PREDICTION OF SOIL SORPTION COEFFICIENT OF CHEMICALS BY MOLECULAR MODELING TECHNIQUE

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การทำนายสัมประสิทธิ์การดูดซับสารเคมีของดินด้วยเทคนิคการสร้างแบบจำลองเชิงโมเลกุล

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วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต
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Thesis Title	PREDICTION OF SOIL SORPTION COEFFICIENT OF CHEMICALS BY MOLECULAR MODELING TECHNIQUE
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วศิน พิทักษ์ตระกูล : การทำนายสัมประสิทธิ์การดูดซับสารเคมีของดินด้วยเทคนิคการสร้างแบบจำลองเชิงโมเลกุล. (PREDICTION OF SOIL SORPTION COEFFICIENT OF CHEMICALS BY MOLECULAR MODELING TECHNIQUE) อ.ที่ปรึกษาหลัก : รศ. ดร. สมศักดิ์ เพียรวณิช

มลพิษทางดิน เป็นหนึ่งในมลพิษที่ได้รับผลกระทบจากการกระทำของธรรมชาติและมนุษย์ ซึ่งส่วนใหญ่เกิดจากการใช้ยาฆ่าแมลง และปุ๋ยเคมี เพื่อให้พืชออกผลผลิตและเติบโตมาอย่างงดงาม แต่ก็ทำให้ดินนั้นได้ดูดซับสารเคมีเอาไว้ ในงานวิจัยนี้จึงได้ศึกษาหาสมบัติของสารเคมีที่มีผลต่อการดูดซับสารของดิน และหาแบบจำลองเพื่อทำนายค่าสัมประสิทธิ์การดูดซับสารของดิน (K_{OC}) ด้วยเทคนิคการหาความสัมพันธ์เชิงปริมาณระหว่างโครงสร้างกับสมบัติ (QSPR) โดยเริ่มจากการนำสารทั้งหมดจำนวน 1,327 สาร มาสร้างโครงสร้าง 3 มิติ และทำการคำนวณปรับโครงสร้างด้วยวิธีเซมิ-เอ็มพิริกัล พีเอ็ม 7 จากนั้นนำมาคำนวณค่าสมบัติทางเคมีกายภาพ จำนวนรวม 1,536 สมบัติ ใช้วิธีการวิเคราะห์การถดถอยเชิงเส้นพหุคูณในการหาสมบัติของสารที่มีผลต่อการดูดซับสารเคมีของดิน และสร้างแบบจำลอง QSPR ซึ่งแบบจำลองที่ได้มีความสัมพันธ์และประสิทธิภาพที่ดีในการทำนาย โดยมีค่า r^2 = 0.762 และ q^2 = 0.761

สาขาวิชา เคมี ลายมือชื่อนิสิต .....

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Wasin Pithaktrakool : PREDICTION OF SOIL SORPTION COEFFICIENT OF CHEMICALS BY MOLECULAR MODELING TECHNIQUE. Advisor: Assoc. Prof. SOMSAK PIANWANIT, Ph.D.

Soil pollution is one of the pollutions caused by nature and human activities, which are mostly the use of insecticide and chemical fertilizer to make plants grow well and produce more products. However, these chemicals are absorbed by soil. In this research work, properties of chemical compound affecting soil sorption were analyzed, and model that can predict soil sorption coefficient of chemicals (K_{OC}) was examined by using quantitative structure property relationship (QSPR) technique. Totally 1,327 compounds were selected, and their three-dimensional structures were constructed. Semi-empirical PM7 method was used for geometry optimization calculations. A total of 1,536 physicochemical properties were computed. Multiple linear regression was employed to analyze properties of compound affecting soil sorption and to find QSPR model. The obtained model has a good relationship and predictive ability with r^2 = 0.762 and q^2 = 0.761.

Field of Study: Chemistry Student's Signature .....

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Wasin Pithaktrakool

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LIST OF ABBREVIATIONS

QSPR	Quantitative structure-property relationship
K_{OC}	soil sorption coefficient
MW	Molecular weight
logP	Octanol-water partition coefficient
HBA	Hydrogen bond acceptor
HBC	Hydrogen bond donor
nRB	number of Rotatable bonds
TE	Total energy
MD	Molecular density
MV	Molecular volume
MA	Molecular area
MP	Mean polarizability
MF	Molecular flexibility
MR	Molecular refractivity
NBE	Non-bond energy
Ob	Orbitals
DM	Dipole moment
QM	Quadrupole moment
WI	Wiener index
ZI	Zegrab index

KI	Kappa index
CHI	Chi index
nAtom	number of all atoms
nEle	number of elements
nRing	number of rings
VR2_Dzi	normalized Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential
MDEO-11	molecular distance edge between primary O and primary O
IC0	0-ordered neighborhood information content
nHRing	number of hetero rings
nG12FAHRing	number of 12-or-greater-membered aliphatic fused hetero ring
AXp-4dv	4-ordered averaged Chi path weighted by valence electrons
C3SP3	SP3 carbon bound to 3 other carbons

CHAPTER 1
INTRODUCTION

1.1 Overview

Nowadays, many chemicals are absorbed into the soil by several processes both naturally occurring causes such as acid rain, volcano eruptions, earthquake, tsunami, and anthropogenic causes such as landfill, mining, industrial waste, agricultural activities (using insecticides and herbicides to protect the crops from insects and pests). In these activities, a large number of chemicals in the soil are residues, and they cause soil pollution that affects the plants and other living things that live in the soil. Finally, it is a health hazard to animals and humans. Therefore, scientists are interested in studying the quantity of chemicals that were adsorbed in the soil to use the information for planning and controlling the quantity of residual chemicals in the soil. It also assessed the environmental risk and impact of each chemical. However, the experiment for chemisorption measurement in the soil requires a budget of instruments, chemicals, and time-consuming for analysis. Hence, the Quantitative Structure-Property Relationship (QSPR) method has been widely applied in the prediction of soil sorption because it can predict chemical adsorption conveniently and rapidly, save the budget and time, and reduce the use of chemicals that will produce waste.

