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Prediction of Soil Sorption Coefficients with COSMO-RS

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Abstract

Using a general theory for partition coefficients based on quantum chemically derived COSMO-RS (Concuctorlike Screening Model for Real Solvents) σ -moment descriptors, the logarithmic soil sorption coefficients $\log K_{OC}$ of a database of 440 compounds has been successfully correlated, achieving a standard deviation (*rms*) of 0.62 log-units on the training set and a predictive *rms* of 0.72 log-units on a more demanding test set. The quality of this generally applicable predictive approach is almost the same as the quality of a regression of $\log K_{OC}$ with experimental $\log K_{OW}$ values, which are the best correlations currently available. The error of this new predictive method is only about 43% of the error of a recently published model using a different quantum chemically based approach.

Keywords: Soil sorption; COSMO-RS; Prediction; Quantum chemistry;

1. Introduction

The adsorption coefficient of organic molecules to soil is an important property for the estimation of the fate of these compounds in the environment. This is of special relevance for pesticides which to a large extent get in contact with soil when they are applied to the crops. Therefore the soil sorption coefficient K_{OC} has become a standard parameter in the regulatory process of pesticides. Due to the large variation of different kinds of soils, the K_{OC} is normalized with respect to the soil content of organic carbon, because usually the organic components of the soil are most active with respect to adsorption. The usual definition is [1]

$$K_{OC} = \frac{C_{soil}}{C_W} \tag{1}$$

where C_{soil} is the concentration of compound X (in g/[g of organic carbon]) in the soil phase, and C_w denotes the concentration of X (in g/[g per gram of water]) in the aqueous phase.

The experimental measurement of K_{OC} is expensive, time-consuming, and often related with considerable experimental error or noise resulting from differences in soils and sometimes in temperature. Hence, there is a great need for reliable calculation methods which

can be used for the prediction of K_{OC} for new pesticides or to validate experimental data. Many methods have been reported which are based on correlations of $\log K_{OC}$ with other experimental data, especially with experimental $\log K_{OW}$ data, water solubilities, melting points, etc. [1 - 3].

In this paper we specially focus on pure predictive methods, which do not depend on other experimental data for the special compound under consideration. The advantages of such methods are that no time-consuming and expensive measurements have to be done for a new pesticide, and even more that they can be applied even for pesticide candidates which have not yet been synthesized. Methods of this kind have mainly be developed based on topological indices [2,3,5]. Meylan et al. [6] introduced a much broader applicable combination of topological indices with group contributions for polar groups [called PC-KOCWIN, further on). This method appears to have considerable predictive power. Nevertheless it cannot be applied for compounds with polar fragments, for which no group contributions have been fitted before. Thus it is not applicable to pesticides with new heterocyles or with other rare polar groups.

Recently, Winget et.al. published a study in which they try to predict K_{OC} using the universal solvation models SMx [7] which is based on quantum chemical calculations in combination with a dielectric continuum model. In this study 440 compounds are considered. The advantage of this approach is that it can be applied to almost any neutral organic compound because of the generality of the underlying quantum chemistry. But the reported predictive accuracy of about 1.6 log-units (*rms*) is much worse than for other methods currently available.

In this paper we present a new model for the prediction of K_{OC} , which is based on another universal solvation model, the COnductor-like Screening MOdel for Real Solvents, COSMO-RS, [8-11], which is more rigorous than the SMx-models used in ref. [7] in two regards:

COSMO-RS is based on density functional calculations which are more reliable than semiempirical and Hartree-Fock quantum chemical methods used in the context of SMx in ref.[7].
COSMO-RS is based on a quite rigorous thermodynamic concept for molecular interaction, which replaces the insufficient dielectric approximation [9,10]. Thus it enables the treatment of mixtures and of variable temperature without the need for new solvent parameters.

COSMO-RS has successfully been used for accurate prediction of many kinds of thermodynamic liquid-liquid and liquid-vapor equilibrium properties, including vapor pressure, solubility and many kinds of partition coefficients. By a generalization of the COSMO-RS theory [12] it has been shown that any kind of logarithmic partition coefficient can be expressed as a linear function of a small number of COSMO-RS descriptors, the σ -moments (see below). While the direct calculation of partition coefficients can only be used for solvent phases of known molecular composition, the σ -moment approach is applicable to situations of chemically less well defined phases. In this way physiological partition coefficients [12] and adsorption coefficients to activated carbon [13] have been successfully correlated.

2. Methodology and Theory

2.1. Koc Data.

The data sets used in this study are exactly the same as those used in the study of Winget et al. [7]. They consist of a training set of 387 compounds (Set1) that arises from a data collection of Meylan et al. [6], and a test of 53 compounds (Set2) selected from a data set of Sabljic et al. [2]. At one place a subset (SetPOW) of 316 compounds out of Set1 is used which is defined by the availability of experimental octanol-water partition coefficients (SetPow) according to ref. [7].

The full data set includes neutral compounds of very different classes, spanning the typical range of pesticide compounds. The elements C, H, N, O, S, P, F, Cl, Br, and I are represented in the data set. Molecular weights are rather equally distributed in the range of 50 to 400, with a minimum value of 32 and a maximum of 546. Most experimental values of $\log K_{OC}$ are in the range of 1.5 to 5, and the extremes are 0 and 6.5, respectively.

2.2. COSMO and COSMO-RS

COSMO-RS [8-11] is a theory combining quantum theory, dielectric continuum models, the concept of surface interactions, and statistical thermodynamics. Since a full derivation of the theory of COSMO-RS is beyond the scope of this article, a short summary of the essentials will be given here. The reader interested in details is referred to the references [8-11]. COSMO-RS considers the a liquid system as an ensemble of molecules of different kinds, including solvent and solute. For each kind of molecules X a density functional calculation with the dielectric continuum solvation model COSMO [8] is performed in order to get the total energy E^{X}_{COSMO} and the polarization (or screening) charge density (SCD) σ , that the dielectric continuum or conductor, respectively, produces on the molecular surface. σ is an good local descriptor of molecular surface polarity [12].

For the purpose of an efficient statistical thermodynamics calculation the liquid ensemble of molecules now is considered as an ensemble of pair-wise interacting molecular surfaces. The most important parts of the specific interaction between molecular surfaces, i.e. electrostatics ES and hydrogen bonding HB, are expressed by the SCDs σ and σ' of the contacting surface pieces:

$$E_{ES}(\sigma,\sigma') = \frac{\alpha'}{2}(\sigma+\sigma')^2$$
⁽²⁾

and

$$E_{HB}(\sigma,\sigma') = c_{HB} \min\{0,\sigma\sigma' + \sigma_{HB}^2\}$$

The three parameters α' , c_{HB} , and σ_{HB} have been adjusted to a large number of thermodynamic data. Since all relevant interactions depend on σ , the distribution functions (histograms) $p^X(\sigma)$ are required for the statistical thermodynamics. These σ -profiles can easily be derived from

(3)

the COSMO output. Note, that the σ -profiles provide a vivid picture of the molecular polarity (see Figure 1, and a discussion given in refs. [8] and [10]). Furthermore we need the σ -profile ps(σ) of the ensemble S, which is simply calculated as a sum of the molecular σ -profiles weighted by mol-fractions.



Figure 1: σ -profiles of different solvents. These profiles show the amount of molecular surface in a given interval of polarization charge density σ .

The chemical potentials of the compounds in the solvent are calculated by a novel, exact and very efficient statistical thermodynamics procedure. The first step is the iterative solution of the equation

$$\boldsymbol{\mu}_{S}(\boldsymbol{\sigma}) = -\frac{RT}{a_{eff}} \ln\left\{ \int d\boldsymbol{\sigma}' \, p_{S}(\boldsymbol{\sigma}') \exp\left(\frac{a_{eff}}{RT}(\boldsymbol{\mu}_{S}(\boldsymbol{\sigma}') - E(\boldsymbol{\sigma}, \boldsymbol{\sigma}'))\right) \right\}$$
(4)

where $E(\sigma,\sigma')$ is the sum of the contributions from eqs. 2 and 3. This implicit equation, in which a_{eff} denotes an effectively independent piece of molecular area, can be solved by iteration within milliseconds on a personal computer. It yields the function $\mu_S(\sigma)$ (σ potential) which tells how much the solvent S likes surface of polarity σ . This is a very characteristic function for each solvent. We call it the σ -potential of solvent S. Examples are given in Figure 2.



Figure 2: σ -potentials of solvents. These curves show the chemical potential (y-axis) of a piece of surface of polarization charge density σ in a solvent. Thus they the affinity of a solvent for surface of polarity σ .

Such σ -potentials describe the solvent behavior regarding electrostatics, HB-affinity, and hydrophobicity. In a second step the σ -potential is integrated over the surface of each compound X, yielding the chemical potential of X in S:

$$\boldsymbol{\mu}_{S}^{X} = \int p^{X}(\boldsymbol{\sigma})\boldsymbol{\mu}_{S}(\boldsymbol{\sigma})d\boldsymbol{\sigma} + \boldsymbol{\mu}_{comb\,S}^{X}$$
(5)

In this equation the surface integral is evaluated as an σ -integral, making use of the σ -profile of the solute X. The combinatorial contribution $\mu^{X}_{comb,S}$ in eq. 5 takes into account size and shape effects of solute and solvent [11]. Usually it is small compared to the first term in eq. 5 which results from the surface interactions. It is sufficient to consider the combinatorial part as a solvent specific constant, here.

As a result of this series of relatively simple steps, starting from a quantum chemical calculation for each compound we found a general expression for the chemical potential of a compound X in any solvent S, which may be a pure compound or a mixture. This allows us to calculate any partition coefficient as well as solubility. Based on density functional COSMO calculations, the few parameters required in COSMO-RS, have been fitted to a large set of experimental data [9], covering 215 diverse chemical compounds and the properties ΔG_{hydr} , log P_{vapor} , and the aqueous partition coefficients with octanol, hexane, benzene, and ether. Note, that the properties ΔG_{hydr} and log P_{vapor} involve the gas-phase, which requires a small addendum to the steps given above that is not of interest here. However, since log S_{aq} is the difference of $\Delta G_{hydr}/RT$ and ln P_{vapor} , aqueous solubility was implicitly taken into account in the parameterization of COSMO-RS. The initial COSMO-RS parameterization yielded a *rms* of 0.3 log-units for the diverse partition and solubility properties of small and medium sized molecules [9]. In recent parameterizations the error has been reduced to about 0.23 log-units.

2.3 Extension of COSMO-RS to chemically undefined phases

As shown in Chapter 2.2, COSMO-RS is a reliable method for the a priori prediction of thermophysical data and phase equilibria of pure fluids and liquid mixtures of well defined composition. Nevertheless, there are several thermodynamic equilibria of industrial importance, which involve one or more phases, which are either chemically less defined, or which are disordered, but not really liquid, or both. Since in such phases no surface composition function $p_S(\sigma)$ is available, the σ -potential $\mu_S(\sigma)$ of the phase S and the chemical potentials μ_S^X of solutes X in these phases cannot be directly calculated by COSMO-RS. But an indirect treatment of such phases by COSMO-RS is enabled by the following extension:

Consideration of a large number of different solvents led to the finding (see as well figure 2) that σ -potentials can be described very well by a Taylor-like expansion of the form

$$\boldsymbol{\mu}_{S}(\boldsymbol{\sigma}) \cong \sum_{i=-2}^{m} c_{S}^{i} f_{i}(\boldsymbol{\sigma})$$
(6)

with

$$f_i(\boldsymbol{\sigma}) = \boldsymbol{\sigma}^i \quad \text{for } i \ge 0 \tag{7}$$

and

$$f_{-2/-1}(\sigma) = f_{acc/don}(\sigma) \cong \begin{cases} 0 & if \quad \pm \sigma < \sigma_{hb} \\ \mp \sigma + \sigma_{hb} & if \quad \pm \sigma > \sigma_{hb} \end{cases}$$
(8)

The highest order of the polynomial contributions (eq. 6) required for a sufficient description of σ -potentials typically is m = 3. The hydrogen bonding contributions expressed by eq. 8 are necessary to describe the acceptor and donor behavior of the solvent. As can be seen in figure 2, this behavior corresponds to an almost linear descent in the σ -potentials starting from some threshold σ_{HB} . The functions $f_{\text{acc}}(\sigma)$ and $f_{\text{don}}(\sigma)$ are well capable of describing just these features of the σ -potentials. Using this Taylor expansion, we may characterize each solvent (at fixed temperature, usually room temperature) by the set of σ -coefficients c^i_S . Obviously any difference between the σ -potentials of two solvents is of the same kind of expansion, with coefficients $c^i_{S,S'}$ being just the difference of the coefficients of the two solvents. Partition coefficients are connected with the pseudo-chemical potentials by the equation

$$kT\ln K_{S,S'}^X = \left[\mu_{S'}^X - \mu_S^X\right] \tag{9}$$

Using eq. 5 for $\mu_s(\sigma)$, we thus find that any partition coefficient between two solvents S and S' should be expressible in the form

$$\ln K_{S,S'}^{X} = \frac{1}{kT} \Big[c_{S,S'} + \int p^{X}(\boldsymbol{\sigma}) (\boldsymbol{\mu}_{S'}(\boldsymbol{\sigma}) - \boldsymbol{\mu}_{S}(\boldsymbol{\sigma})) d\boldsymbol{\sigma} \Big]$$

$$\cong \widetilde{c}_{S,S'} + \int p^{X}(\boldsymbol{\sigma}) \sum_{i=-2}^{m} \widetilde{c}_{S,S'}^{i} f_{i}(\boldsymbol{\sigma}) d\boldsymbol{\sigma} = \widetilde{c}_{S,S'} + \sum_{i=-2}^{m} \widetilde{c}_{S,S'}^{i} M_{i}^{X}$$
(10)

where the combinatorial contributions have been subsumed in $\tilde{c}_{s,s'}$ and the σ -moments M_i^X of the solute X are defined by

$$M_i^X = \int p^X(\boldsymbol{\sigma}) f_i(\boldsymbol{\sigma}) d\boldsymbol{\sigma}$$
(11)

Eq. 10 implies that any logarithmic partition coefficient can be represented as a linear combination of σ -moments. As a consequence, the set of σ -moments M_i^X , i = 0,2,3, complemented by the hydrogen bond moments $M_{acc}^X (=M_{-2}^X)$ and $M_{don}^X (=M_{-1}^X)$ should be a very good and almost complete set of molecular descriptors for a linear regression analysis of any partition problem. Note, that the first moment M_I^X usually is of no importance, because it is just the negative of the total charge of the molecule. Hence, for neutral compounds M_I^X trivially vanishes. By definition of the σ -profiles the zero-th moment M_0^X is identical with the molecular surface. The second moment is an excellent measure of the overall electrostatic polarity of the solute, and the third moment is a measure of the asymmetry of the sigma profile. The hydrogen bond moments are quantitative measures of the acceptor and donor capacities of the compound X, respectively. Since the organic soil phase involved in the soil sorption coefficients is of unknown chemical composition, this σ -moment approach is well suited to generate a predictive K_{OC} model.

