5-Tetrachloroaniline	2.21
634-90-2	1,2,3,5-Tetrachlorobenzene	3.59
634-91-3	3,4,5-Trichloroaniline	2.36
634-93-5	2,4,6-TRICHLOROANILINE	2.00
636-28-2	1,2,4,5-Tetrabromobenzene	3.59
636-30-6	2,4,5-Trichloroaniline	2.33
680-31-9	HEXAMETHYLPHOSPHORAMIDE	-0.30
696-44-6	BENZENAMINE, N,3-DIMETHYL-	0.86
709-98-8	Propanil	1.84
732-11-6	S-[(1,3-Dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]O,O-dimethyl ester, Phosphorodithioic acid	0.26
732-26-3	Phenol, 2,4,6-tris(1,1-dimethylethyl)-	4.14
760-23-6	3,4-DICHLORO-1-BUTENE	1.11
764-13-6	2,5-DIMETHYL-2,4-HEXADIENE	2.32
767-00-0	Benzonitrile, 4-hydroxy-	0.91
782-74-1	2,2'-DICHLOROHYDRAZOBENZENE	3.66
839-90-7	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(2-hydroxyethyl)-	0.20
873-63-2	3-Chlorobenzenemethanol	1.29
877-10-1	1,2,4,5-Tetrachloro-3,6-dimethylbenzene	3.62
877-11-2	Pentachloromethyl benzene	3.83
879-39-0	1,2,3,4-Tetrachloro-5-nitrobenzene	1.90
920-66-1	2-Propanol, 1,1,1,3,3,3-hexafluoro-	0.40

CAS	NAME	log BCF
938-22-7	Benzene, 1,2,3,5-tetrachloro-4-methoxy-	3.34
938-86-3	Benzene, 1,2,3,4-tetrachloro-5-methoxy-	3.67
947-04-6	Azacyclotridecan-2-one	0.41
947-72-8	9-Chlorophenanthrene	3.49
950-37-8	S-((5-Methoxy-2-oxo-1,3,4-thiadiazol-3(2H)-yl)methyl)O,O-dimethyl ester phosphorodithioic acid	0.74
961-11-5	Phosphoric acid, 2-chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl ester	1.61
962-58-3	Diethyl-6-methyl-2-(1-methylethyl)-4-pyrimidinyl ester phosphoric acid	-0.35
1163-19-5	Benzene, 1,1 -oxybis[2,3,4,5,6-pentabromo-	3.38
1212-29-9	THIOUREA, N,N'-DICYCLOHEXYL-	0.64
1241-94-7	Phosphoric acid, 2-ethylhexyl diphenyl ester	2.49
1321-74-0	Benzene, diethenyl-	2.51
1330-78-5	Phosphoric acid, tris(methylphenyl) ester	2.90
1460-02-2	1,3,5-TRI-TERT-BUTYLBENZENE	4.36
1490-04-6	Cyclohexanol, 5-methyl-2-(1-methylethyl)-	1.18
1502-22-3	Cyclohexanone, 2-(1-cyclohexen-1-yl)-	0.70
1544-19-0	NL-33	4.35
1570-64-5	2-METHYL-4-CHLOROPHENOL	1.33
1582-09-8	Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-	3.36
1623-19-4	TRIALLYLPHOSPHATE	0.08
1631-58-9	4-(N,N-DIMETHYLAMINO)-1,2-DITHIOLANE	1.72
1634-04-4	Propane, 2-methoxy-2-methyl-	0.18
1634-78-2	Malaoxon	0.05
1712-70-5	4-ISOPROPENYL-CHLOROBENZENE	2.84
1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]dioxin	4.99
1746-81-2	Monolinuron	1.15
1805-32-9	3,4-DICHLOROBENZYL ALCOHOL	0.54
1825-21-4	Pentachloroanisole	4.16
1825-31-6	1,4-dichloronaphthalene	3.75
1836-77-7	CHLORNITROFEN	3.31
1843-05-6	Methanone, [2-hydroxy-4-(octyloxy)phenyl]phenyl-	1.90
1897-45-6	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro-	1.80
1912-24-9	1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-N-(1-methylethyl)-	0.90
2042-14-0	3-NITRO-P-CRESOL	1.00