1.2 Quantitative structure-property relationship

The Quantitative Structure-Property Relationship (QSPR) method is a chemical information technique about the mathematical model that shows a correlation between chemical structure and property. This method can develop a mathematical model that connects with the physicochemical properties of a molecule by using chemometric methods to explain the physicochemical properties. [1]

The molecular descriptors of a molecule are shown in the numeric equation and then these molecular descriptors are used to calculate the physicochemical properties of the molecule. [2] The molecular descriptors can be estimated physicochemical properties, and are divided into many classes such as constitutional descriptors (molecular weight, total number of atoms, functional group), topological descriptors (connectivity index, Wiener index, Balaban index), electrostatic descriptors (polarizability, dipole moment), geometrical descriptors (molecular volume, molecular surface area), thermodynamic descriptors (vibrational frequencies, translational frequencies, rotational frequencies), and quantum chemical descriptors (HOMO/LUMO energies, standard heat of formation). [3]

The QSPR models can be developed by first collecting the data: the data is collected and used to create the 3D structures for calculating molecular descriptors. Second, building the model: built QSPR model by the quantitative relationship between something's values and structural properties. And last, validation of the QSPR model by validating both the internal and the external QSPR model. [4]

1.3 The soil sorption coefficient

In general, soil sorption is experimentally measured as the organic carbon-water partition coefficient or soil sorption coefficient (K_{OC}). K_{OC} value can be calculated from the ratio between the concentrations of dissolved chemicals in the soil and the concentration of dissolved chemicals in the water compared to the organic carbon content of a soil as shown in the equation below. From the equation, it seems that K_{OC} may relate with an octanol-water partition coefficient (log P). Therefore, there are several QSPR publications that used log P as descriptor to predict the value of K_{OC}. The soil sorption coefficient is applied in an environmental risk assessment and is important for the characterization of the dispersion of chemicals in the soil phase and water phase. [5]

$$K_{oc} = \frac{\text{concentration of chemical in soil}}{\text{concentration of chemical in water}} \times \frac{100}{\text{\% organic carbon content of soil}}$$

1.4 Literature reviews

There are several research on the QSPR models of soil sorption coefficient.

In 1994, Lohninger [6] built QSPR models of a training set of 120 pesticides and analyzed them with multiple linear regression (MLR) and neural network methods. The QSPR model was obtained from 11 structural parameters. It consisted of 2 topological parameters and 9 structural fragment parameters. And resultant prediction in a test set of 81 pesticides was similar to the model that used the water solubility parameter.

In 2003, Eduardo et. al. [7] built QSPR models of 82 organic compounds that included polar, non-polar, saturated, unsaturated, aliphatic, aromatic, and polycyclic aromatic compounds. The best correlation of the QSPR model had r^2 = 0.94 with 5 parameters, namely molecular weight, the number of benzene rings, and the number of nitrogen, oxygen, and sulfur atoms. It was found that this QSPR model used simple parameters that were calculated from the molecular formula and the calculation of these parameters did not need to use quantum theory and software in calculation. Furthermore, this model could be good and predicted the soil sorption coefficient in a data set of 43 organic compounds.

In 2005, Irish et. al. [8] studied the QSPR model of 344 compounds of organic pollutants that different classes. The QSPR was built from each of the classes and all 344 compounds. It found that the QSPR models from each of the classes were better than all compounds, and some QSPR models used log K_{OW} parameter, whereas some QSPR models did not use log K_{OW} parameter too.

In 2007, Pablo et. al. [9] studied the QSPR model of 163 non-ionic organic pesticides and used 1,247 theoretical descriptors to analyze the correlation with statistical methods that they contained forward stepwise regression (FSR), genetic

algorithm (GA), and the replacement method (RM). It was found that the QSPR models contained 6 descriptors without logP parameter in these methods.

In 2009, Nasser et. al. [10] studied the QSPR models of 124 pesticides and used 1,457 descriptors to analyze the correlation with linear regression (multiple linear regression, MLR) and non-linear regression (artificial neural network, ANN). It was found that the QSPR models contained 7 descriptors without logP parameter.

In 2013, Ralpho et. al. [11] studied the QSPR model of 143 pesticides by using log P that were calculated from different algorithms. It was found the algorithm used to calculate logP parameter had effect on the performance of the QSPR model. Therefore, the best model obtained from logP parameter was a suitable calculation.

In 2014, Yonghua et. al. [12] studied the QSPR model of 964 several organic compounds to analyze with 3 statistical methods: multiple linear regression (MLR), local lazy regression (LLR), and Least squares support vector machine (LV-SVM). The QSPR model contained 4 parameters that included logP descriptor in this model. And the QSPR model from the LS-SVM method analysis has the highest efficiency compared to MLR and LLR methods.

In 2019, Carlos et al. [13] studied the QSPR of a training set of 639 non-ionic organic compounds, then they built the QSPR model by using only logP parameter, but a training set was changed the size for studying the effect of sized and the statistical quality. It was found that the sizes of the training set had not affected the efficiency in the prediction of QSPR model.

All of the research articles, some research works used logP parameter while some research did not. Therefore, this research would like to know the parameter that affects soil sorption by using quantitative structure-property relationship methods to know the factor of soil sorption.

1.5 Objectives

This research aims to find physicochemical properties that affect soil sorption and to find QSPR modeling for predicting soil sorption coefficient.

CHAPTER 2
COMPUTATIONAL EXPERIMENT

2.1 Materials

2.1.1 Personal Computer

2.2.2 HyperChem Professional 8.0 software

2.2.3 MOPAC 2016 software

2.2.4 Materials studio software

2.2.5 Mordred software [14]

2.2 Computational method

2.2.1 Finding the QSPR Models

2.2.2.1 Collected Data Set

To research, study and collect data from 1994-2019 research articles [6-13] that included chemical names, chemical structures, chemical formulas, CAS no., and soil sorption coefficient (log K_{OC}). It is a total of 1,327 compounds.

2.2.2.2 Built the Chemical Structure

The 2D, and 3D structures of all 1,327 compounds were built in HyperChem Professional 8.0 software. Geometry optimizations were performed with the semi-empirical PM7 method in MOPAC 2016 software. A total of 1,536 physicochemical properties were calculated in Material Studio software and Mordred software.

2.2.2.3 Built the QSPR Model

1,327 compounds were divided into a training set of 928 compounds and a test set of 399 compounds. The QSPR model was built using the training set by a correlation between log K_{OC} and physicochemical properties and analyzed with the multiple linear regression (MLR) method in Materials Studio software.

2.2.2.4 Validation of the QSPR Model

The QSPR model that was obtained from the calculation in step 2.2.2.3 is analyzed to validate its efficiency using compounds in the test set. The predicted log K_{oc} values are compared with their corresponding experimental values.

2.2.2.5 Adjustment of the QSPR Model

One of the major disadvantages of MLR method is its sensitivity to outliers. Therefore, it is usually necessary to adjust the QSPR model by omitting some outliers to improve the performance of the model.

CHAPTER 3
RESULTS & DISCUSSIONS

3.1 Division of chemicals to a training set and a test set

After chemical structures that were built in 3D, computed geometry optimization with semi-empirical PM7, and calculated physicochemical properties in Materials Studio and Mordred software, and a data set of 1,327 compounds was divided into 2 groups, namely a training set of 928 compounds and a test set of 399 compounds, it showed in Appendix A and B.

3.2 Construction of quantitative structure-property relationship models

The quantitative structure-property relationship models constructed for the correlation between the soil sorption coefficient and the physicochemical properties, 24 physicochemical properties in Materials Studio software and 1,519 physicochemical properties in Mordred software.

3.2.1 Construction of QSPR model from Materials Studio software

3.2.1.1 Using 1 physicochemical property

The model 1 was constructed the correlation between the log K_{OC} of the training set and AlogP98 (Octanol-Water Partition Coefficient) property that related to the model 1.