2.4. Calculations

Density functional COSMO calculations have been done for all compounds. Starting from the optimized geometries used by Winget et. al. [7], the geometries of all compounds have been optimized by the semi-empirical AM1/COSMO [14,8] method using the MOPAC2000 program [15]. Using the geometries thus optimized, the COSMO polarization charge densities σ on the molecular surfaces have been computed on density functional level with the COSMO extension of Turbomole program package [16, 17] using Becke-Perdew density functional theory [18, 19] with split valence polarization basis set. Finally, the σ moments have been calculated using the COSMO*therm* program [20]. The σ -moments of all 440 compounds considered in this paper are provided as supplementary material together with calculated and exp. values of log K_{OV} and log K_{OC}

A multi-linear regression was performed on the 387 compounds of the training set (Set 1) using a self-written multi-linear regression routine which automatically evaluates the predictivity of the model by leave-one-out cross-validation. The regression coefficients and standard deviations are referred to as r^2 and rms, and their analogs from cross-validation are noted as q^2 and qms.

3. Results and Discussion

The multi-linear regression of the experimental $\log K_{OC}$ value vs. 5 σ -moments yielded the model equation

$$\log K_{oc} = 0.0168(\pm 8)M_0 - 0.017(\pm 2)M_2 - 0.040(\pm 4)M_3 + 0.19(\pm 5)M_{acc} - 0.27(\pm 5)M_{don} + 0.37(\pm 14)$$

$$(N = 387, r^2 = 0.71, rms = 0.62, q^2 = 0.70, qms = 0.63, F = 189)$$
(12)

This model will be referred to as COSMO-KOC, further on. The results are graphically shown in Figure 3. On the chemically more demanding test set of 53 compounds COSMO-KOC achieves a rms deviation of 0.72. These results are significantly better than those achieved by Winget et al. [7]. They got rms = 1.36 on the training set and rms = 1.62 on the test set. Note, that the number of adjusted parameters is very similar in both models, i.e. 5 in their model and 6 in COSMO-KOC. The applicability of COSMO-KOC can be assumed to be even broader than that of the method of Winget et al.



Figure 3: Experimental vs. calculated soil sorption coefficients. Values on x-axis are by the COSMO-KOC model (see eq. 12).

In order to compare the quality of COSMO-KOC with methods based on other experimental data we considered the 316 compounds (SetKOW) for which experimental octanol-water partition coefficients are reported in ref. 6. A linear regression of $\log K_{oc}$ with respect to these experimental values yields

$$\log K_{oc} = 0.63(\pm 2) \log K_{ow} + 0.80(\pm 6)$$
(13)
(N = 316, r² = 0.77, rms = 0.56)

We call this the KOW-KOC model. On the same subset COSMO-KOC yields a *rms* of 0.59 (without re-fitting). Thus both models can be considered as almost equally accurate. In Figure 4 an analysis of the error distribution of both models is given. The deviations from experiment of the two methods are clearly correlated ($r^2 = 0.54$). Because COSMO-KOC and KOW-KOC models are absolutely independent, this error correlation may either be caused by a common systematic of the errors of the models, or it may be due to experimental error or experimental noise, resulting from different soil samples and eventually different temperatures. We consider the latter to be more likely, because the intrinsic accuracy of the COSMO-RS approach for logarithmic partition coefficients is about 0.3 log-units (*rms*). But we may keep in mind, that both COSMO-KOC and KOW-KOC derive the log K_{OC} -values from models of liquid partition. Hence there is some chance, that special effects arising from the fact that soil is a solid phase, may be missed by both models.



Figure 4: Error correlation of the two models COSMO-KOC (see eq. 12) and KOW-KOC (see eq. 13). The full line is the regression line.

The error distribution curve of COSMO-KOC for all 440 compounds would be best described by a Gaussian error function which is centered at $\delta = \text{COSMO-KOC} - \log K_{\text{OC,exp}} =$ 0.06 log-units and which has a width of 0.83 log-units. While on the positive side the error distribution is very to this Gaussian distribution, there are significantly more large negative deviations, i.e. large underestimations, than expected from a purely Gaussian distribution. A large number of these large underestimations arise from polycyclic aromatic hydrocarbons and their aza-derivatives. Interestingly, these classes show about the same underestimation in the KOW-KOC model. Hence it is likely, that some special adsorption effects are present in soil sorption of large, rigid compounds like polycyclic aromatic hydrocarbons that are not captured in pseudo-liquid partition models. Surprisingly simple alcohols appear to get overestimated systematically by about 0.8 log-units, without a significant trend in chain lengths. Again, the same feature can be found in the KOW-KOC model, with an even larger deviation of about 1.0 log-unit. For the 35 phosphate compounds in the dataset COSMO-KOC tends to overestimate the $\log K_{OC}$ significantly. The overall largest overestimation (2 log-units) is for phosalone, which is a phosphate. Since we have carefully checked the conformation of this outlier, no reason for this overestimation is obvious at the moment.

We also compared our method with the PC-KOCWIN estimation method of Meylan et al. [6]. For this we made use of a list of 430 estimated $\log K_{OC}$ values from PC-KOCWIN, which have been made available for this study by Meylan. On all 430 compounds the *rms* of PC-KOCWIN is 0.48. On a subset of 368 compounds, which we could merge with the structures of our data set, we found an *rms* deviation of 0.49, while COSMO-KOC gives a *rms* error of 0.62 on this set. It is remarkable, that there is almost no error correlation ($r^2 =$

0.04) between these two methods. For some compounds for which COSMO-KOC and KOW-KOC consistently find a large deviation from the experimental results, PC-KOCWIN finds almost zero error. Others, for which COSMO-KOC and KOW-KOC are in reasonable agreement with experiment, are large outliers in PC-KOCWIN. This behavior probably arises from the bias in the development of PC-KOCWIN. Polar fragment corrections have been defined only by the apparent necessity, i.e. based on the deviations to experiment. This procedure bears the danger that some experimental error has been fitted into polar group corrections, while for other compounds necessary corrections are missing. Since KOW-KOC and COSMO-KOC do not have any group-specific contributions they are not subject to such bias.

4. Summary

COSMO-KOC is a new and almost generally applicable method for the a priori prediction of soil sorption coefficients. It is based on σ -moments as molecular descriptors, which are derived from quantum chemical density functional calculations combined with the continuum solvation model COSMO. The underlying σ -moment approach is theoretically well justified and has been successfully validated for other partition coefficients. The *rms* of COSMO-KOC from experimental data is about 0.65 log-units. Hence it is about as accurate as prediction methods based on experimental values of log K_{OW} . It is likely that a large portion of the deviations arises from experimental error.

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Suppl. Material

Molecule logKo	/c exp.	COSMO)-KOC	deviatio	n	logKOW	/exp	KOW-KOC	deviation
Training Set									
methanol	0.4	0.4093	0.0093	-0.7	0.3599	-0.0401			
1-decanol	2.6	3.0777	0.4777	4.6	3.7095	1.1095			
1-propanol	0.5	1.0356	0.5356	0.3	0.9919	0.4919			
ethanol 0.2	0.7403	0.5403	-0.3	0.6127	0.4127				
1-butanol	0.5	1.3083	0.8083	0.9	1.3711	0.8711			
1-nonanol	1.9	2.7829	0.8829	4	3.3303	1.4303			
1-hexanol	1	1.8973	0.8973	2	2.0663	1.0663			
1-pentanol	0.7	1.5974	0.8974	1.5	1.7503	1.0503			
1-heptanol	1.1	2.1824	1.0824	2.6	2.4455	1.3455			
1-octanol	1.6	2.6914	1.0914	3	2.6983	1.0983			
benzo[f]quinolin	e	4.6	2.7004	-1.8996					
3-methylcholant	hrene	6.2	4.3155	-1.8845	6.4	4.8471	-1.3529		
7H-dibenzo[c,g]	carbazole	6	4.1669	-1.8331					
asulam 2.5	0.7114	-1.7886	-0.3	0.6127	-1.8873				
benzo[a]pyrene	6	4.2388	-1.7612	6.2	4.7207	-1.2793			
tetracene	5.8	4.0512	-1.7488	5.9	4.5311	-1.2689			
13H-dibenzo[a,i]	carbazol	e	6	4.3107	-1.6893	6.4	4.8471	-1.1529	
2,3,7,8-TCDDx	6.5	4.8643	-1.6357	4.4	3.5831	-2.9169			
dibenz[a,h]anthra	acene	6.3	4.6974	-1.6026	6.5	4.9103	-1.3897		
2,3,5-trimethylph	nenol	3.6	2.1922	-1.4078					
acridine 4.1	2.7073	-1.3927	3.4	2.9511	-1.1489				
tebuthiurony	2.8	1.4291	-1.3709						
pyrene 4.9	3.5602	-1.3398	5.1	4.0255	-0.8745				
9-methylanthrace	ene	4.8	3.4808	-1.3192	5.1	4.0255	-0.7745		
5-indanol	3.4	2.1179	-1.2821						
benz[a]anthracer	ne	5.3	4.0217	-1.2783	5.8	4.4679	-0.8321		
thiabendazole	3.2	1.9701	-1.2299						
7,12-dimethylber	nzanthrac	cene	5.4	4.2024	-1.1976	5.8	4.4679	-0.9321	
6-aminochrysene	e 5.2	4.014	-1.186	5	3.9623	-1.2377			
mevinphos	2.3	1.1204	-1.1796	1.2	1.5607	-0.7393			
2-aminoanthrace	ne	4.5	3.3518	-1.1482					
quinoline	3.1	1.9995	-1.1005	2	2.0663	-1.0337			
methomyl	1.3	0.2099	-1.0901	0.5	1.1183	-0.1817			
phenazine	3.4	2.3517	-1.0483	2.8	2.5719	-0.8281			
fluoranthene	4.6	3.5907	-1.0093	5.1	4.0255	-0.5745			
4-aminobenzoic	acid	2	1.0259	-0.9741	0.8	1.3079	-0.6921		
anthracene	4.3	3.3517	-0.9483	4.6	3.7095	-0.5905			
mirex 6	5.0625	-0.9375	5.3	4.1519	-1.8481				
1-napthylamine	3.5	2.6238	-0.8762	2.2	2.1927	-1.3073			
fluorene 3.9	3.0285	-0.8715	4.2	3.4567	-0.4433				
p-cresolp	2.7	1.8471	-0.8529	2	2.0663	-0.6337			
1-naphthol	3.3	2.4481	-0.8519	2.8	2.5719	-0.7281			
benzo[b]thiopher	ne	3.5	2.6504	-0.8496	3.1	2.7615	-0.7385		
2,3,4,5,6,2',5'-PC	СВо	6	5.2017	-0.7983					
diflubenzuron	3.8	3.0202	-0.7798	3.9	3.2671	-0.5329			