CAS	NAME	log BCF
2050-74-0	1,8-dichloronaphthalene	3.79
2050-76-2	2,4-DICHLORO-1-NAPHTHOL	1.35
2051-24-3	Decachlorobiphenyl	4.24
2104-64-5	Ethyl p-nitrophenyl phenylphosphonothioate	2.97
2104-96-3	Bromophos	3.59
2122-19-2	PROPYLENE THIOUREA	1.00
2173-57-1	Naphthalene, 2-(2-methylpropoxy)-	2.80
2212-67-1	Hexahydro-1H-azepine-1-carbothioic acid, S-Ethyl ester	1.41
2216-51-5	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, [1R-(1à,2 ,5à)]-	0.89
2216-69-5	Naphthalene, 1-methoxy-	2.21
2234-13-1	Octachloronaphthalene	2.58
2243-62-1	1,5-DIAMINONAPHTHALENE	0.65
2255-17-6	Dimethylphosphoric acid 3-Methyl-4-nitrophenyl	0.44
2385-85-5	Mirex	4.31
2460-49-3	Phenol, 4,5-dichloro-2-methoxy-	2.03
2463-84-5	O-(2-Chloro-4-nirtophenyl) O,O-dimethyl ester phosphorothioic acid	1.89
2497-06-5	Disulfoton sulfone	0.70
2497-07-6	Disulfoton sulfoxide	0.00
2498-66-0	BENZ (A) ANTHRACENE-7,12-DIONE	1.69
2531-84-2	Phenanthrene, 2-methyl-	3.48
2539-17-5	Phenol, 2,3,4,5-tetrachloro-6-methoxy-	3.08
2581-34-2	3-METHYL-4-NITROPHENOL	1.06
2597-03-7	alpha-[(Dimethoxyphosphinothioyl)thio] benzeneacetic acid, Ethyl ester	1.69
2631-40-5	N-METHYL-2-ISOPROPYLPHENYLCARBAMATE	0.95
2636-26-2	O-(4-Cyanophenyl)O,O-dimethyl ester, Phosphorothioic acid	1.56
2655-14-3	N-ME-3,5-DIMETHYLPHENYL CARBAMATE	0.40
2668-24-8	Phenol, 2,3,4-trichloro-6-methoxy-	1.97
2668-47-5	[1,1 -Biphenyl]-4-ol, 3,5-bis(1,1-dimethylethyl)-	3.78
2691-41-0	Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine (HMX)	-0.30
2921-88-2	Phosphorothioic acid, O,O-diethyl O-(3,5,6-trichloro-2-pyridinyl) ester	3.18
3089-11-0	1,3,5-Triazine-2,4,6-triamine, N,N,N,N,N ,N -hexakis(methoxymethyl)-	0.54
3209-22-1	Benzene, 1,2-dichloro-3-nitro-	2.16
3229-00-3	PROPANE, 1,3-DIBROMO-2,2-BIS(BROMOMETHYL)-	1.94

CAS	NAME	log BCF
3268-87-9	1,2,3,4,5,6,7,8-Octachlorodibenzo-p-dioxin	3.12
3296-90-0	1,3-Propanediol, 2,2-bis(bromomethyl)-	0.68
3319-31-1	1,2,4-Benzenetricarboxylic acid, tris(2-ethylhexyl) ester	1.17
3380-34-5	Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-	1.72
3389-71-7	Hexachloronorbornadiene	3.81
3481-20-7	2,3,5,6-Tetrachloroaniline	2.52
3761-41-9	O,O-Dimethyl O-[3-methyl-4-(methylsulfinyl)phenyl]ester phosphorothioic acid	0.12
3761-42-0	O,O-Dimethyl O-[3-methyl-4-(methylsulfonyl)phenylester phosphorothioic acid	0.51
3766-81-2	2-(1-Methylpropyl)phenol, Methylcarbamate	1.41
3811-49-2	2-Methoxy-4H-1,3,2-benzodioxaphosphorin-2-sulfide	1.31
3846-71-7	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-	3.81
3864-99-1	Phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-	3.57
4101-68-2	1,2-DIBROMODECANE	1.78
4130-42-1	Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-	3.46
4390-04-9	Nonane, 2,2,4,4,6,8,8-heptamethyl-	3.82
4821-19-6	2,6-DICYCLOEHXYLPHENOL	3.02
4883-72-1	N-CYCLOHEXYL-N-NITROSO HYDROXYLAMINE	0.60
4904-61-4	1,5,9-CYCLODODECATRIENE	3.92
5103-71-9	alpha (cis) Chlordane	4.34
5124-25-4	Benzenesulfonamide, 3-nitro-N-phenyl-4-(phenylamino)-	1.61
5428-54-6	PHENOL, 2-METHYL-5-NITRO-	0.85
5510-99-6	2,6-DI-SEC-BUTYLPHENOL	2.39
5566-34-7	2,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene	4.30
5707-44-8	4-Ethylbiphenyl	2.82
6130-75-2	Benzene, 1,2,4-trichloro-5-methoxy-	2.81
6165-51-1	Benzene, 1,4-dimethyl-2-(1-phenylethyl)-	2.86
6639-30-1	2,4,5-Trichlorotoluene	3.87
6731-36-8	Peroxide, (3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)	3.96
6842-15-5	1-Propene, tetramer	3.25
6936-40-9	Benzene, 1,2,4,5-tetrachloro-3-methoxy-	3.69
7756-94-7	1-Propene, 2-methyl-, trimer	3.42
10315-98-7	N-ISOBUTYLMORPHOLINE	0.25
10605-21-7	Carbamic acid, 1H-benzimidazol-2-yl-, methyl ester	0.40