Before adjusted Model 1: $\log K_{OC} = 0.503 * AlogP98 + 1.386$

$n = 928$, $r^2 = 0.598$, $q^2 = 0.596$

After adjusted Model 1: $\log K_{OC} = 0.5800 * AlogP98 + 1.236$

$n = 860$, $r^2 = 0.757$, $q^2 = 0.756$

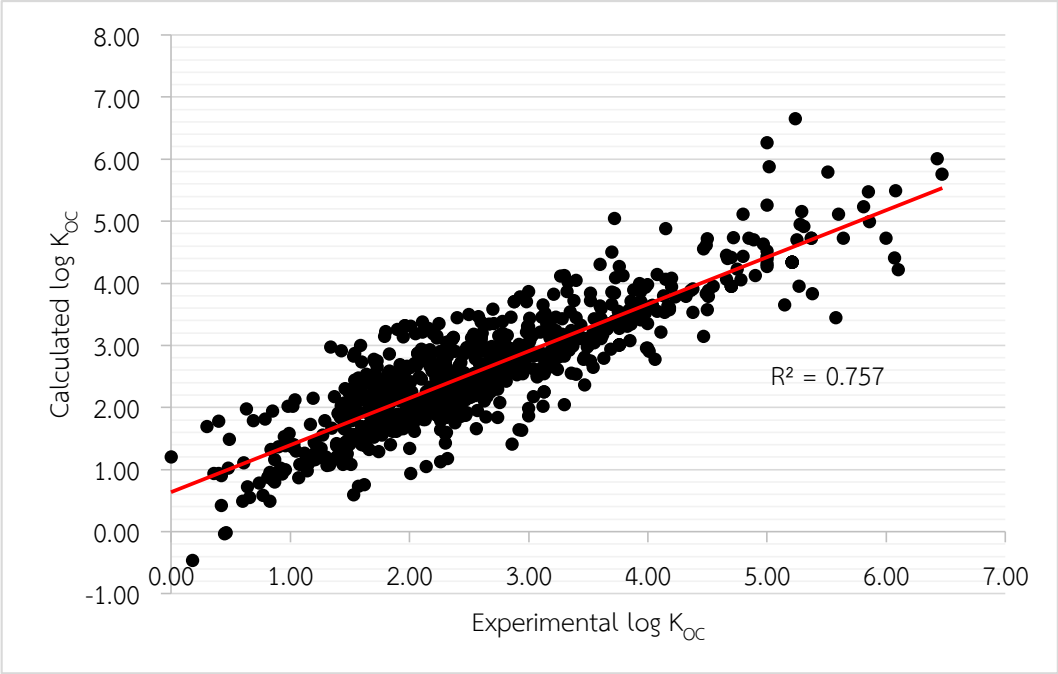

Figure 3.1 Scatter plot of the calculated vs experimental log K_{OC} of a training set of model 1

And model 1 was validated in the test set of 399 compounds.

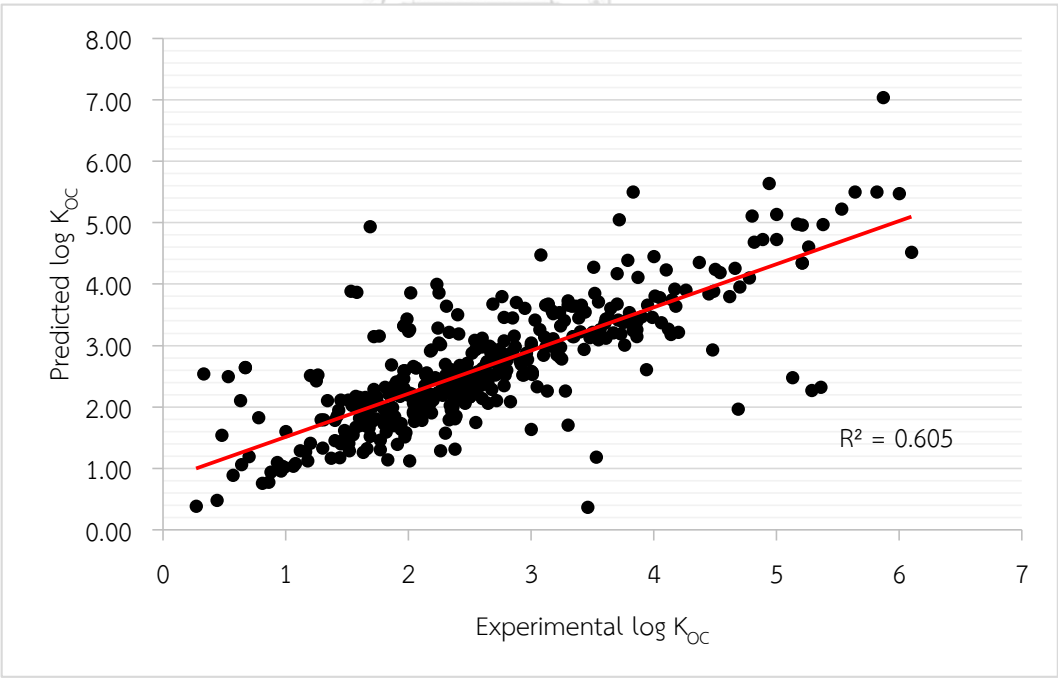

Figure 3.2 Scatter plot of the predicted vs experimental log K_{OC} of a test set of model 1

3.2.1.2 Using 17 physicochemical properties

The model 2 was constructed the correlation between the log K_{OC} of a training set and 17 physicochemical properties that consist of MW (Molecular weight), AlogP98 (Octanol-Water Partition Coefficient), HBA (Hydrogen Bond Acceptor), HBD (Hydrogen Bond Donor), nRB (Number of Rotatable Bond), TE (Total Energy), MD (Molecular Density), MV (Molecular Volume), MA (Molecular Area), MP (Mean polarizability), MF (Molecular flexibility), NBE (Non-bond Energy), Ob (Orbitals), DM (Dipole Moment), MR (Molecular refractivity), WI (Wiener index), and ZI (Zagreb index). It found that the physicochemical properties, namely ALogP98 (Octanol-Water Partition Coefficient), HBA (Hydrogen Bond Acceptor), MF (Molecular Flexibility), and ZI (Zagreb Index) related to the correlation of the model 2.