3.5-dimetry lptmp2.82.0330.76692.42.3191-enty lmap trimap3.83.037-0.76034.43.5830.2169quinto zenev4.33.540-0.75044.63.70954.50buty lbenzy lptm14.23.4420.75734.33.5190.6801phenol2.41.65151.75030.64970.73034.33.303-0.26972-methy lpap trimo2.41.65770.742320.6630.3337-0.26972-methy lpap trimo3.62.86410.75591.75030.6497-1.1052-methy lpap trimo4.94.1987-0.70134.63.7095-1.1052-methy lpap trimo4.90.4987-0.66931.31.62390.59212-methy lpap trimo2.41.73310.66691.81.30790.5921carbendazim2.41.24480.66520.81.30790.59213-nitrober zamide 1.91.24480.65185.84.6790.3213-nitrober zamide 1.91.24480.65121.80780.3021-1.30293-nitrober zamide 1.91.24480.65121.80780.3021-0.32212.24 + CEN4.83.0370.50210.5021-0.512-0.5123-acety lattrace3.30.56090.81.30790.3261-0.12923-acety lattrace3.40.56135.2630.5240.512-0.5123-settrace3	phenanthrene	4.1	3.3255	-0.7745	4.5	3.6463	-0.4537	
1-ethylmaphthaler3.83.0379.76234.443.5810.2169urra<	3,5-dimethylpher	nol	2.8	2.0331	-0.7669	2.4	2.3191	
unea0.50.20010.70012.70.90411.4041quintoznev3.54060.75033.70950.51090.5109butyl benzyl pit-late0.55051.75030.64070.75751.75030.6407diethylacetamid1.80.55750.74050.30.90190.8081p-nirophenol2.41.65770.74250.3010.91090.70132-methylnaphthaler3.80.80810.70194.43.58310.2169pentrophenol4.92.83070.66691.501.50300.6497carbendazim2.41.7310.66620.81.30790.5921carbendazim2.40.73140.66620.81.30790.5921dibenzothiopenzemid-191.23480.66520.81.30790.5921carbendazim2.411.2440.65610.81.30790.59212.2;4-PCBo4.80.5122.02720.2830.32710.5921social2.11.48470.65120.83.02170.5921social2.11.48470.57570.62631.5070.5211social2.11.48470.57570.5031.5070.5021social2.11.8270.57573.2673.26710.5292social2.11.8290.57631.5070.52630.5021social2.11.5290.57573.2673.26710.5292sociop	1-ethylnaphthale	ne	3.8	3.0377	-0.7623	4.4	3.5831	-0.2169
quintozener4.33.54060.75744.63.70950.5091btuty berzy linthike4.23.44270.75734.33.51990.6801phenel2.41.65570.74630.49910.8081pnirtophenol2.41.65570.74232.2.06630.33372-methy haptthike3.63.68410.71594.43.53010.21692-mity haptthike3.83.08910.71094.43.5310.21692-mithox ychor4.91.9370.66931.301.62391.87612-mithox ychor4.91.73310.66971.5300.6497carbendazin1.73410.66520.81.30700.5921dibenzothiopher4.03.3360.41693.5310.41693-nitrobenzami1.940.65515.84.7070.59212.2.4 - PCB4.4483.5840.65185.84.6700.59212.2.4 - PCB2.41980.58120.6280.30710.59213-sitrobenzami1.940.58120.62810.30710.5921soci2.11.48870.58120.57810.3214soci2.11.5810.56185.84.7070.321soci2.11.5820.57810.57810.57810.5781soci3.31.22190.57810.57810.57810.5781soci3.51.7570.56430.81.30700.5921 <td>urea 0.5</td> <td>-0.2601</td> <td>-0.7601</td> <td>-2.7</td> <td>-0.9041</td> <td>-1.4041</td> <td></td> <td></td>	urea 0.5	-0.2601	-0.7601	-2.7	-0.9041	-1.4041		
buty benzy l phtN is 1.4.23.4270.75734.33.51990.6801phenol2.41.65771.75030.69170.99190.8011p-intro-phenol2.41.65770.742320.66630.33372-methy l maphtN is 11.65770.742320.66630.33030.26972-ethy l maphtN is 13.602.68010.71034.1030.26910.35810.2169benzidins3.541.63790.66691.501.62391.61900.6191carbendazim2.401.73310.66620.81.30700.5921carbendazim1.2440.65610.861.30700.59213.nitro-bernzmi is 11.2440.65185.804.61090.33213.nitro-bernzmi is 10.580230.60571.30700.59212.924 · IST1.44870.65185.804.61090.32113.01701.41870.65121.57713.26710.13213.02171.57810.57753.26710.13213.02171.57810.57753.26710.13213.02171.57810.57753.26710.13213.02171.5290.57753.26710.13213.02171.5290.57511.5790.57513.02171.5290.57511.5990.56123.03171.5290.57511.5990.26113.041111.5290.57511.5990.2715 </td <td>quintozenev</td> <td>4.3</td> <td>3.5406</td> <td>-0.7594</td> <td>4.6</td> <td>3.7095</td> <td>-0.5905</td> <td></td>	quintozenev	4.3	3.5406	-0.7594	4.6	3.7095	-0.5905	
phenol2.41.64440.75561.51.75030.64747diethylacetamide1.81.05750.74250.30.20160.33330.26972-methylaphthalme3.62.86140.71594.3.50310.21692-methylaphthalme3.62.86140.71594.3.50310.2169methoxychlor4.904.19870.70134.63.70951.19050.5191carbendazim2.41.73310.66691.51.5070.59210.5191dibenzothiopheme1.23480.65520.81.30790.59210.41693-nitrobenzamide I.91.2440.6550.81.30790.59210.41693-nitrobenzamide I.91.2440.6550.81.30790.59210.33212,2;4-PCBo4.41780.5185.84.46790.33210.41693-nitrobenzamide I.91.2440.6550.81.30790.5921sioci2.11.48870.5120.5781.51.5sincer3.10.58023.50.50713.93.26710.13299-acetylamhace1.63.0210.5781.30790.59211.51-horthylamphthace1.63.0210.57830.51.51.51-horthylamphthace1.63.0370.52260.57671.51.51-horthylamphthace1.63.0370.52260.57671.51.51-horthylamphthace<	butyl benzyl phth	alate	4.2	3.4427	-0.7573	4.3	3.5199	-0.6801
diethylacetamide1.81.05350.74650.30.99190.8081p-nitrophenol2.41.65777.742322.0663-0.33372-methylnaphthalene3.62.8641-0.735943.3000.26972-ethylnaphthalene3.83.8010.71094.43.5831-0.2169methoxychlor4.94.1987-0.70134.63.7005-1.8761benzidine3.52.8307-0.66931.31.6239-1.8761carbendazim2.41.7331-0.66691.51.7503-0.64974-nitrobenzamide I.91.244-0.6560.81.3079-0.59212.2.4.PCBO4.84.1482-0.65185.84.479-0.33212.acetonaphtome2.92.272-0.628storid2.11.4887-0.6113storid2.11.4887-0.6131storid3.11.4887-0.6131storid3.11.4887-0.5189-acetylanthracene3.63.0217-0.5781-methylaphthalene3.63.0217-0.5630.563-1-methylaphthalene3.63.037-0.56430.563-3.5-dinitrobenzamide1.81.337-0.56430.563-1-methylaphthalene3.63.0273.5	phenol 2.4	1.6444	-0.7556	1.5	1.7503	-0.6497		
p-nirophenol2.41.6577-0.74232.2.0663-0.33372-methylnaphthalere3.62.8641-0.73594.3.303-0.26072-ethylnaphthalere3.83.0891-0.71034.43.5811-0.2169methoxychlor4.94.1987-0.66931.31.6239-1.8761carbendazim2.401.7331-0.66650.81.3079-0.5921carbendazim1.91.244-0.6560.81.3079-0.59212.4-nitrobenzamide I.91.244-0.6560.81.3079-0.59212.1421.4887-0.61132.4.1720.4887-0.6122.4.178-0.5185.84.4679-0.3321-2.4.1780.560375.693-0.3071-0.13292-acetylamtracere3.63.0217-0.5782.9acetylamtracere3.63.0217-0.5782.9acetylamtracere3.42.8224-0.5781-methylraphthalere3.63.0217-0.5631-methylraphthalere3.63.0217-0.5781-methylraphthalere3.63.0217-0.5781-methylraphthalere3.63.0217-0.5781-methylraphthalere3.63.0217-0.5781-methylraphthalere3.63.0217 </td <td>diethylacetamide</td> <td>1.8</td> <td>1.0535</td> <td>-0.7465</td> <td>0.3</td> <td>0.9919</td> <td>-0.8081</td> <td></td>	diethylacetamide	1.8	1.0535	-0.7465	0.3	0.9919	-0.8081	
2-methylnaphthalene 3.6 2.8641 -0.7359 4 3.303 -0.2097 2-ethylnaphthalene 3.8 3.0891 -0.7109 4.4 3.5831 -0.2169 methoxychlor 4.9 4.1987 -0.7013 4.6 3.7095 -1.1905 benzidine 3.5 2.8307 -0.6693 1.3 1.6239 -1.8761 carbendazim 2.4 1.7331 -0.6669 1.5 1.7503 -0.6447 4-nitrobenzamide 1.9 1.244 -0.6518 5.8 4.4679 -0.3321 2-acetonaphthone 2.9 2.272 -0.628 -0.3021 -0.1329 2-acetonaphthone 3.6 3.0217 -0.5783 -0.1329 -0.1329 9-acetylanthracene 3.6 3.0217 -0.5783 -0.1329 -0.5921 1-butylamine 1.9 1.3231 -0.5649 0.8 1.3079 -0.9921 3-strictobenzamide 2.3 1.7357 -0.5643 0.8 1.3079 -0.9921	p-nitrophenol	2.4	1.6577	-0.7423	2	2.0663	-0.3337	
2-ethylnaphthalene 3.8 3.0891 -0.7109 4.4 3.5831 -0.2169 methoxychlor 4.9 4.1987 -0.7013 4.6 3.7095 -1.1905 benzidine 3.5 2.807 -0.6693 1.3 1.6239 -1.8761 carbendazim 2.4 1.7331 -0.66652 0.8 1.3079 -0.5921 dibenzothiophene 4 3.36 -0.6644 4.4 3.5831 -0.4169 3-nitrobenzamide 1.9 1.244 -0.6518 5.8 4.4679 -0.3321 2.acetonaphthome 2.9 2.72 -0.668 -0.3017 - - storil 2.1 1.4887 -0.613 - -0.5783 - - storil 3.3 2.629 0.5769 0.8 1.3079 -0.5921 - 1-butylamine 1.9 1.3231 -0.5769 0.8 1.3079 -0.5921 aldrin 4.7 4.1337 -0.5637 0.8 1.3079 -0.5921 aldrin 4.7 1.8718 -0.5282 <t< td=""><td>2-methylnaphtha</td><td>lene</td><td>3.6</td><td>2.8641</td><td>-0.7359</td><td>4</td><td>3.3303</td><td>-0.2697</td></t<>	2-methylnaphtha	lene	3.6	2.8641	-0.7359	4	3.3303	-0.2697
methoxychlor 4.9 4.1987 -0.7013 4.6 3.7095 -1.1905 benzidine 3.5 2.8307 -0.6693 1.3 1.6239 -1.8761 carbendazin 2.4 1.7331 -0.6669 1.5 1.7503 -0.6497 4-nitrobenzamide1.9 1.244 -0.656 0.8 1.3079 -0.5921 2.2;4-PCBo 4.8 4.1482 -0.6518 5.8 4.4679 -0.5921 2.2;4-PCBo 4.8 4.1482 -0.6518 5.8 4.4679 -0.3321 2-acetomaphthome 2.9 2.272 -0.628	2-ethylnaphthale	ne	3.8	3.0891	-0.7109	4.4	3.5831	-0.2169
benzidine 3.5 2.8307 -0.6693 1.3 1.6239 -1.8761 carbendazim 2.4 1.7331 -0.6669 1.5 1.7503 -0.6497 4-nitrobenzamide 1.9 1.2348 -0.652 0.8 1.3079 -0.5921 dibenzothiophene 4 3.336 -0.664 4.4 3.5831 -0.4169 3-nitrobenzamide 1.9 1.244 -0.656 0.8 1.3079 -0.5921 2.2;4-PCB0 4.8 4.1482 -0.6518 5.8 4.4679 -0.3321 2-acetonaphthone 2.9 2.272 -0.628 isocil 2.1 1.4887 -0.6113 styrene 3 2.4198 -0.5802 3 2.6983 -0.3017 9-acetylanthracene 3.6 3.0217 -0.5783 -tolrothalonil 3.3 2.722 -0.578 1-methylnaphthalene 3.4 2.8224 -0.5776 3.9 3.2671 -0.1329 1-butylamine 1.9 1.3231 -0.569 0.8 1.3079 -0.5921 1-butylamine 1.9 1.3231 -0.5663 7 5.2263 0.5263 3,5-dinitrobenzamide 2.3 1.737 -0.5643 0.8 1.3079 -0.9921 9-anthracenemethanol 3.6 3.0373 -0.5627 chlorsulfuron 2.7 2.1549 -0.5451 2.1 2.1295 -0.5705 carbaryl 2.4 1.8718 -0.528 2.3 2.2559 -0.1441 4-acetylbiphenyl 3.2 2.6822 -0.5178 3,4,5-trichlorophenol 3.6 3.0924 -0.5076 4.1 3.3935 -0.2065 isopropalin 4.9 4.4079 -0.4921 iodobenzene 3.1 2.6142 -0.4858 3.3 2.8879 -0.2121 DNOCj 2.4 1.9183 -0.4817 2.1 2.1295 -0.2705 methabenzthiazuron 2.8 2.3337 -0.4663 4-methylbenzamide 1.8 1.3404 -0.4559 5.4 4.2151 -0.3849 4-methylbenzamide 1.8 1.3404 -0.4559 5.4 2.151 -0.3849 -1.5607 -0.2393 2,2;5-PCB0 4.6 4.1441 -0.4559 5.4 4.2151 -0.3849 -1.5607 -0.2393 2,2;5-PCB0 4.6 4.1441 -0.4559 5.4 4.2151 -0.3849 -1.5607 -0.2393 2,2;5-PCB0 4.6 1.444 -0.4559 5.4 4.2151 -0.3849 -1.5607 -0.2393 2,2;5-PCB0 4.6 1.444 -0.4559 5.4 4.2151 -0.3849 -1.5607 -0.2393 2,2;5-PCB0 4.6 1.444 -0.4559 5.4 4.2151 -0.3849 -1.5607 -0.2393 2,2;5-PCB0 4.6 1.144 -0.4559 5.4 4.2151 -0.3849 -1.5607 -0.2393 -2.510705phenol 3.6 2.9961 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 -1.5607 -0.3292 -2.61070phenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4703 -2.61070phenol 2.6	methoxychlor	4.9	4.1987	-0.7013	4.6	3.7095	-1.1905	
carbendazim 2.4 1.7331 -0.6669 1.5 1.7503 -0.6497 4-nitrobenzamide 1.9 1.2348 -0.6652 0.8 1.3079 -0.5921 dibenzothiophene 4 3.336 -0.6644 4.4 3.5831 -0.4169 3-nitrobenzamide 1.9 1.244 -0.6518 5.8 4.4679 -0.3321 2.acetonaphthone 2.9 2.272 -0.628 -0.3017 - social 2.1 1.4887 -0.6113 -	benzidine	3.5	2.8307	-0.6693	1.3	1.6239	-1.8761	
Anitrobenzamide 1.91.2348-0.66520.81.3079-0.5921dibenzothiophene43.36-0.6644.43.5831-0.41693-nitrobenzamide 1.91.244-0.6560.81.3079-0.59212.2'.4-PCBo4.84.1482-0.65185.84.4679-0.33212.acetonaphthone2.92.272-0.628-0.50213-acetylanthracene3.63.0217-0.5783-acetylanthracene3.63.0217-0.5783-horothalonil3.32.722-0.5781-methylnaphthalene3.42.8224-0.57763.93.2671-0.13291-butylamine1.91.3231-0.57690.81.3079-0.9921aldrin4.74.1337-0.566375.22630.52633,5-dinitrobenzamide2.31.7357-0.56430.81.3079-0.99219-antracenemethanol3.63.0373-0.5027-0.5705-carbaryl 2.41.8718-0.52822.32.2559-0.14414-acetylbiphenyl 3.22.6822-0.51783,4,5-trichlorophenol3.63.0924-0.50764.13.3935-0.2025iodobenzne3.12.6142-0.48583.32.8879-0.2121DNOCj 2.41.9183-0.48172.12.1295-0.2705methabenzthiazuron2.82.3337-0.4663-4.methylbenzamide1.81.3404-0.4596	carbendazim	2.4	1.7331	-0.6669	1.5	1.7503	-0.6497	
Initiality Initiality <thinitiality< th=""> Initiality Initiali</thinitiality<>	4-nitrobenzamide	19	1 2348	-0.6652	0.8	1 3079	-0 5921	
anitrobanopienie 1 <th1< th=""> 1 1</th1<>	dibenzothiophene		4	3 336	-0 664	4.4	3 5831	-0 4169
$\begin{array}{l c c c c c c c c c c c c c c c c c c c$	3-nitrobenzamide		1 244	-0.656	0.8	1 3079	-0 5921	0.110)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2 2' 4-PCBo	4.8	4 1482	-0.6518	5.8	4 4679	-0.3321	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2,2,4-1 CD0	ч.0 2	7 Q	2 272	-0.628	 -077	-0.3321	
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4-acetylbiphenyl 3.22.6822-0.51783,4,5-trichlorophenol3.6 3.0924 -0.5076 4.1 3.3935 -0.2065isopropalin 4.9 4.4079 -0.4921-0.4921-0.2121-0.0205iodobenzene 3.1 2.6142-0.4858 3.3 2.8879 -0.2121DNOCj 2.4 1.9183 -0.4817 2.1 2.1295 -0.2705 -0.2393aemethylbenzamide1.8 1.3404 -0.4596 1.2 1.5607 -0.23932,2',5-PCBo4.6 4.1441 -0.4559 5.4 4.2151 -0.3849 dieldrin 4.1 3.6513 -0.4487 5 3.9623 -0.1377 carbazole 3.4 2.9557 -0.4443 3.6 3.0775 -0.3225 n-butylbenzene 3.4 2.9661 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 3,4-dichlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 3.2 2.8663 -0.0337 ethyl 4-methylbenzoate 2.6 2.1919 -0.4081 -0.4705 ethyl 4-methylbenzoate 2.5 2.1076 -0.3924 -0.3524 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid m	carbaryl 2.4	1.8718	-0.5282	2.3	2.2559	-0.1441		
3,4,5-trichlorophenol3.6 3.0924 -0.5076 4.1 3.3935 -0.2065 isopropalin 4.9 4.4079 -0.4921 0.4921 iodobenzene 3.1 2.6142 -0.4858 3.3 2.8879 -0.2121 DNOCj 2.4 1.9183 -0.4817 2.1 2.1295 -0.2705 methabenzthiazuron 2.8 2.3337 -0.4663 4-methylbenzamide 1.8 1.3404 -0.4596 1.2 1.5607 -0.2393 $2,2',5-PCBo$ 4.6 4.1441 -0.4559 5.4 4.2151 -0.3849 dieldrin 4.1 3.6513 -0.4487 5 3.9623 -0.1377 carbazole 3.4 2.9557 -0.4443 3.6 3.0775 -0.3225 n-butylbenzene 3.4 2.9661 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 $3,4$ -dichlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 3.5199 -0.3371 ethyl 4-methylbenzoate 2.6 2.1919 -0.4019 2 2.0663 -0.0337 ethyl 4-methylbenzoate 2.5 2.1076 -0.3824 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1	4-acetylbiphenyl	3.2	2.6822	-0.5178				
isopropalin 4.9 4.4079 -0.4921 iodobenzene 3.1 2.6142 -0.4858 3.3 2.8879 -0.2121 DNOCj 2.4 1.9183 -0.4817 2.1 2.1295 -0.2705 methabenzthiazuron 2.8 2.3337 -0.4663 4-methylbenzamide 1.8 1.3404 -0.4596 1.2 1.5607 -0.2393 2,2',5-PCB0 4.6 4.1441 -0.4559 5.4 4.2151 -0.3849 dieldrin 4.1 3.6513 -0.4487 5 3.9623 -0.1377 carbazole 3.4 2.9557 -0.4443 3.6 3.0775 -0.3225 n-butylbenzene 3.4 2.9661 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 3,4-dichlorophenol 3.1 2.6852 -0.4148 3.2 2.8247 -0.2753 2-chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 ethyl 4-methylbenzoate 2.6 2.1919 -0.4081 4-bromophenylurea 2.1 1.6981 -0.4019 2 2.0663 -0.0337 ethyl 4-nitrobenzoate 2.5 2.1076 -0.3924 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3-nitroacetanilide 1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401	3,4,5-trichloroph	enol	3.6	3.0924	-0.5076	4.1	3.3935	-0.2065
iodobenzene 3.1 2.6142 -0.4858 3.3 2.8879 -0.2121 DNOCj 2.4 1.9183 -0.4817 2.1 2.1295 -0.2705 methabenzthiazuron 2.8 2.3337 -0.4663 4-methylbenzamide 1.8 1.3404 -0.4596 1.2 1.5607 -0.2393 2,2',5-PCBo 4.6 4.1441 -0.4559 5.4 4.2151 -0.3849 dieldrin 4.1 3.6513 -0.4487 5 3.9623 -0.1377 carbazole 3.4 2.9557 -0.4443 3.6 3.0775 -0.3225 n-butylbenzene 3.4 2.9661 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 3,4-dichlorophenol 3.1 2.6852 -0.4148 3.2 2.8247 -0.2753 2-chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 ethyl 4-methylbenzoate 2.6 2.1919 -0.4081 4-bromophenylurea 2.1 1.6981 -0.4019 2 2.0663 -0.0337 ethyl 4-nitrobenzoate 2.5 2.1076 -0.3924 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3-nitroacetanilide 1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401	isopropalin	4.9	4.4079	-0.4921				
DNOCj 2.4 1.9183 -0.4817 2.1 2.1295 -0.2705 methabenzthiazuron 2.8 2.3337 -0.4663 4-methylbenzami 1.8 1.3404 -0.4596 1.2 1.5607 -0.2393 2,2',5-PCBo 4.6 4.1441 -0.4559 5.4 4.2151 -0.3849 dieldrin 4.1 3.6513 -0.4487 5 3.9623 -0.1377 carbazole 3.4 2.9557 -0.4443 3.6 3.0775 -0.3225 n-butylbenzene 3.4 2.9661 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 3,4-dichlorophenol 3.1 2.6852 -0.4148 3.2 2.8247 -0.2753 2-chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl 4-methylbenzoate 3 2.59 -0.41 4-bromophenylurea 2.6 2.1919 -0.4081 4-bromophenylurea 2.6 2.1919 -0.4019 2 2.0663 -0.0337 ethyl 4-methylbenzoate 2.5 2.1076 -0.3924 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3-nitroacetanilide1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401	iodobenzene	3.1	2.6142	-0.4858	3.3	2.8879	-0.2121	
methabenzthiazuron2.82.3337-0.46634-methylbenzamide1.81.3404-0.45961.21.5607-0.23932,2',5-PCBo4.64.1441-0.45595.44.2151-0.3849dieldrin 4.13.6513-0.448753.9623-0.1377carbazole3.42.9557-0.44433.63.0775-0.3225n-butylbenzene3.42.9661-0.43394.43.58310.1831benzoic acid phenyl ester3.22.7708-0.4292-3,4-dichlorophenol3.12.6852-0.41483.22.8247-0.27532-chlorophenol2.62.1884-0.41162.12.1295-0.4705ethyl 4-methylbenzoate3.2.59-0.414-bromophenylurea2.11.6981-0.401922.0663-0.0337ethyl 4-nitrobenzoate2.52.1076-0.38242,3,4,6-tetrachlorophenol3.73.3116-0.38844.33.5199-0.1801methiocarb2.31.9309-0.36912.92.63510.3351benzoic acid methyl ester2.11.7348-0.36522.12.12950.02953-nitroacetanilide1.91.5391-0.36091.51.7503-0.1497naphthalene32.6584-0.34163.42.9511-0.0489	DNOCj 2.4	1.9183	-0.4817	2.1	2.1295	-0.2705		
4-methylbenzamide1.81.3404-0.45961.21.5607-0.23932,2',5-PCBo4.64.1441-0.45595.44.2151-0.3849dieldrin 4.13.6513-0.44875 3.9623 -0.1377carbazole3.42.9557-0.44433.6 3.0775 -0.3225n-butylbenzene3.42.9661-0.43394.4 3.5831 0.1831benzoic acid phenyl ester3.2 2.7708 -0.4292-0.47053,4-dichlorophenol3.1 2.6852 -0.4148 3.2 2.8247 -0.27532-chlorophenol2.6 2.1884 -0.4116 2.1 2.1295 -0.4705ethyl 4-methylbenzoate3 2.59 -0.41-0.4019 2 2.0663 -0.0337ethyl 4-methylbenzoate2.6 2.1919 -0.4019 2 2.0663 -0.0337ethyl 4-nitrobenzoate 2.5 2.1076 -0.3824 $2,3,4,6$ -tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3-nitroacetanilide 1.9 1.5391 -0.3609 1.5 1.7503 -0.1497naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489	methabenzthiazu	ron	2.8	2.3337	-0.4663			
2,2',5-PCBo4.64.1441-0.45595.44.2151-0.3849dieldrin4.13.6513-0.44875 3.9623 -0.1377carbazole3.42.9557-0.4443 3.6 3.0775 -0.3225n-butylbenzene 3.4 2.9661-0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 3.4 2.8247 -0.27532-chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705ethyl octanoate 3 2.59 -0.41 2.1295 -0.4705ethyl 4-methylbenzoate 2.6 2.1919 -0.4081 -0.4019 2 $2,3,4,6$ -tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801methiocarb 2.3 1.9309 -0.3601 2.9 2.6551 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3 -nitroacetanilide 1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489	4-methylbenzam	ide	1.8	1.3404	-0.4596	1.2	1.5607	-0.2393
dieldrin4.13.6513 -0.4487 5 3.9623 -0.1377 carbazole 3.4 2.9557 -0.4443 3.6 3.0775 -0.3225 n-butylbenzene 3.4 2.9661 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 $3,4$ -dichlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 2 -chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 -0.4019 2 2.0663 -0.0337 ethyl 4-methylbenzoate 2.6 2.1919 -0.4019 2 2.0663 -0.0337 ethyl 4-nitrobenzoate 2.5 2.1076 -0.3924 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6551 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3 -nitroacetanilide 1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489	2,2',5-РСВо	4.6	4.1441	-0.4559	5.4	4.2151	-0.3849	
carbazole 3.4 2.9557 -0.4443 3.6 3.0775 -0.3225 n-butylbenzene 3.4 2.9661 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 3,4-dichlorophenol 3.1 2.6852 -0.4148 3.2 2.8247 -0.2753 2-chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 2.1 2.1295 -0.4705 ethyl 4-methylbenzoate 2.6 2.1919 -0.4081 - - - 4-bromophenylurea 2.1 1.6981 -0.4019 2 2.0663 -0.0337 ethyl 4-nitrobenzoate 2.5 2.1076 -0.3924 - - 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0	dieldrin 4.1	3.6513	-0.4487	5	3.9623	-0.1377		
n-butylbenzene 3.4 2.9661 -0.4339 4.4 3.5831 0.1831 benzoic acid phenyl ester 3.2 2.7708 -0.4292 3,4-dichlorophenol 3.1 2.6852 -0.4148 3.2 2.8247 -0.2753 2-chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 ethyl 4-methylbenzoate 2.6 2.1919 -0.4081 4-bromophenylurea 2.1 1.6981 -0.4019 2 2.0663 -0.0337 ethyl 4-nitrobenzoate 2.5 2.1076 -0.3924 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3-nitroacetanilide1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401	carbazole	3.4	2.9557	-0.4443	3.6	3.0775	-0.3225	
benzoic acid phenyl ester 3.2 2.7708 -0.4292 $3,4$ -dichlorophenol 3.1 2.6852 -0.4148 3.2 2.8247 -0.2753 2 -chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 -0.4081 4 -bromophenylurea 2.6 2.1919 -0.4081 4 -bromophenylurea 2.5 2.1076 -0.3924 $2,3,4,6$ -tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 0.1801 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 3 -nitroacetanilide 1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489	n-butylbenzene	3.4	2.9661	-0.4339	4.4	3.5831	0.1831	
3,4-dichlorophenol 3.1 2.6852 -0.4148 3.2 2.8247 -0.2753 2-chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 2.1295 -0.4705 ethyl 4-methylbenzoate 2.6 2.1919 -0.4081	benzoic acid pher	nyl ester	3.2	2.7708	-0.4292			
2-chlorophenol 2.6 2.1884 -0.4116 2.1 2.1295 -0.4705 ethyl octanoate 3 2.59 -0.41 -0.4081 4-bromophenylurea 2.1 1.6981 -0.4019 2 2.0663 -0.0337 ethyl 4-nitrobenzoate 2.5 2.1076 -0.3924 -0.1801 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3-nitroacetanilide1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401 -0.0489	3,4-dichlorophen	ol	3.1	2.6852	-0.4148	3.2	2.8247	-0.2753
ethyl octanoate 3 2.59 -0.41 ethyl 4-methylbenzoate 2.6 2.1919 -0.4081 4-bromophenylurea 2.1 1.6981 -0.4019 2 2.0663 -0.0337 ethyl 4-nitrobenzoate 2.5 2.1076 -0.3924 2 2.0663 -0.1801 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3-nitroacetanilide1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401 -0.0489	2-chlorophenol	2.6	2.1884	-0.4116	2.1	2.1295	-0.4705	
ethyl 4-methylbenzoate2.62.1919-0.40814-bromophenylurea2.11.6981-0.401922.0663-0.0337ethyl 4-nitrobenzoate2.52.1076-0.3924-0.3924-0.18012,3,4,6-tetrachlorophenol3.73.3116-0.38844.33.5199-0.1801methiocarb2.31.9309-0.36912.92.63510.3351benzoic acid methyl ester2.11.7348-0.36522.12.12950.02953-nitroacetanilide1.91.5391-0.36091.51.7503-0.1497naphthalene32.6584-0.34163.42.9511-0.0489ethyl 4-hydroxybenzoate2.21.8599-0.3401-0.3401	ethyl octanoate	3	2.59	-0.41				
4-bromophenylurea 2.1 1.6981 -0.4019 2 2.0663 -0.0337 ethyl 4-nitrobenzoate 2.5 2.1076 -0.3924 -0.3924 2,3,4,6-tetrachlorophenol 3.7 3.3116 -0.3884 4.3 3.5199 -0.1801 methiocarb 2.3 1.9309 -0.3691 2.9 2.6351 0.3351 benzoic acid methyl ester 2.1 1.7348 -0.3652 2.1 2.1295 0.0295 3-nitroacetanilide1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401 -0.0489	ethyl 4-methylbe	nzoate	2.6	2.1919	-0.4081			
ethyl 4-nitrobenzoate2.52.1076-0.39242,3,4,6-tetrachlorophenol3.73.3116-0.38844.33.5199-0.1801methiocarb2.31.9309-0.36912.92.63510.3351benzoic acid methyl ester2.11.7348-0.36522.12.12950.02953-nitroacetanilide1.91.5391-0.36091.51.7503-0.1497naphthalene32.6584-0.34163.42.9511-0.0489ethyl 4-hydroxybenzoate2.21.8599-0.3401-0.3401	4-bromophenylu	rea	2.1	1.6981	-0.4019	2	2.0663	-0.0337
2,3,4,6-tetrachlorophenol3.73.3116-0.38844.33.5199-0.1801methiocarb2.31.9309-0.36912.92.63510.3351benzoic acid methyl ester2.11.7348-0.36522.12.12950.02953-nitroacetanilide1.91.5391-0.36091.51.7503-0.1497naphthalene32.6584-0.34163.42.9511-0.0489ethyl4-hydroxybenzoate2.21.8599-0.3401	ethyl 4-nitrobenz	oate	2.5	2.1076	-0.3924			
methiocarb2.31.9309-0.36912.92.63510.3351benzoic acid methyl ester2.11.7348-0.36522.12.12950.02953-nitroacetanilide1.91.5391-0.36091.51.7503-0.1497naphthalene32.6584-0.34163.42.9511-0.0489ethyl 4-hydroxybenzoate2.21.8599-0.3401-0.3401	2,3,4,6-tetrachlor	ophenol	3.7	3.3116	-0.3884	4.3	3.5199	-0.1801
benzoic acid methyl ester2.11.7348-0.36522.12.12950.02953-nitroacetanilide1.91.5391-0.36091.51.7503-0.1497naphthalene32.6584-0.34163.42.9511-0.0489ethyl 4-hydroxybenzoate2.21.8599-0.3401-0.3401	methiocarb	2.3	1.9309	-0.3691	2.9	2.6351	0.3351	
3-nitroacetanilide1.9 1.5391 -0.3609 1.5 1.7503 -0.1497 naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401	benzoic acid met	hyl ester	2.1	1.7348	-0.3652	2.1	2.1295	0.0295
naphthalene 3 2.6584 -0.3416 3.4 2.9511 -0.0489 ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401	3-nitroacetanilide	e1.9	1.5391	-0.3609	1.5	1.7503	-0.1497	
ethyl 4-hydroxybenzoate 2.2 1.8599 -0.3401	naphthalene	3	2.6584	-0.3416	3.4	2.9511	-0.0489	
	ethyl / hydroyyh	enzoate	2.2	1.8599	-0.3401			