CAS	NAME	log BCF
12002-48-1	Benzene, trichloro-	3.00
12789-03-6	Chlordane (technical)	4.43
13116-53-5	PROPANE, 1,2,2,3-TETRACHLORO-	1.57
13358-11-7	N-(2-ETHYLHEXYL)-1-ISOPROPYL-4-METHYLBICYCLO[2,2	2.97
13475-82-6	Heptane, 2,2,4,6,6-pentamethyl-	2.94
13540-50-6	PHENYL XYLYLMETHANE	3.14
13674-84-5	2-Propanol, 1-chloro-, phosphate (3:1)	0.90
13674-87-8	2-Propanol, 1,3-dichloro-, phosphate (3:1)	1.08
13936-21-5	2-PENTYLANTHRAQUINONE	2.94
14816-18-3	3,5-Dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile, 4-ethoxy-7-phenyl-, 4-sulfide	2.91
15087-24-8	3-Benzylidene camphor	2.50
15258-73-8	BENZENEMETHANOL, 2,6-DICHLORO-	0.47
15862-07-4	2,4,5-Trichloro-1,1'-biphenyl	3.78
15972-60-8	Alachlor	1.12
16219-75-3	ETHYLIDENE NORBORNENE	2.04
16605-91-7	2,3-Dichloro-1,1'-biphenyl	3.98
17109-49-8	Phosphorodithioic acid, S,S-Diphenyl O-propyl ester	1.51
17700-09-3	1,2,3-Trichloro-4-nitrobenzene	2.20
18181-70-9	Phosphorothioic acid, O-(2,5-Dichloro-4-iodophenyl) O,O-dimethyl ester	3.62
18708-70-8	1,3,5-Trichloro-2-nitrobenzene	2.47
18854-01-8	Phosphorothioic acid, O,O-Diethyl-O-(5-phenyl-3-isoxazolyl)ester	2.61
19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	3.92
19666-30-9	3-[2,4-Dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one	3.08
20020-02-4	1,2,3,4-Tetrachloronaphthalene	3.70
21564-17-0	Thiocyanic acid, (2-benzothiazolylthio)methyl ester	2.32
21609-90-5	Leptophos	3.78
24019-05-4	Sulcofuron	1.87
25154-52-3	Phenol, nonyl- (mixed isomers)	2.19
25154-54-5	DINITROBENZENES	1.16
25265-71-8	Propanol, oxybis-	0.53
25311-71-1	2-[[Ethoxy[(1-methylethyl)amino]phosphinothioyl]oxy]benzoic acid 1-methylethyl ester	2.12
25321-09-9	DIISOPROPYLBENZENE (mixture)	3.26
25321-14-6	Benzene, methyldinitro-	1.09

CAS	NAME	log BCF
25323-68-6	TRICHLOROBIPHENYL	4.23
25512-42-9	DICHLOROBIPHENYL	3.75
26087-47-8	Phosphorothioic acid, O,O-Bis(1-methylethyl)S-(phenylmethyl)ester	0.94
26444-49-5	Phosphoric acid, methylphenyl diphenyl ester	2.51
26601-64-9	HEXACHLOROBIPHENYL	3.77
26603-23-6	Benzenamine, ar-octyl-N-(octylphenyl)-	1.54
26761-40-0	1,2-Benzenedicarboxylic acid, diisodecyl ester	1.16
26898-17-9	Benzene, methylbis(phenylmethyl)-	4.00
26914-33-0	TETRACHLOROBIPHENYL	4.10
28106-30-1	Benzene, ethenylethyl-	2.69
28249-77-6	Diethylcarbamothioic acid, S-[(4-Chlorophenyl)methyl]ester	2.23
28575-17-9	Diethylbiphenyl	3.76
28680-45-7	Heptachloronorbornene	4.05
29082-74-4	Octachlorostyrene	3.91
29253-36-9	ISOPROPYLNAPHTHALENE	2.78
29761-21-5	Phosphoric acid, isodecyl diphenyl ester	2.83
30171-80-3	Oxirane, [(dibromomethylphenoxy)methyl]-	1.11
32598-13-3	3,3',4,4'-Tetrachloro-1,1'-biphenyl	4.62
32669-06-0	2-CHLOROETHYLBENZHYDRYL ETHER	2.51
32861-85-1	2,4-Dichloro-1-(3-methoxy-4-nitrophenoxy)benzene	3.59
33423-92-6	1,3,6,8-Tetrachlorodibenzo-p-dioxin	3.76
33576-92-0	O,O-Dimethyl-O-phenylphosphorothioate	1.89
34883-39-1	2,5-Dichloro-1,1'-biphenyl	3.98
34883-41-5	3,5-Dichloro-1,1'-biphenyl	3.77
35065-27-1	2,2',4,4',5,5'-Hexachloro-1,1'-biphenyl	5.43
35367-38-5	DIFLUBENZURON	2.20
35693-99-3	2,2',5,5'-Tetrachloro-1,1'-biphenyl	4.26
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	3.67
35860-37-8	Naphthalene, tris(1-methylethyl)-	3.70
36065-30-2	2,4,6-TRIBROMOPHENYL(2-METHYL-2,3-DIBROMOPROPYL)	4.28
36335-67-8	(1-Methylpropyl)phosphoramidothioic acid, O-Ethyl O-(5-methyl-2-nitrophenyl)ester	2.46
36734-19-7	3-(3,5-Dichlorophenyl)-N-(1-methylethyl)-2,4-dioxo-1-imidazolidinecarboxamide	2.53
37680-65-2	2,2',5-Trichloro-1,1'-biphenyl	4.23