Before adjusted Model 2: $\log K_{OC} = 0.475 * AlogP98 - 0.0879 * HBA + 0.0204 * MF + 0.00347 * ZI + 1.422$

$n = 928, r^2 = 0.614, q^2 = 0.610$

After adjusted Model 2: $\log K_{OC} = 0.519 * AlogP98 - 0.0957 * HBA + 0.0172 * MF + 0.00458 * ZI + 1.376$

$n = 694, r^2 = 0.802, q^2 = 0.793$

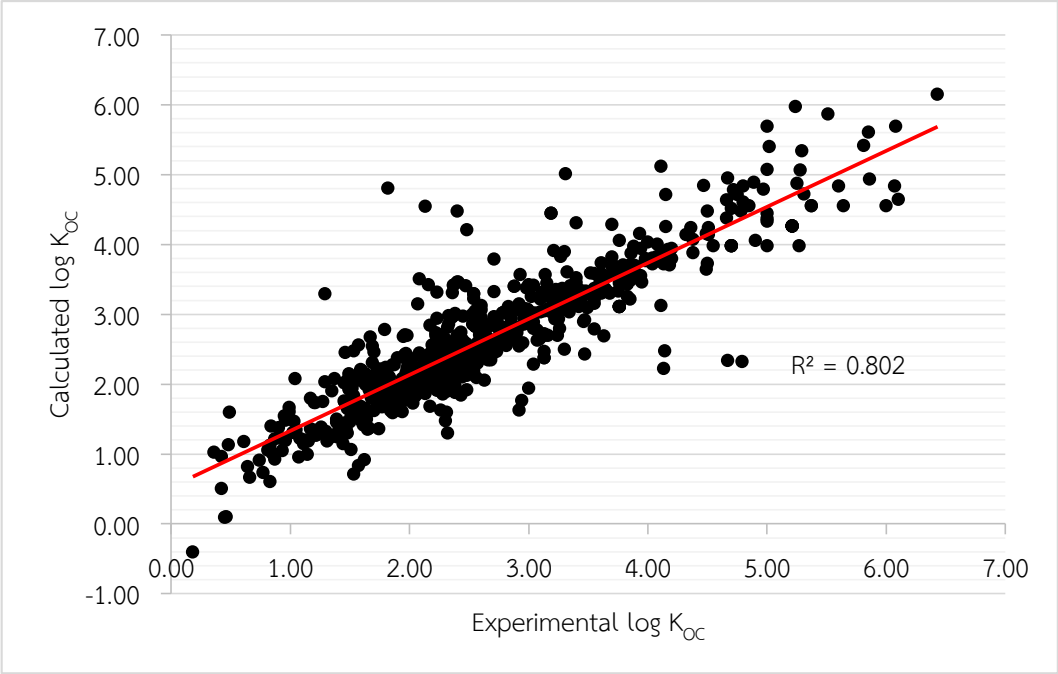

Figure 3.3 Scatter plot of the calculated vs experimental log K_{OC} of a training set of model 2

And model 2 was validated in the test set of 399 compounds.

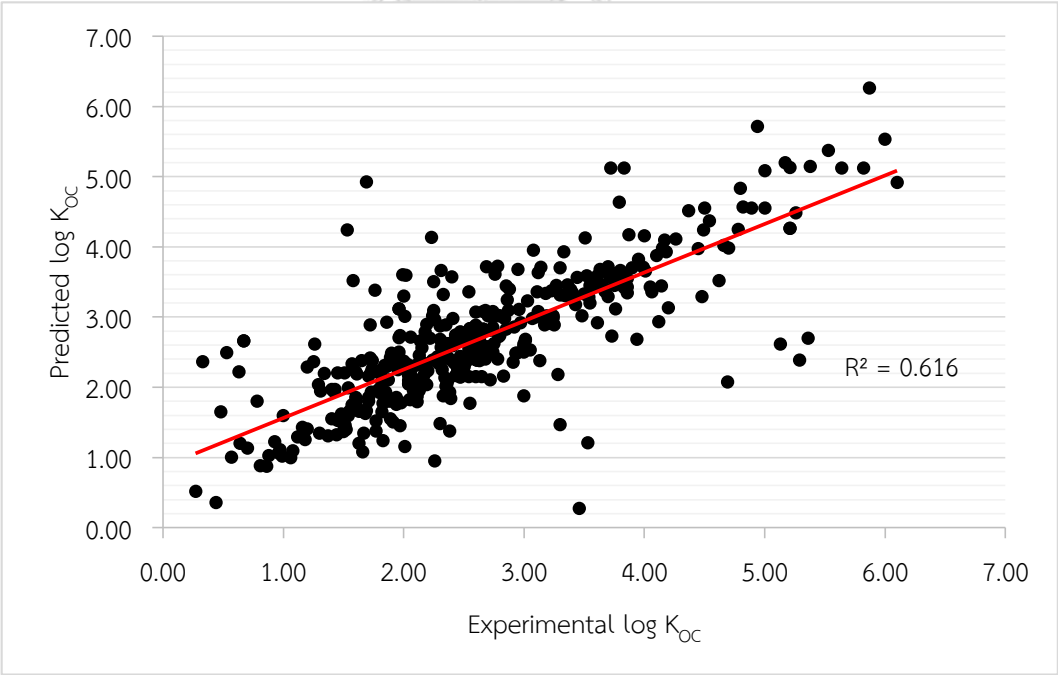

Figure 3.4 Scatter plot of the predicted vs experimental log K_{OC} of a test set of model 2

3.2.1.2 Using 24 physicochemical properties

The model 3 was constructed the correlation between the log K_{OC} of a training set and 24 physicochemical properties that consist of MW (Molecular weight), AlogP98 (Octanol-water partition coefficient), HBA (Hydrogen Bond Acceptor), HBD (Hydrogen Bond Donor), nRB (Number of Rotatable Bond), TE (Total Energy), MD (Molecular Density), MV (Molecular Volume), MA (Molecular Area), MP (Mean polarizability), MF (Molecular flexibility), NBE (Non-bond Energy), Ob (Orbitals), DM (Dipole Moment), QM (Quadrupole moment), MR (Molecular refractivity), WI (Wiener index), and ZI (Zagreb index), J (Balaban index), KI (Kappa index), ChI (Chi index), nAtom (Number of all atoms), nEle (Number of Elements), and nRing (Number of rings). It found that the physicochemical properties, namely AlogP98 (Octanol-water partition coefficient), HBA (Hydrogen Bond Acceptor), nRB (Number of Rotatable Bond), TD (Total Dipole), QM-zz (Quadrupole ZZ), and WI (Wiener index) related to the correlation of the model 3.