benzamide	1.5	1.1602	-0.3398	0.7	1.2447	-0.2553		
1,2,4,5-tetrameth	ylbenzen	ie	3.1	2.7612	-0.3388	4.1	3.3935	0.2935
2,4,5,2',4',5'-PCB	ю	5.6	5.2643	-0.3357	7.1	5.2895	-0.3105	
2-nitrobenzamide	e1.4	1.0661	-0.3339	-0.1	0.7391	-0.6609		
di-n-butyl phthala	ate	3.1	2.7716	-0.3284	4.4	3.5831	0.4831	
2,4,5-trichloroph	enol	3.4	3.0737	-0.3263	4	3.3303	-0.0697	
butralin 3.9	3.5763	-0.3237						
pentachloropheno	ol	3.8	3.4806	-0.3194	5.1	4.0255	0.2255	
azoxybenzene	3.5	3.1811	-0.3189					
1,2,3-trimethylbe	nzene	2.8	2.4825	-0.3175	3.6	3.0775	0.2775	
pyridineu	1.6	1.2884	-0.3116	0.6	1.1815	-0.4185		
chlorpyrifos	3.7	3.391	-0.309	5	3.9623	0.2623		
phthalic acid	1.1	0.791	-0.309	1	1.4343	0.3343		
p.p'-DDTs	5.4	5.0964	-0.3036	6.1	4.6575	-0.7425		
ethvl heptanoate	2.6	2.2967	-0.3033					
2.5.2'.5'-PCBo	4.9	4.6005	-0.2995	5.2	4.0887	-0.8113		
N-methylbenzam	ide	14	1 1127	-0.2873	0.9	1 3711	-0.0289	
2 4 4'-PCBo	46	4 3135	-0.2865	57	4 4047	-0 1953	0.020)	
benzoic acid ethy	l ester	2.3	2 0178	-0.2822	2.5	2 3823	0.0823	
ethyl pentanoate	2	1 7188	-0.2812	0.2022	2.3	2.3025	0.0025	
chloroyurona	2 3 5	2 2222	0.2728	3 7	2 8217	0 6753		
3 mathyl 4 brom	J.J onhonylı	J.2212	-0.2728	5.2 2.1276	0.2724	-0.0755	1 2872	0.0177
folgat 2.2	2 02 40	0.2651	2.4	2.1270	-0.2724	2.3	2.3823	-0.0177
Totpet 5.5	5.0549 1 0	-0.2031	0.2617	2.0247	-0.4755			
binhanal2.2	2.0	2.3365	-0.2017	2 2 (71	0.0220			
Dipnenyi5.5	3.0404	-0.2596	3.9	3.20/1	-0.0329	0 4000		
N-methylaniline	2.3	2.0412	-0.2588	1./	1.8/6/	-0.4233		
3-chlorophenol	2.5	2.2429	-0.25/1	2.5	2.3823	-0.11//	0.0100	
4-aminonitrobenz	zene	1.9	1.6526	-0.2474	1.4	1.68/1	-0.2129	
1 1 1	• •	0 0	0.0400			0.0050		
chlorpropham	2.8	2.5562	-0.2438	3.3	2.8879	0.0879		
chlorpropham diphenyl ether	2.8 3.3	2.5562 3.0562	-0.2438 -0.2438	3.3 4.2	2.8879 3.4567	0.0879 0.1567		
chlorpropham diphenyl ether 3-phenyl-1,1-dim	2.8 3.3 nethylure	2.5562 3.0562 a	-0.2438 -0.2438 2.1	3.3 4.2 1.8563	2.8879 3.4567 -0.2437	0.0879 0.1567		
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo	2.8 3.3 hethylure 4.1	2.5562 3.0562 a 3.8616	-0.2438 -0.2438 2.1 -0.2384	3.3 4.2 1.8563 5.1	2.8879 3.4567 -0.2437 4.0255	0.0879 0.1567 -0.0745		
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz	2.8 3.3 nethylure 4.1 tidine	2.5562 3.0562 a 3.8616 4.3	-0.2438 -0.2438 2.1 -0.2384 4.0692	3.3 4.2 1.8563 5.1 -0.2308	2.8879 3.4567 -0.2437 4.0255 3.5	0.0879 0.1567 -0.0745 3.0143	-1.2857	
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene	2.8 3.3 nethylure: 4.1 tidine 2.9	2.5562 3.0562 a 3.8616 4.3 2.6711	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289	3.3 4.2 1.8563 5.1 -0.2308 3.7	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407	0.0879 0.1567 -0.0745 3.0143 0.2407	-1.2857	
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic	2.8 3.3 hethylure 4.1 tidine 2.9 acid	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559	-1.2857 0.4559	
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate	2.8 3.3 nethylure. 4.1 tidine 2.9 acid 1.8	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455	-1.2857 0.4559	
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene	2.8 3.3 nethylure 4.1 cidine 2.9 acid 1.8 2.1	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2189	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601	-1.2857 0.4559	
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo	2.8 3.3 nethylure 4.1 tidine 2.9 acid 1.8 2.1 3.9	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2189 -0.2178	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727	0.0879 0.1567 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273	-1.2857 0.4559	
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole	2.8 3.3 nethylure. 4.1 tidine 2.9 acid 1.8 2.1 3.9 3.4	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2178 -0.2145	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273	-1.2857 0.4559	
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho	2.8 3.3 nethylure. 4.1 cidine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 vlurea	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2189 -0.2178 -0.2145 2	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4	-1.2857 0.4559 1.6871	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb	2.8 3.3 nethylure: 4.1 cidine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 vlurea 2.8964	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2189 -0.2178 -0.2145 2 -0.2036	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4	-1.2857 0.4559 1.6871	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi	2.8 3.3 nethylure: 4.1 cidine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 durea 2.8964 1.4	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2178 -0.2145 2 -0.2036 1.1968	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871	-1.2857 0.4559 1.6871 0.2871	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone	2.8 3.3 nethylure. 4.1 cidine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 Jurea 2.8964 1.4 2.4973	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879	-1.2857 0.4559 1.6871 0.2871	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe	2.8 3.3 nethylure. 4.1 tidine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 enzeneac	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 /lurea 2.8964 1.4 2.4973 2.8	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775	-1.2857 0.4559 1.6871 0.2871 0.2775	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone	2.8 3.3 nethylure. 4.1 cidine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 mzeneac 1.8	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 vlurea 2.8964 1.4 2.4973 2.8 1.6033	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2189 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135	-1.2857 0.4559 1.6871 0.2871 0.2775	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea	2.8 3.3 hethylure: 4.1 didine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 onzeneac 1.8 1.5	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 Aurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921	-1.2857 0.4559 1.6871 0.2871 0.2775	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea 3,4-dichlorophen	2.8 3.3 hethylure. 4.1 didine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 mzeneac 1.8 1.5 ylurea	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 Jurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111 2.5	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889 2.3232	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8 -0.1768	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079 2.6	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921 2.4455	-1.2857 0.4559 1.6871 0.2871 0.2775 -0.0545	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea 3,4-dichlorophen endrin 4.1	2.8 3.3 nethylure. 4.1 cidine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 nzeneac 1.8 1.5 ylurea 3.9257	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 /lurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111 2.5 -0.1743	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889 2.3232 5	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8 -0.1768 3.9623	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079 2.6 -0.1377	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921 2.4455	-1.2857 0.4559 1.6871 0.2871 0.2775 -0.0545	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea 3,4-dichlorophen endrin 4.1 3,5-dinitroaniline	2.8 3.3 nethylure: 4.1 cidine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 nzeneac 1.8 1.5 ylurea 3.9257 2.5	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 vlurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111 2.5 -0.1743 2.3272	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2189 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889 2.3232 5 -0.1728	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8 -0.1768 3.9623 1.9	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079 2.6 -0.1377 2.0031	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921 2.4455 -0.4969	-1.2857 0.4559 1.6871 0.2871 0.2775 -0.0545	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea 3,4-dichlorophen endrin 4.1 3,5-dinitroaniline anthracene-9-carl	2.8 3.3 hethylure: 4.1 didine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 onzeneac 1.8 1.5 ylurea 3.9257 2.5 boxylic a	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 Aurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111 2.5 -0.1743 2.3272 cid	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889 2.3232 5 -0.1728 2.7	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8 -0.1768 3.9623 1.9 2.5277	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079 2.6 -0.1377 2.0031 -0.1723	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921 2.4455 -0.4969 3.5	-1.2857 0.4559 1.6871 0.2871 0.2775 -0.0545 3.0143	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea 3,4-dichlorophen endrin 4.1 3,5-dinitroaniline anthracene-9-carl neburonn	2.8 3.3 hethylure. 4.1 didine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 nzeneac 1.8 1.5 ylurea 3.9257 2.5 boxylic a 3.4	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 Jurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111 2.5 -0.1743 2.3272 cid 3.2352	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889 2.3232 5 -0.1728 2.7 -0.1648	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8 -0.1768 3.9623 1.9 2.5277 3.8	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079 2.6 -0.1377 2.0031 -0.1723 3.2039	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921 2.4455 -0.4969 3.5 -0.1961	-1.2857 0.4559 1.6871 0.2871 0.2775 -0.0545 3.0143	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea 3,4-dichlorophen endrin 4.1 3,5-dinitroaniline anthracene-9-carl neburonn aldicarb 1 5	2.8 3.3 nethylure. 4.1 didine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 nzeneac 1.8 1.5 ylurea 3.9257 2.5 boxylic a 3.4 1.3387	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 Jurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111 2.5 -0.1743 2.3272 cid 3.2352 -0.1613	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889 2.3232 5 -0.1728 2.7 -0.1648 1.1	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8 -0.1768 3.9623 1.9 2.5277 3.8 1.4975	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079 2.6 -0.1377 2.0031 -0.1723 3.2039 -0.0025	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921 2.4455 -0.4969 3.5 -0.1961	-1.2857 0.4559 1.6871 0.2871 0.2775 -0.0545 3.0143	-0.3129
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea 3,4-dichlorophen endrin 4.1 3,5-dinitroaniline anthracene-9-carl neburonn aldicarb 1.5 3-bromophenylure	2.8 3.3 hethylure: 4.1 didine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 snzeneac 1.8 1.5 ylurea 3.9257 2.5 boxylic a 3.4 1.3387 rea	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 flurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111 2.5 -0.1743 2.3272 cid 3.2352 -0.1613 2.1	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2189 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889 2.3232 5 -0.1728 2.7 -0.1648 1.1 1.9428	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8 -0.1768 3.9623 1.9 2.5277 3.8 1.4975 -0.1572	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079 2.6 -0.1377 2.0031 -0.1723 3.2039 -0.0025 2.1	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921 2.4455 -0.4969 3.5 -0.1961 2.1295	-1.2857 0.4559 1.6871 0.2871 0.2775 -0.0545 3.0143 0.0295	-0.3129 0.3143
chlorpropham diphenyl ether 3-phenyl-1,1-dim 2,4'-PCBo 3,3'-dichlorobenz n-propylbenzene 4-methylbenzoic diethyl phthalate nitrobenzene 2,2'-PCBo methazole 3-chloro-4-metho chloroneb 4-hydroxybenzoi benzophenone 1,3,5-trimethylbe acetophenone phenylurea 3,4-dichlorophen endrin 4.1 3,5-dinitroaniline anthracene-9-carl neburonn aldicarb 1.5 3-bromophenylur	2.8 3.3 hethylure: 4.1 didine 2.9 acid 1.8 2.1 3.9 3.4 oxypheny 3.1 c acid 2.7 onzeneac 1.8 1.5 ylurea 3.9257 2.5 boxylic a 3.4 1.3387 rea nzene	2.5562 3.0562 a 3.8616 4.3 2.6711 1.8 1.5807 1.8811 3.6822 3.1855 Jurea 2.8964 1.4 2.4973 2.8 1.6033 1.3111 2.5 -0.1743 2.3272 cid 3.2352 -0.1613 2.1 3.3	-0.2438 -0.2438 2.1 -0.2384 4.0692 -0.2289 1.5751 -0.2193 -0.2178 -0.2145 2 -0.2036 1.1968 -0.2027 2.6011 -0.1967 -0.1889 2.3232 5 -0.1728 2.7 -0.1648 1.1 1.9428 3.1462	3.3 4.2 1.8563 5.1 -0.2308 3.7 -0.2249 2.6 1.8 4.7 1.7963 -0.2032 3.3 -0.1989 1.6 0.8 -0.1768 3.9623 1.9 2.5277 3.8 1.4975 -0.1572 -0.1538	2.8879 3.4567 -0.2437 4.0255 3.5 3.1407 2.3 2.4455 1.9399 3.7727 -0.2037 1.4 2.8879 3.6 1.8135 1.3079 2.6 -0.1377 2.0031 -0.1723 3.2039 -0.0025 2.1 4.1	0.0879 0.1567 -0.0745 3.0143 0.2407 2.2559 0.6455 -0.1601 -0.1273 1.4 1.6871 0.1879 3.0775 0.0135 -0.1921 2.4455 -0.4969 3.5 -0.1961 2.1295 3.3935	-1.2857 0.4559 1.6871 0.2871 0.2775 -0.0545 3.0143 0.0295 0.0935	-0.3129 0.3143