CAS	NAME	log BCF
38444-93-8	2,2',3,3'-Tetrachloro-1,1'-biphenyl	4.23
38640-62-9	Naphthalene, bis(1-methylethyl)-	3.27
39001-02-0	1,2,3,4,5,6,7,8-Octachlorodibenzofuran	2.89
39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	4.00
40321-76-4	1,2,3,7,8-Pentachlorodibenzo-p-dioxin	4.26
41122-70-7	4'-n-HEXYL-4-CYANOBIPHENYL	3.52
42240-73-3	2,2',3,3'-TETRACHLORO-4,4'-DIAMINODIPHENYLMETHAN	3.43
50375-10-5	Benzene, 1,2,4-trichloro-3-methoxy-	2.52
50512-35-1	Bis(1-methylethyl)ester, 1,3-Dithiolan-2-ylidene propanedioic acid	1.57
51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	3.61
52315-07-8	Cypermethrin	2.62
54135-80-7	Benzene, 1,2,3-trichloro-4-methoxy-	2.96
54135-81-8	Benzene, 1,2,5-trichloro-3-methoxy-	3.05
54135-82-9	Benzene, 1,2,3-trichloro-5-methoxy-	3.09
55720-37-1	1,3,7-trichloronaphthalene	4.43
56348-72-2	1,1'-Oxybis[3,4-dichlorobenzene]	4.51
57018-04-9	O-(2,6-Dichloro-4-methylphenyl) O,O-dimethyl ester, Phosphorothioic acid	2.86
57057-83-7	Phenol, 3,4,5-trichloro-2-methoxy-	2.41
57117-31-4	2,3,4,7,8-Pentachlorodibenzofuran	4.13
57117-39-2	2,3,6,7-Tetrachlorodibenzofuran	2.72
57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	3.58
57117-43-8	2,3,4,6,7-Pentachlorodibenzofuran	3.57
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	3.94
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	3.93
59080-33-0	2,4,6-tribromobiphenyl	3.87
59080-37-4	2,2',5,5'-tetrabromobiphenyl	4.97
59261-08-4	2,2',4,4',6,6'-hexabromobiphenyl	4.66
59365-60-5	1-CHLORO-2-(1,2-ETHANEDIOL)BENZENE	0.54
59722-76-8	9,10-Anthracenedione, 1-amino-2-(4-bromophenoxy)-4-hydroxy-	2.05
60782-58-3	TRIHEXYLSILANOL	2.70
60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	3.98
66332-96-5	N-[3-(1-Methylethoxy)phenyl]-2-(trifluoromethyl)benzamide	1.29
67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	3.45

CAS	NAME	log BCF
69806-40-2	Haloxyfop-methyl	1.23
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	3.90
75627-02-0	1,2,4,6,7,9-Hexachlorodibenzofuran	2.96
79060-60-9	1,2,3,4,6,7-Hexachlorodibenzofuran	2.78
84852-15-3	Phenol, 4-nonyl-, branched,	2.40
92341-06-5	1,2,3,6,7,9-Hexachlorodibenzofuran	3.20
119168-77-3	Tebufenpyrad	1.15
NA - 1	Octaethylene glycol monotridecyl ether	1.50
NA - 2	NL-83	2.96
NA - 3	NL-63B	3.71
NA - 4	NL-63A	3.92
NA - 5	NL-93	3.76
NA - 6	NL-133	3.19
NA - 7	NL-123	2.85