Before adjusted Model 3: $\log K_{OC} = 0.476 * \text{AlogP98} - 0.0744 * \text{HBA} - 0.0180 * \text{nRB} - 0.0367 * \text{TD} + 0.00732 * \text{QM-zz} + 0.000430 * \text{WI} + 1.682$

$n = 928$, $r^2 = 0.622$, $q^2 = 0.616$

After adjusted Model 3: $\log K_{OC} = 0.563 * \text{AlogP98} - 0.0670 * \text{HBA} - 0.0214 * \text{nRB} - 0.0449 * \text{TD} + 0.00798 * \text{QM-zz} + 0.000341 * \text{WI} + 1.539$

$n = 838$, $r^2 = 0.800$, $q^2 = 0.795$

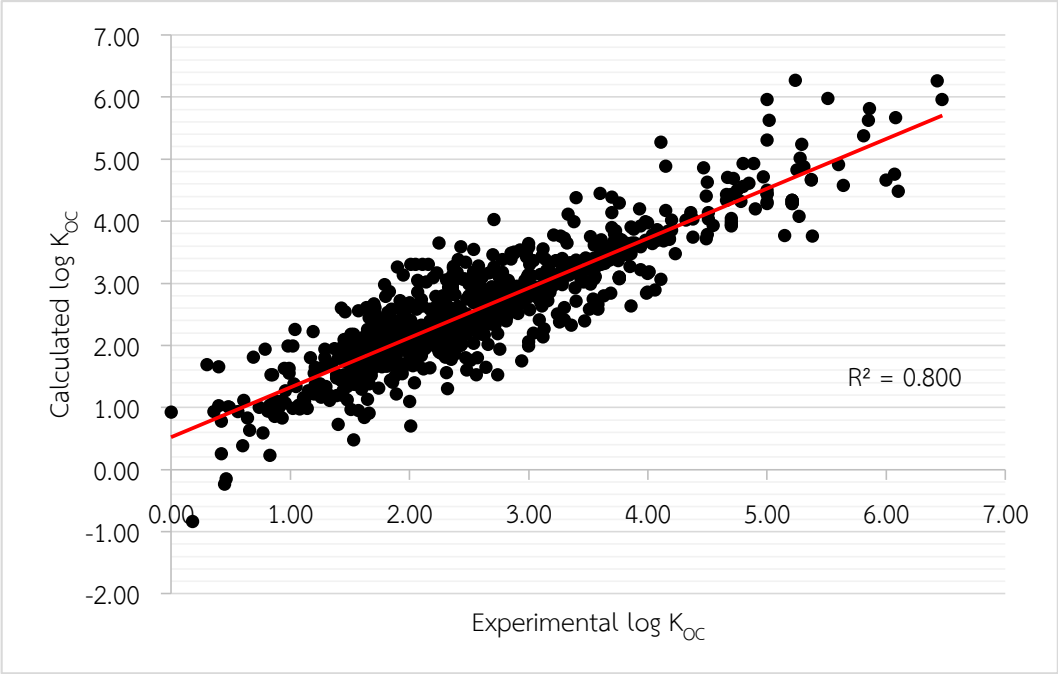

Figure 3.5 Scatter plot of the calculated vs experimental log K_{OC} of a training set of model 3

And model 3 was validated in the test set of 399 compounds.

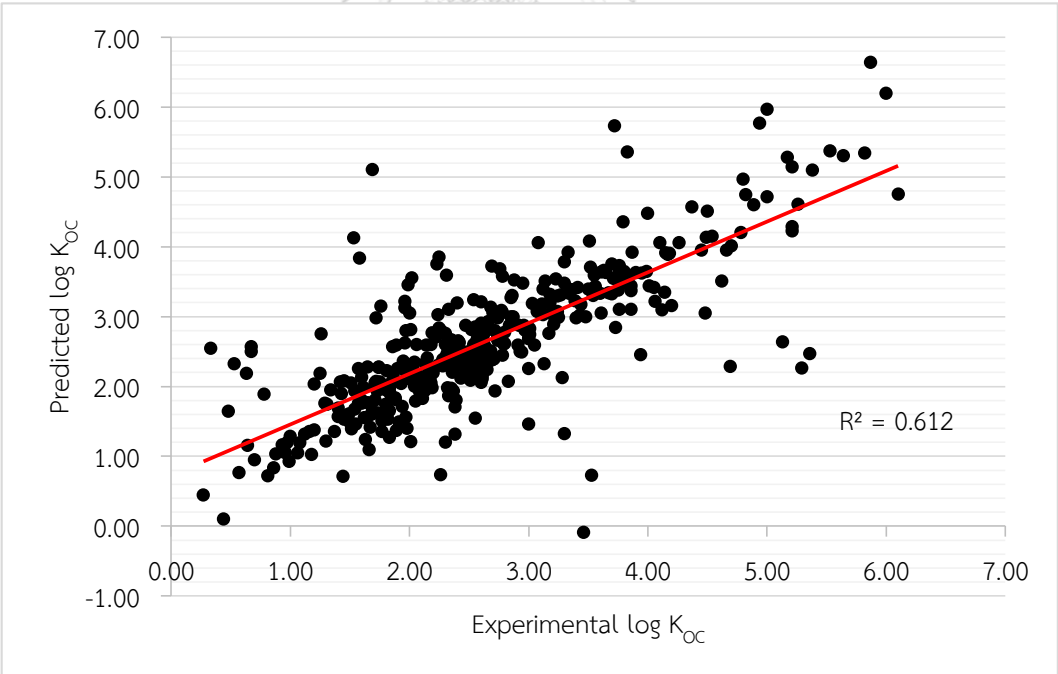

Figure 3.6 Scatter plot of the predicted vs experimental log K_{OC} of a test set of model 3

3.2.2 Construction of QSPR model from Mordred software

3.2.2.1 Using 1 physicochemical property

The model 4 was constructed the correlation between the log K_{OC} of a training set and SlogP (Octanol-Water Partition Coefficient) property that related to the model 4.

Before adjusted Model 4: $\log K_{OC} = 0.505 * SlogP + 1.410$

$n = 928, r^2 = 0.552, q^2 = 0.549$

After adjusted Model 4: $\log K_{OC} = 0.638 * SlogP + 1.152$

$n = 834, r^2 = 0.762, q^2 = 0.761$

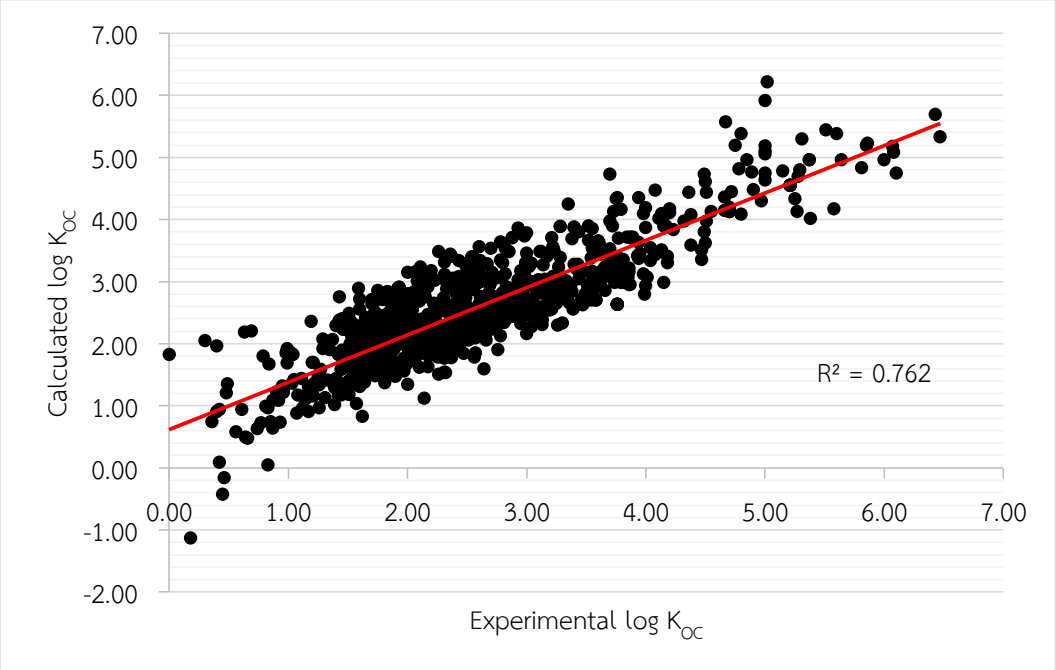

Figure 3.7 Scatter plot of the calculated vs experimental log K_{OC} of a training set of model 4