3-fluorophenylurea	a	1.8	1.6536	-0.1464	1.3	1.6239	-0.1761	
3-chlorophenylure	a	2	1.8542	-0.1458	1.8	1.9399	-0.0601	
3-bromoacetanilide	e	2	1.859	-0.141	2.2	2.1927	0.1927	
2-chlorobiphenyl 3	3.5	3.3636	-0.1364	4.5	3.6463	0.1463		
diamidaphos 1	.5	1.3722	-0.1278					
oxamyl 1 0).8734	-0.1266	-0.5	0.4863	-0.5137			
prometon 2	2.6	2.4748	-0.1252	3	2.6983	0.0983		
??chlordane 4	1.8	4.6767	-0.1233					
nitralin 3 2	2.8786	-0.1214						
4-bromophenol 2	2.4	2.2835	-0.1165	2.5	2.3823	-0.0177		
4-phenoxyphenylu	rea	2.6	2.4842	-0.1158	2.8	2.5719	-0.0281	
3-methylphenylure	ea	1.6	1.4865	-0.1135	1.3	1.6239	0.0239	
phenylacetic acid 1	.4	1.2868	-0.1132	1.4	1.6871	0.2871		
2,4-dichlorophenol	1	2.8	2.687	-0.113	3.2	2.8247	0.0247	
3-chloroacetanilide	e	1.9	1.7918	-0.1082	2.1	2.1295	0.2295	
3,6-dichlorosalicyl	ic acid	2.3	2.1942	-0.1058				
norflurazon 3	3.3	3.1979	-0.1021	2.3	2.2559	-1.0441		
N,N-dimethylanili	ne	2.3	2.1999	-0.1001	2.4	2.3191		
methyl chloramber	n	2.7	2.6032	-0.0968				
aldicarb sulfone 0).5	0.4058	-0.0942	-0.6	0.4231	-0.0769		
ethvl hexanoate 2	2.1	2.0061	-0.0939					
methyl N-phenylca	arbamat	e	1.7	1.6065	-0.0935	1.8	1.9399	0.2399
4-fluorophenvlurea	a a	1.5	1.4081	-0.0919	1	1.4343	-0.0657	
hexanoic acid 1	.5	1.4086	-0.0914	1.9	2.0031	0.5031		
2.2'-biquinoline 4	L	3.9194	-0.0806	4.3	3.5199	-0.4801		
cvanazine 2	2.3	2.2242	-0.0758	2.1	2.1295	-0.1705		
benzoic acid 1	.5	1.4291	-0.0709	1.9	2.0031	0.5031		
ethyl 3.5-dinitrobe	nzoate	2.7	2.6354	-0.0646				
azobenzene 3	3.3	3.2358	-0.0642	3.8	3.2039	-0.0961		
2-chlorophenylure	a	1.6	1.5363	-0.0637	1.3	1.6239	0.0239	
pebulated 2	2.8	2.762	-0.038	3.8	3.2039	0.4039		
veratrolead 2	2	1.9859	-0.0141	1.7	1.8767	-0.1233		
2.3-dichlorophenol	1	2.6	2.5862	-0.0138	3	2.6983	0.0983	
1.4-dimethylbenze	nei	2.4	2.3923	-0.0077	3.2	2.8247	0.4247	
metribuzin 2	2	1.9985	-0.0015	1.7	1.8767	-0.1233		
captafol 3.3 3	3 2986	-0.0014	3.2	2.8247	-0 4753	0.1200		
3-methyl-4-fluoror	henvlu	rea	1.8	1 8059	0.0059	16	1 8135	0.0135
thiobencarb aa 3	3	3 3166	0.0166	3.4	2 9511	-0 3489	1.0155	0.0155
nvroxychlor 3	3.5	3 5204	0.0204	5.1	2.7511	0.5107		
3-(3 4-dichlorophe	nvl)-1-1	nethvlur	-9 -9	25	2 5218	0.0218		
	, ii ji i i	incentyren	cu	2.0	2.5210	0.0210		
bromobenzene 2	2.5	2 5235	0.0235	2.9	2 6351	0 1351		
bromobenzene 2 2 3 4 2' 3' 4'-PCBo	2.5	2.5235 5	0.0235	2.9 0.0358	2.6351 7.1	0.1351	0 2895	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze	2.5 ene	2.5235 5 2.4	0.0235 5.0358 2.4436	2.9 0.0358 0.0436	2.6351 7.1 2.6	0.1351 5.2895 2.4455	0.2895	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8	2.5 ene 8593	2.5235 5 2.4 0.0593	0.0235 5.0358 2.4436 0.9	2.9 0.0358 0.0436 1.3711	2.6351 7.1 2.6 -0.4289	0.1351 5.2895 2.4455	0.2895 0.0455	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace	2.5 ene 8593 etanilide	2.5235 5 2.4 0.0593	0.0235 5.0358 2.4436 0.9 1.4	2.9 0.0358 0.0436 1.3711 1.4658	2.6351 7.1 2.6 -0.4289 0.0658	0.1351 5.2895 2.4455	0.2895 0.0455	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace toluene 2.1 2	2.5 ene 8593 etanilide 2.1684	2.5235 5 2.4 0.0593 c 0.0684	0.0235 5.0358 2.4436 0.9 1.4 2.7	2.9 0.0358 0.0436 1.3711 1.4658 2 5087	2.6351 7.1 2.6 -0.4289 0.0658 0.4087	0.1351 5.2895 2.4455	0.2895 0.0455	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace toluene 2.1 2 carbofuran 1	2.5 ene 8593 etanilide 2.1684 8	2.5235 5 2.4 0.0593 0.0684 1.8719	0.0235 5.0358 2.4436 0.9 1.4 2.7 0.0719	2.9 0.0358 0.0436 1.3711 1.4658 2.5087 2	2.6351 7.1 2.6 -0.4289 0.0658 0.4087 2.0663	0.1351 5.2895 2.4455 0.2663	0.2895 0.0455	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace toluene 2.1 2 carbofuran 1 4-biphenylmethano	2.5 ene 8593 etanilide 2.1684 8	2.5235 5 2.4 0.0593 2.0.0684 1.8719 2.6	0.0235 5.0358 2.4436 0.9 1.4 2.7 0.0719 2.6738	2.9 0.0358 0.0436 1.3711 1.4658 2.5087 2 0.0738	2.6351 7.1 2.6 -0.4289 0.0658 0.4087 2.0663	0.1351 5.2895 2.4455 0.2663	0.2895 0.0455	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace toluene 2.1 2 carbofuran 1 4-biphenylmethano 2-chlorobenzamide	2.5 ene 8593 etanilide 2.1684 8 ol	2.5235 5 2.4 0.0593 0.0684 1.8719 2.6 1.5	0.0235 5.0358 2.4436 0.9 1.4 2.7 0.0719 2.6738 1 5774	2.9 0.0358 0.0436 1.3711 1.4658 2.5087 2 0.0738 0.0774	2.6351 7.1 2.6 -0.4289 0.0658 0.4087 2.0663	0.1351 5.2895 2.4455 0.2663	0.2895 0.0455	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace toluene 2.1 2 carbofuran 1 4-biphenylmethano 2-chlorobenzamide simazine 2	2.5 ene 8593 etanilide 2.1684 8 ol e 2.1	2.5235 5 2.4 0.0593 0.0684 1.8719 2.6 1.5 2.1806	0.0235 5.0358 2.4436 0.9 1.4 2.7 0.0719 2.6738 1.5774 0.0806	2.9 0.0358 0.0436 1.3711 1.4658 2.5087 2 0.0738 0.0774 2.1	2.6351 7.1 2.6 -0.4289 0.0658 0.4087 2.0663	0.1351 5.2895 2.4455 0.2663	0.2895 0.0455	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace toluene 2.1 2 carbofuran 1 4-biphenylmethano 2-chlorobenzamide simazine 2 2,4,6-trichloropher	2.5 ene 8593 etanilide 2.1684 8 e 2.1 nol	2.5235 5 2.4 0.0593 0.0684 1.8719 2.6 1.5 2.1806 3	0.0235 5.0358 2.4436 0.9 1.4 2.7 0.0719 2.6738 1.5774 0.0806 3.0817	2.9 0.0358 0.0436 1.3711 1.4658 2.5087 2 0.0738 0.0774 2.1 0.0817	2.6351 7.1 2.6 -0.4289 0.0658 0.4087 2.0663 2.1295 3.8	0.1351 5.2895 2.4455 0.2663 0.0295 3.2039	0.2895 0.0455 0.2039	
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace toluene 2.1 2 carbofuran 1 4-biphenylmethano 2-chlorobenzamide simazine 2 2,4,6-trichloropher 2-methoxy-3 5 6-tr	2.5 ene 8593 etanilide 2.1684 8 ol e 2.1 nol	2.5235 5 2.4 0.0593 0.0684 1.8719 2.6 1.5 2.1806 3 pyridine	0.0235 5.0358 2.4436 0.9 1.4 2.7 0.0719 2.6738 1.5774 0.0806 3.0817 3	2.9 0.0358 0.0436 1.3711 1.4658 2.5087 2 0.0738 0.0774 2.1 0.0817 3.0877	2.6351 7.1 2.6 -0.4289 0.0658 0.4087 2.0663 2.1295 3.8 0.0877	0.1351 5.2895 2.4455 0.2663 0.0295 3.2039 4.3	0.2895 0.0455 0.2039 3.5199	0.5199
bromobenzene 2 2,3,4,2',3',4'-PCBo 4-bromonitrobenze aniline 1.8 1 3-methylphenylace toluene 2.1 2 carbofuran 1 4-biphenylmethano 2-chlorobenzamide simazine 2 2,4,6-trichloropher 2-methoxy-3,5,6-tr pyrazon 2.1 2	2.5 ene 8593 etanilide 2.1684 8 ol e 2.1 nol richloro 2.1965	2.5235 5 2.4 0.0593 2.6 1.5 2.1806 3 pyridine 0.0965	0.0235 5.0358 2.4436 0.9 1.4 2.7 0.0719 2.6738 1.5774 0.0806 3.0817 3 1.1	2.9 0.0358 0.0436 1.3711 1.4658 2.5087 2 0.0738 0.0774 2.1 0.0817 3.0877 1.4975	2.6351 7.1 2.6 -0.4289 0.0658 0.4087 2.0663 2.1295 3.8 0.0877 -0.6025	0.1351 5.2895 2.4455 0.2663 0.0295 3.2039 4.3	0.2895 0.0455 0.2039 3.5199	0.5199

4-methoxyacetanilide 1.4 1.4969 0.0969 1.1 1.4975 0.0975 diallate 3.3 3.4038 0.1038 methyl N-(3,4-dichlorophenyl)carbonate 2.7 2.8045 0.1045 3.3 2.8879 0.1879 hexachlorobenzene 3.7 3.8054 0.1054 5.4 4.2151 0.5151 4-nitrobenzoic acid 1.5 1.6112 0.1112 1.6 1.8135 0.3135 terbacil 1.7 1.8123 0.1123 1.9 2.0031 0.3031 2-fluorophenylurea 1.3 1.4171 0.1171 0.9 1.3711 0.0711 methyl parathion 3 3.1192 0.1192 3 2.6983 -0.3017 EPTCl 2.4 2.5237 0.1237 3.2 2.8247 0.4247 1.7242 0.1242 1.3 1.6239 0.0239 2-chloroacetanilide 1.6 dichlorobenil 2.4 2.527 0.127 2.8 2.5719 0.1719 2,6-dinitro-n-propyl-?????trifluoro-p-toluidine 3.6 3.7303 0.1303 1,2-dimethylbenzeneg 2.2 2.3342 0.1342 3.1 2.7615 0.5615 3.2 3.3382 0.1382 3 2.6983 -0.5017 disulfoton ethyl N-phenylcarbamate 1.8 1.9409 0.1409 2.3 2.2559 0.4559 ethyl phenylacetate 2.0435 0.1435 2.3 2.2559 0.3559 1.9 dinitramine 3.6 3.744 0.144 1,2,4-trichlorobenzene 3.1 3.2486 0.1486 4.1 3.3935 0.2935 1-naphthalenemethanol 2.2 2.3488 0.1488 2.4 2.3191 propachlort 2.4 2.5494 0.1494 2.2 2.1927 -0.20732.8 2.9535 0.1535 3.3 2.8879 0.0879 trietazine carbophenothion 4.7 4.8563 0.1563 5.3 4.1519 -0.5481 4-methylaniline 1.9 2.0582 0.1582 1.4 1.6871 -0.2129benzene 1.8 1.9604 0.1604 2.1 2.1295 0.3295 2.6605 0.1605 3.3 2.8879 0.3879 2.5 metolachlor n-propyl N-phenylcarbamate 2.12.2606 0.1606 2.8 2.5719 0.4719 pirimicarb 1.9 2.0619 0.1619 1.7 1.8767 -0.0233 chlornitrofen 3.9 4.064 0.164 4.2 3.4567 -0.4433 1-dodecanol 3.5 3.6671 0.1671 5.2 4.0887 0.5887 trichlorfon 1.9 2.0702 0.1702 0.5 1.1183 -0.7817 2.9 3.0752 0.1752 3.4 2.9511 0.0511 prometryn cycloate 2.5 2.6769 0.1769 4.1 3.3935 0.8935 3-methoxyphenyl-1,1-dimethylurea 1.7 1.884 0.184 1,3-dimethylbenzeneh 2.2 2.3857 0.1857 3.2 2.8247 0.6247 1.9 2.0928 3-(3-chlorophenyl)-1-methylurea 0.1928 monolinuron 2.12.2964 0.1964 2.3 2.2559 0.1559 1.4 1.5976 0.1976 1.2 1.5607 0.1607 acetanilide 3.5 3.6993 0.1993 5.1 pentachlorobenzene 4.0255 0.5255 3-(3-chloro-4-methoxyphenyl)-1-methylurea 1.8 2.0001 0.2001 3-phenyl-1-methylurea 1.3 1.5094 0.2094 1.1 1.4975 0.1975 3,4-dichloronitrobenzene 2.5 2.7101 0.2101 3.1 2.7615 0.2615 2.8178 0.2178 3.4 1,2-dichlorobenzene 2.6 2.9511 0.3511 2.7 2.9236 0.2236 3.1 2.7615 0.0615 chlorbromuron 2.2 2.4237 0.2237 3.1 2.7615 0.5615 ethylbenzene maleic hydrazine 0.5 0.7241 0.2241 -0.8 0.2967 -0.2033 3.6245 0.2245 triallate 3.4 4.9253 0.2253 4.7207 0.0207 p,p'-DDEr 4.7 6.2 0.2325 3.8 n-pentyl N-phenylcarbamate 2.6 2.8325 3.2039 0.6039 dipropetryn 3.1 3.3361 0.2361 molinate1.9 2.1366 0.2366 3.2 2.8247 0.9247 n-butyl N-phenylcarbamate 2.3 2.5385 0.2385 3.3 2.8879 0.5879 diphenylamine 2.8 3.0402 0.2402 3.4 2.9511 0.1511 acetic acid 0 0.2414 0.2414 -0.3 0.6127 0.6127 3-(trifluroromethyl)acetanilide 1.8 2.0578 0.2578 2.4 2.3191