And model 4 was validated in the test set of 399 compounds.

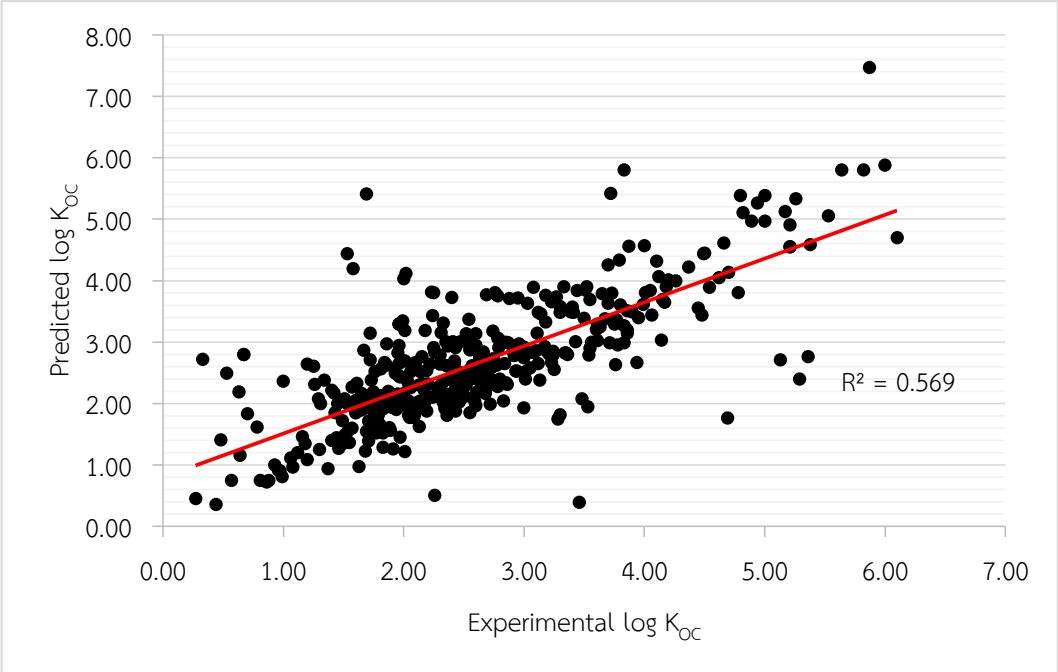

Figure 3.8 Scatter plot of the predicted vs experimental log K_{OC} of a test set of model 4

3.2.2.2 Using 1,519 physicochemical properties

The model 5 was constructed the correlation between the log K_{OC} of a training set and 1,519 physicochemical properties such as SlogP (Octanol-Water Partition Coefficient), VR2_Dzi (Normalized Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential), MDEO-11 (Molecular Distance Edge between primary O and primary O), IC0 (0-ordered neighborhood information content), nAtom (Number of all Atoms), nHRing (Number of Rings), nG12FAHRing (Number of 12-or-Greater-Membered Aliphatic Fused Hetero ring), AXp-4dv (4-ordered averaged Chi path weighted by valence electron), C3SP3 (SP3 Carbon bound to 3 other Carbon), etc. It found that the physicochemical properties, namely SlogP (Octanol-Water Partition Coefficient), MDEO-11 (Molecular Distance Edge between primary O and primary O), IC0 (0-ordered neighborhood information content), nHRing (Number of Rings), nG12FAHRing (Number of 12-or-Greater-Membered Aliphatic Fused Hetero ring),

and C3SP3 (SP3 Carbon bound to 3 other Carbon) related to the correlation of the model 5.

Before adjusted Model 5: $\log K_{OC}$ = 0.530 * SlogP + 0.345 * MDEO-11 - 0.913 * IC0 + 0.253 * nHRing + 1.628 * nG12FAHRing - 0.256 * C3SP3 + 2.597

n = 928, r^2 = 0.637, q^2 = 0. 623

After adjusted Model 5: $\log K_{OC}$ = 0.631 * SlogP + 0.345 * MDEO-11 - 0.933 * IC0 + 0.147 * nHRing + 1.378 * nG12FAHRing - 0.143 * C3SP3 + 2.434

n = 840, r^2 = 0.804, q^2 = 0.802

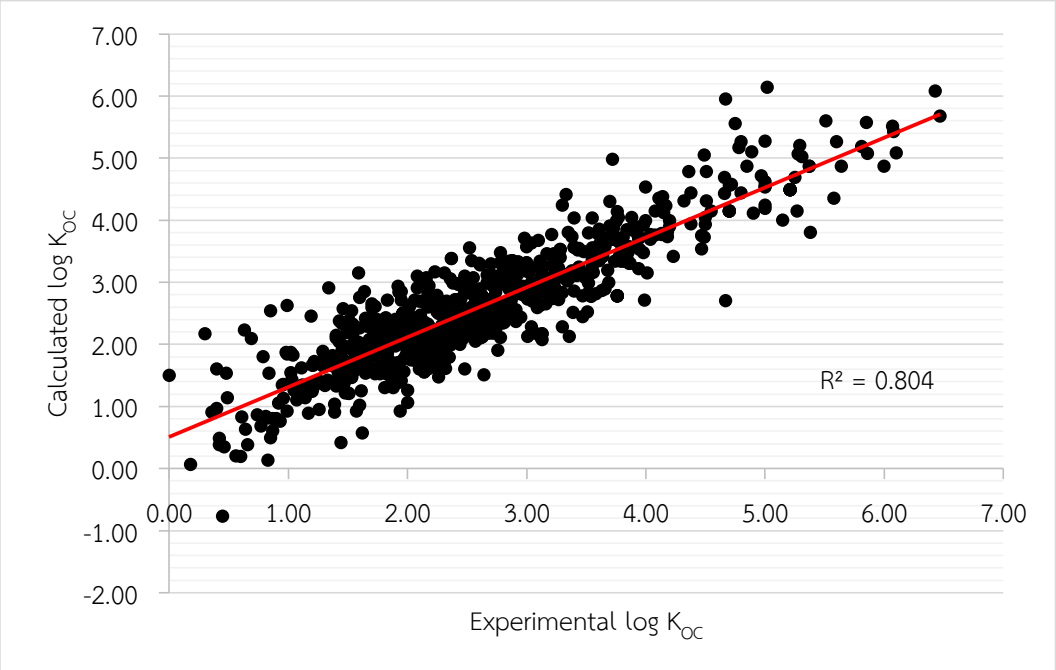

Figure 3.9 Scatter plot of the calculated vs experimental log K_{OC} of a training set of model 5

And model 5 was validated in a test set of 399 compounds.