3-chloro-4-bromonitrobenzene 2.6 2.8609 0.2609 3.2 2.8247 0.2247 0.2623 2.8247 0.3247 fenamiphos 2.5 2.7623 3.2 3,5-dimethyl-4-bromophenyl-1,1-dimethylurea 2.5 2.7657 0.2657 3,4-dichloroacetanilide 2.3 2.571 0.271 2.8 2.5719 0.2719 di-2-ethylhexyl phthalate 4.9 5.1787 0.2787 6.5 4.9103 0.0103 ametryn 2.6 2.8876 0.2876 3 2.6983 0.0983 3-phenyl-1-cyclopropylurea 1.7 2.0045 0.3045 1.6 1.8135 0.1135 1,3-dichlorobenzene 2.9093 0.3093 3.5 3.0143 0.4143 2.6 methyl N-(3-chlorophenyl)carbamate 2.4107 0.3107 2.12.7615 0.3615 2.7108 0.3108 3.1 tetrachloroethylene 2.4 2.9511 0.1511 napropamide 2.8 3.1117 0.3117 3.4 4-bromoacetanilide 1.9 2.212 0.312 2.2 2.1927 0.2927 ethion 4.1 4.4142 0.3142 5.1 4.0255 -0.0745 alachlor 2.3 2.6153 0.3153 3.5 3.0143 0.7143 tetrachloroguaiacol 2.9 3.2176 0.3176 4.6 3.7095 0.8095 1,4-dichlorobenzene 2.6 2.9228 0.3228 3.4 2.9511 0.3511 3-aminonitrobenzene 1.7 2.0242 0.3242 1.4 1.6871 -0.0129 3.2 3.5262 0.3262 3.7 3.1407 -0.0593 parathion 2,3,4,2',5'-PCBo 4.5 4.8289 0.3289 6.4 4.8471 0.3471 1,2,3,5-tetrachlorobenzene 3.2 3.5404 0.3404 4.6 3.7095 0.5095 captan 2.3 2.6428 0.3428 2.4 2.3191 2,4,5,2',5'-PCBo 4.6 4.9434 0.3434 6.5 4.9103 0.3103 2.5488 0.3488 2.5 2.3823 0.1823 atrazine 2.2 1.9497 0.3497 1.6 3-fluoroacetanilide 1.6 1.8135 0.2135 chlorobenzene 2.12.4604 0.3604 2.8 2.5719 0.4719 3-(trifluoromethyl)phenylurea 2 2.3605 0.3605 2.3 2.2559 0.2559 linuron 2.6 2.962 0.362 3 2.6983 0.0983 leptophos 4.5 4.8621 0.3621 6.2 4.7207 0.2207 3.4 3.7799 0.3799 niclosamide sec-phenethyl alcohol 1.5 1.8831 0.3831 2.2904 0.3904 2.1 2.1295 0.2295 bromacil 1.9 3.2671 ipazine 2.9 3.2976 0.3976 3.9 0.3671 2.2982 2.4455 0.5455 3-phenyl-1-cyclopentylurea 1.9 0.3982 2.6 propoxur 1.7 2.1016 0.4016 1.5 1.7503 0.0503 6-chloropicolinic acid 0.9 1.3025 0.4025 -1.7 -0.2721 -1.1721 BMPCb 1.7 2.1097 0.4097 2.9 2.6351 0.9351 3-methyl-4-bromoaniline 2.3 2.7119 0.4119 2.5 2.3823 0.0823 4-methoxyphenyl-1,1-dimethylurea 1.4 1.8124 0.4124 0.4207 1.4 1.5 1.9207 4-fluoroacetanilide 1.6871 0.1871 3-fluorophenyl-1,1-dimethylurea 1.8 2.2262 0.4262 1.4 1.6871 -0.1129 1,3,5-trichlorobenzene 2.9 3.3268 0.4268 4.2 3.4567 0.5567 5.2296 0.4296 6.6 permethrin 4.8 4.9735 0.1735 1.7 2.1356 0.4356 1,2-dichloropropane 3-methylaniline 1.6 2.04 0.44 1.4 1.6871 0.0871 methyl chlorpyrifos 3.5 3.948 0.448 4.2 3.4567 -0.0433 diuron 2.4 2.8487 0.4487 2.8 2.5719 0.1719 1.9523 0.4523 anisole 1.5 2.12.1295 0.6295 dimeton-S-methyl 1.5 1.9626 0.4626 1 1.4343 -0.0657 fenuron 1.4 1.8741 0.4741 1 1.4343 0.0343 3-phenyl-1-cycloheptylurea 2.6983 0.2983 2.8819 0.4819 3 2.4 4-chloroaniline 2 2.4897 0.4897 1.8 1.9399 -0.0601 2.594 3.2039 1.1039 benzoic acid butyl ester 2.10.494 3.8 metobromuron 2.5953 0.4953 2.4 2.3191 2.1 2.1997 0.4997 2 1.2-dibromoethane 1.7 2.0663 0.3663

3-chloro-4-metho	oxyanilin	e	1.9	2.4067	0.5067	1.9	2.0031	0.1031	
propazine	2.4	2.9122	0.5122	3	2.6983	0.2983			
4,5,6-trichlorogu	aiacol	2.8	3.3174	0.5174	3.8	3.2039	0.4039		
monuron	1.9	2.4272	0.5272	2	2.0663	0.1663			
1,1,1-trichloroeth	nane	1.9	2.4431	0.5431	2.5	2.3823	0.4823		
4-methylphenyl-	1,1-dime	thylurea	1.5	2.0483	0.5483				
dimethyl phthala	te	1.6	2.1538	0.5538	1.7	1.8767	0.2767		
profluralin	3.9	4.4602	0.5602	6.3	4.7839	0.8839			
4-bromoaniline	2	2.5619	0.5619	2.1	2.1295	0.1295			
trichloroethylene	2	2.5682	0.5682	2.5	2.3823	0.3823			
1,2-dichloroethar	ne	1.5	2.0686	0.5686	1.5	1.7503	0.2503		
3-trifluoromethy	l-4-nitrop	ohenol	2.1	2.6691	0.5691	2.3	2.2559	0.1559	
chlortoluron	2	2.571	0.571	2.4	2.3191				
propylene glycol	methyl e	ether acet	ate	0.4	0.9717	0.5717			
benzyl alcohol	1.1	1.6736	0.5736	1.1	1.4975	0.3975			
diazinon 2.8	3.3815	0.5815	3.3	2.8879	0.0879				
3,5-dimethylpher	nyl-1,1-d	imethylu	rea	1.7	2.2824	0.5824			
dicambaf	1.5	2.0886	0.5886	2.2	2.1927	0.6927			
chlorimuron	2	2.59	0.59						
butyranilide	1.7	2.2906	0.5906	1.9	2.0031	0.3031			
3,5-dichloroanili	ne	2.5	3.0908	0.5908	2.7	2.5087	0.0087		
fenitrothion	2.6	3.1938	0.5938	3.4	2.9511	0.3511			
metoxuron	1.7	2.2944	0.5944	1.6	1.8135	0.1135			
azinphos methyl	2.3	2.9059	0.6059	2.6	2.4455	0.1455			
IBPm 2.1	2.7096	0.6096	3.3	2.8879	0.7879				
tetrachlorometha	nez	1.9	2.5115	0.6115	2.7	2.5087	0.6087		
2,6-dinitro-?????	?trifluoro	o-p-toluic	line	2.6	3.2147	0.6147	2.3	2.2559	-0.3441
dichloromethane	1.4	2.0229	0.6229	1.2	1.5607	0.1607			
3-(trifluoromethy	l)aniline	2.4	3.0271	0.6271	2.4	2.3191			
phorate 2.7	3.3309	0.6309	3.6	3.0775	0.3775				
crotoxyphos	2	2.6377	0.6377	3.3	2.8879	0.8879			
3-chlorophenyl-1	,1-dimet	hylurea	1.8	2.4378	0.6378				
oxadiazon	3.5	4.1389	0.6389	4.8	3.8359	0.3359			
picloram	1.3	1.9626	0.6626	0.3	0.9919	-0.3081			
1,2-dibromo-3-cl	nloroprop	pane	2.1	2.7723	0.6723				
2,3,4,5-tetrachlor	oaniline	3	3.6742	0.6742	4.2	3.4567	0.4567		
3,4-dichloroanili	ne	2.3	2.9776	0.6776	2.6	2.4455	0.1455		
3,5,6-trichloro-2-	pyridino	12.1	2.8022	0.7022	2.7	2.5087	0.4087		
2,3,4-trichloroan	iline	2.6	3.3084	0.7084	3.4	2.9511	0.3511		
EPNk 3.1	3.8086	0.7086	4.6	3.7095	0.6095				
trichloroacetamic	le	1	1.7251	0.7251	1	1.4343	0.4343		
terbuthylazine	2.3	3.0319	0.7319	3.1	2.7615	0.4615			
3,5 dinitrobenzoi	c aicd	1.5	2.2354	0.7354	1.6	1.8135	0.3135		
propham	1.8	2.5531	0.7531	2.4	2.3191				
1,1,2-trichloroeth	nane	1.9	2.6623	0.7623	1.9	2.0031	0.1031		
piperophos	3.4	4.1702	0.7702						
4-fluorophenyl-1	,1-dimet	hylurea	1.4	2.1862	0.7862				
gamma-BHC	3.3	4.0867	0.7867	3.7	3.1407	-0.1593			
dichlorvos	1.7	2.4874	0.7874	1.4	1.6871	-0.0129			
trifluralin	4.1	4.9012	0.8012	5.3	4.1519	0.0519			
2,4-Dd 1.6	2.4177	0.8177	2.7	2.5087	0.9087	0.00.15			
nitrapyrin	2.5	3.3382	0.8382	3.2	2.8247	0.3247			
terbutos 2.8	3.6469	0.8469	3.9	3.2671	0.4671	0.00.11			
агрһа-ВНС	3.3	4.168	0.868	3.8	3.2039	-0.0961			

nuometuron	2	2.9207	0.9207	2.3	2.2559	0.2559	
dimethoate	1.2	2.1231	0.9231	0.7	1.2447	0.0447	
DCIPe 1.7	2.63	0.93					
benefin 4	4.9328	0.9328	5.3	4.1519	0.1519		
beta-BHC	3.5	4.4338	0.9338	3.8	3.2039	-0.2961	
chloramben	1.3	2.2396	0.9396				
trichloromethane	ab	1.6	2.5921	0.9921	1.9	2.0031	0.4031
chlorthiamid	2	3.0259	1.0259				
silvex 1.8	2.8363	1.0363					
methyl isothiocy	anate	0.8	1.9126	1.1126	0.9	1.3711	0.5711
pronoamide	2.3	3.4512	1.1512				
fluchloralin	3.6	4.7817	1.1817				
2,4,5-Tw	1.9	3.0921	1.1921	3.1	2.7615	0.8615	
triclopyr 1.4	2.7087	1.3087					
chlorfenvinphos	2.5	3.8367	1.3367				
1,1,2,2-tetrachlor	roethane	1.9	3.2845	1.3845	2.4	2.3191	
methidathion	1.5	3.1187	1.6187	2.3	2.2559	0.7559	
phosalone	2.6	4.5778	1.9778	4.3	3.5199	0.9199	
Test set							
aldicarb sulfoxid	e	0.6	0.319	-0.281			
amitrole 1 2	0 1575	-1 0425					
bromodichlorom	ethane	1.0125	2 6337	0.8337			
butachlor	2.9	3 536	0.636	0.0557			
butylate 2.1	2.9	0.769	0.050				
carbonhenothion	2.007 methyl	47	1 3688	0 3312			
catechol 2	1 <i>1 1 1 1 1 1 1 1 1 1</i>	+./ 0.5532	4.3088	-0.3312			
dalarron 0.4	1.4400	1 4117					
diharamaahlaram	1.011/	1.4117	2 7072	0 0072			
	ethane	1.9	2.7072	0.8072			
1,2-dibromoetne	ne	1.0	2.2964	0.0904			
2,4-dichloroanili	ne	2.7	3.0021	0.3021			
2,6-dichloroanili	ne	3.2	2.9342	-0.2658			
2.6-dichlorobenz		~ ~ ~		1 47700			
	amide	0.5	1.9720	1.4728			
1,1-dichloroetha	amide ne	0.5 1.5	2.1213	1.4728 0.6213			
1,1-dichloroethau 1,1-dichloroethau	amide ne ne	0.5 1.5 1.8	2.1213 2.172	1.4728 0.6213 0.372			
1,1-dichloroethar 1,1-dichloroethar dicrotophos	amide ne 1.7	0.5 1.5 1.8 1.2303	1.9728 2.1213 2.172 -0.4697	1.4728 0.6213 0.372			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi	amide ne 1.7 ic acid	0.5 1.5 1.8 1.2303 1.5	2.1213 2.172 -0.4697 2.418	1.4728 0.6213 0.372 0.918			
1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi dinoseb 2.1	amide ne 1.7 ic acid 3.0829	0.5 1.5 1.8 1.2303 1.5 0.9829	2.1213 2.172 -0.4697 2.418	1.4728 0.6213 0.372 0.918			
1,1-dichloroethan 1,1-dichloroethan dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate3.4	amide ne 1.7 ic acid 3.0829 3.4827	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827	2.1213 2.172 -0.4697 2.418	1.4728 0.6213 0.372 0.918			
1,1-dichloroethat 1,1-dichloroethat dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate3.4 endosulfan	amide ne 1.7 ic acid 3.0829 3.4827 4.1	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952	 1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 	1.4728 0.6213 0.372 0.918			
1,1-dichloroethar 1,1-dichloroethar dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113	-0.6048 0.8113	1.4728 0.6213 0.372 0.918			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304	1.4728 0.6213 0.372 0.918 0.1304			
1,1-dichloroethan 1,1-dichloroethan 1,1-dichloroethan dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304	1.4728 0.6213 0.372 0.918			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304	1.4728 0.6213 0.372 0.918 0.1304			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166	-0.6048 0.8113 1.8304	1.4728 0.6213 0.372 0.918 0.1304			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoo dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304	1.4728 0.6213 0.372 0.918			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben malathion	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4 3.1	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421 3.2777	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304 0.9421 0.1777	1.4728 0.6213 0.372 0.918			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben malathion meobal 1.7	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4 3.1 1.6356	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421 3.2777 -0.0644	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304 0.9421 0.1777	1.4728 0.6213 0.372 0.918			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoo dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben malathion meobal 1.7 metalaxyl	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4 3.1 1.6356 1.6	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421 3.2777 -0.0644 1.8729	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304 0.9421 0.1777 0.2729	1.4728 0.6213 0.372 0.918			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzor dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben malathion meobal 1.7 metalaxyl metamitron	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4 3.1 1.6356 1.6 0	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421 3.2777 -0.0644 1.8729 1.3751	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304 0.9421 0.1777 0.2729 1.3751	1.4728 0.6213 0.372 0.918 0.1304			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben malathion meobal 1.7 metalaxyl metamitron 2-methoxypheno	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4 3.1 1.6356 1.6 0 11.6	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421 3.2777 -0.0644 1.8729 1.3751 1.9008	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304 0.9421 0.1777 0.2729 1.3751 0.3008	1.4728 0.6213 0.372 0.918 0.1304			
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoi dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben malathion meobal 1.7 metalaxyl metamitron 2-methoxypheno 3-methoxypheny	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4 3.1 1.6356 1.6 0 11.6 lcarbama	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421 3.2777 -0.0644 1.8729 1.3751 1.9008 tte	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304 0.9421 0.1777 0.2729 1.3751 0.3008 1.4	1.4728 0.6213 0.372 0.918 0.1304	0.0397		
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzoo dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben malathion meobal 1.7 metalaxyl metamitron 2-methoxypheno 3-methoxypheny oryzalin 3.4	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4 3.1 1.6356 1.6 0 11.6 lcarbama 2.1871	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421 3.2777 -0.0644 1.8729 1.3751 1.9008 tte -1.2129	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304 0.9421 0.1777 0.2729 1.3751 0.3008 1.4	1.4728 0.6213 0.372 0.918 0.1304 1.4397	0.0397		
1,1-dichloroethai 1,1-dichloroethai 1,1-dichloroethai dicrotophos 3,4-dinitrobenzor dinoseb 2.1 dyfonate 3.4 endosulfan ethoprophos 3-ethylphenylcar fenac 1.8 imazalil 3.7 isouron 2.5 isoxaben malathion meobal 1.7 metalaxyl metamitron 2-methoxypheny oryzalin 3.4 pentachloroanilin	amide ne 1.7 ic acid 3.0829 3.4827 4.1 1.8 bamate 2.6122 3.4646 1.334 2.4 3.1 1.6356 1.6 0 11.6 lcarbama 2.1871 ne	0.5 1.5 1.8 1.2303 1.5 0.9829 0.0827 3.4952 2.6113 1.7 0.8122 -0.2354 -1.166 3.3421 3.2777 -0.0644 1.8729 1.3751 1.9008 tte -1.2129 4.6	1.9728 2.1213 2.172 -0.4697 2.418 -0.6048 0.8113 1.8304 0.9421 0.1777 0.2729 1.3751 0.3008 1.4 3.8724	1.4728 0.6213 0.372 0.918 0.1304 1.4397 -0.7276	0.0397		

profenophos	3	3.7267	0.7267		
propiconazole	3.4	3.2941	-0.1059		
propyleneglycol	0.4	0.6345	0.2345		
siduron 2.3	2.6706	0.3706			
sulfometuron me	thyl	1.6	1.038	-0.562	
4-t-butylphenylca	arbamate	2.1	2.2118	0.1118	
terbufos sulfone	2.2	3.1643	0.9643		
terbufos sulfoxid	e	2.2	2.9532	0.7532	
terbutryn	2.9	3.3228	0.4228		
2,3,5,6-tetrachlor	oaniline	3.9	3.6731	-0.2269	
2,6,2',6'-tetrachlo	robiphen	yl	5	4.264	-0.736
2,3,4,5-tetrachlor	onitrober	nzene	4.2	3.1664	-1.0336
2,3,5,6-tetrachlor	onitrober	nzene	4	3.4705	-0.5295
tetrachlorophthal	ate	3.3	2.5566	-0.7434	
triadimefon	2.7	2.7969	0.0969		
tribromomethane	2.1	2.7851	0.6851		
tricyclazol	3.1	1.6113	-1.4887		
vernolate	2.3	2.758	0.45		