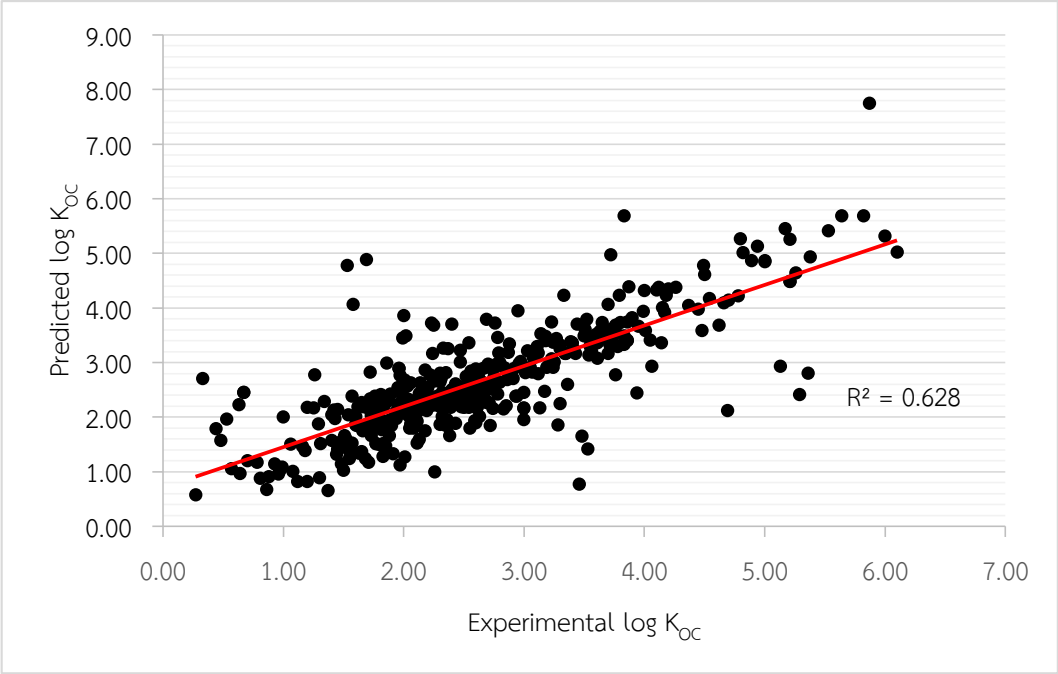

Figure 3.10 Scatter plot of the predicted vs experimental log K_{OC} of a test set of model 5

In this research, the soil sorption strongly depended on logP property. The soil sorption coefficient (log K_{OC}) is related to the logP property in a positive way. It showed that a compound with high logP value is highly absorbed by the soil. This agrees with the research work of Ralpho et. al. (2013) [11], Yonghua et. al. (2014) [12] and Carlos et. al. (2019) [13]. And this data supported the theory of the soil sorption coefficient that it is related to logP property.

Table 3.1 Comparison of physicochemical properties, r^2, and q^2 values all of models

Model	Physicochemical properties	r^2	q^2
1	AlogP98	0.757	0.756
2	AlogP98, HBA, MF, ZI	0.802	0.793
3	AlogP98, HBA, nRB, TD, QM-zz, WI	0.800	0.795
4	SlogP	0.762	0.761
5	SlogP, MDEO-11, IC0, nHRing, nG12FAHRing, C3SP3	0.804	0.802

Table 3.1 summarizes data of all models, in which the physicochemical properties of model 1-3 were calculated in Materials Studio software and those of model 4-5 were calculated in Mordred software. All five QSPR models have the logP property, but the difference in each model was the number of physicochemical properties which were added in the other models. In model 1 that used AlogP98 calculated in Materials Studio 2020 software and model 4 that used SlogP calculated in Mordred software, they have very similar statistical values. However, the model 4 is preferred because the Mordred software is free software so all researchers can use the software conveniently without any restriction. Therefore, model 4 that was log K_{OC} = 0.638 * SlogP + 1.152 with r^2 and q^2 values of 0.762 and 0.761 was chosen. Then, it was validated in the test set giving r^2 value of 0.569. Therefore, model 4 has good statistics and can be applied to compounds with diverse structural classes than previous published QSPR models.

The number of physicochemical properties used in model 2 is 4 while model 3 and 5 used 6 physicochemical properties, and their r^2 values were increased from 0.762 in model 1 to 0.802, 0.800, and 0.804 in model 2, 3, and 5 respectively. The r^2 values were increased by just 5.12 to 5.25 percentage when changing from using only 1 physicochemical property (model 4) to 4 and 6 physicochemical properties (model 2,3, and 5). This increase in r^2 values is statistically not significant, therefore, models 2, 3 and 5 were not chosen.

3.3 Comparison of r^2 and q^2 values of each group by using model 6, 7 and 8

Because model 4 was constructed by using several structural groups, it is interesting to investigate QSPR model for each individual structural group whether using only SlogP property would be adequate, or the addition of other properties into the model would result in a higher efficiency. Therefore, the physicochemical properties, namely MDEO-11, IC0, nHRing, nG12FAHRing and C3SP3, which were

obtained in model 5, were correlated in each group. Statistics for QSPR models of 11 different structural groups are shown in Table 3.2.

Table 3.2 r^2 and q^2 values of model 6 and 7

Gr.	structure	n	*Model 6		Property(ies)	**Model 7	
			r^2	q^2		r^2	q^2
1	PAHs	58	0.344	0.310	SlogP	0.344	0.310
2	Ether	20	0.494	0.339	SlogP	0.494	0.339
3	Alcohol	55	0.922	0.877	SlogP MDEO-11	0.960	0.895
4	Organophosphorus	60	0.278	0.225	SlogP MDEO-11	0.334	0.188
5	Amine	35	0.517	0.403	SlogP IC0	0.723	0.693
6	Nitrile	18	0.738	0.723	SlogP IC0	0.796	0.742
7	Organosulfur	19	0.370	-0.401	SlogP IC0	0.546	-0.407
8	Aliphatic hydrocarbons	149	0.555	0.550	SlogP MDEO-11 IC0	0.647	0.607
9	Carbonyl derivatives	181	0.594	0.582	SlogP MDEO-11 IC0 C3SP3	0.665	0.614
10	Benzene and derivatives	539	0.566	0.562	SlogP MDEO-11 IC0 C3SP3	0.639	0.627
11	Heterocyclic	173	0.326	0.316	SlogP MDEO-11 C3SP3 G12FAHRing	0.417	0.281
12	Other compound	20	-	-	-	-	-

* used only SlogP in model 6

** used some physicochemical properties that obtained in model 5 into model 7

After the model 7 was constructed, it used some physicochemical properties that obtained in model 5, the results showed that the compounds in group 1 and 2 still used only SlogP property but the statistics of these groups were not high. It indicated that these structures may have other factors to affect the soil sorption or may have complicated mechanisms of soil sorption. Model for compounds in group 3, which uses SlogP and MDEO-11, has high efficiency with the values of r^2 = 0.960 and

q^2 = 0.895. Model for compounds in group 4 used the same physicochemical properties as that of group 3, but the statistics of group 4 were lower than group 3. From compounds in group 5, 6, and 7, models of these groups use 2 physicochemical properties, i.e., SlogP and IC0. Model for group 8 has 3 physicochemical properties: SlogP, MDEO-11, and IC0. Models for group 9 and 10 have 4 physicochemical properties, which are SlogP, MDEO-11 IC0, and C3SP3. Model for group 11 uses 4 physicochemical properties, which are SlogP, MDEO-11, C3SP3, and nG12FAHRing.

In the considered model shown in Appendix D, the significantly increased r^2 was a higher percentage of 10 per the addition of 1 property, it was found that group 4, 5, and 7 conformed to this criterion. However, considering q^2 values of groups 4, 5, and 7, the q^2 values of group 4 and 7 were decreased, therefore, addition of physicochemical property in models 4 and 7 did not improve the model, but the q^2 value of group 5 increased significantly. Hence, only group 5, which is amine compounds, has higher efficiency of the QSPR model. The obtained QSPR models have different physicochemical properties in each structural group. Therefore, these results indicated that the soil sorption mechanism was complicated and related to different several properties.

Table 3.3 Comparison of the correlation of model 6, 7 and 8

Gr.	structure	n	Model 6		Model 7		Model 8	
			r^2	q^2	r^2	q^2	r^2	q^2
1	PAHs	58	0.344	0.310	0.344	0.310	0.364	0.290
2	Ether	20	0.494	0.339	0.494	0.339	0.539	-75.26
3	Alcohol	55	0.922	0.877	0.960	0.895	0.960	0.941
4	Organophosphorus	60	0.278	0.225	0.334	0.188	0.347	0.184
5	Amine	35	0.517	0.403	0.723	0.693	0.752	-109.88
6	Nitrile	18	0.738	0.723	0.796	0.742	0.796	-293.13
7	Organosulfur	19	0.370	-0.401	0.546	-0.407	0.633	-0.454
8	Aliphatic hydrocarbons	149	0.555	0.550	0.647	0.607	0.657	0.641
9	Carbonyl derivatives	181	0.594	0.582	0.665	0.614	0.668	0.617
10	Benzene and derivatives	539	0.566	0.562	0.639	0.627	0.640	0.628
11	Heterocyclic	173	0.326	0.316	0.417	0.281	0.431	0.277
12	Other compounds	20	-	-	-	-		

In Table 3.3, Model 6 used only SlogP, Model 7 used some additional physicochemical properties that were obtained in model 5, and model 8 used all physicochemical properties in model 5. All of these models were constructed the correlation of each group between log K_{OC} and physicochemical properties to improve the statistics. The results showed that models for compounds in group 1, 2, 4, 5, 6, 7, and 11 have quite low r^2 values, and their q^2 values were lower than model 6 which used only SlogP and model 7 which used one additional property. Models for compounds in groups 3, 8, 9, 10 and 11 have similar r^2 and q^2 values to model 6 and 7, therefore, they are statistically no different. In summary, first, some physicochemical properties might not be suitable for some structural group and second, the addition of a number of physicochemical properties might decrease the efficiency of model.

CHAPTER 4
CONCLUSIONS

The quantitative structure-property relationship (QSPR) method in this work showed the mathematical model of a correlation between the soil sorption coefficient (log K_{OC}) and physicochemical properties that were calculated in Materials Studio and Mordred software. All of 1,327 several structural compounds, such as aliphatic hydrocarbon, alcohol, ether, carbonyl, amine, benzene derivatives, aromatic hydrocarbon, heterocyclic aromatic hydrocarbon, polycyclic aromatic hydrocarbon etc. were collected in the research article, then the structures were built 3D structure, optimized geometry, calculated physicochemical properties and constructed the models and analyzed model multiple linear regression analysis. It found that the model 4: log K_{OC} = 0.638 * SlogP + 1.152 was selected as the best QSPR model because the physicochemical property was calculated in Mordred software that is free software and values of r^2 and q^2 are 0.762 and 0.761, respectively. The model was validated in a test set, it gave r^2 predicted = 0.569. So, model 4 had better statistics and might be applied to several classes of structures than previous research.

Adding physicochemical properties from model 5 into model 4 could improve r^2 values of group 4 (organophosphorus), 5 (amine), and 7 (organosulfur) but the q^2 values of group 4 and 7 were decreased, whereas the q^2 values of group 5 was significantly increased, so group 5 which is amine compound was higher efficiency of QSPR model. Therefore, the addition of a number of physicochemical properties might be decreased the efficient model. It indicated that the mechanism in the soil sorption of each step was complicated and related to different several properties, therefore, the model also obtained different physicochemical properties of each structural group.

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Appendix

Table A-1 Chemicals list, values of exp log KOC and physicochemical properties in a training set

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0001	2-phenylpropionic acid	2.36	1.957	2	2.387	3	1.722	-5.931	50	156	1.875	0.500	1.357	0.000	0.000	1.000
0002	(4-chloro-2-methylphenoxy)acetic acid	3.86	2.446	4	3.422	4	0.460	0.118	60	266	2.112	0.500	1.650	0.000	0.000	0.000
0003	benzyl bromide	2.97	2.575	1	2.096	1	1.329	-5.841	34	64	2.582	0.000	1.287	0.000	0.000	0.000
0004	[3-(trifluoromethyl)phenyl] urea	1.60	1.683	4	2.640	2	4.863	-1.807	68	309	2.196	0.000	1.992	0.000	0.000	0.000
0005	1,1,1-trichloroethane	2.01	2.029	3	1.814	0	1.724	-1.407	20	16	2.377	0.000	1.561	0.000	0.000	0.000
0006	1,1,2,2-tetrachloroethane	2.68	2.399	4	3.818	1	0.837	1.461	22	29	2.594	0.000	1.500	0.000	0.000	0.000
0007	1,1,2-trichloro-1,2,2-trifluoroethane	3.10	2.786	6	2.295	1	0.684	3.568	38	58	2.919	0.000	1.561	0.000	0.000	0.000
0008	1,1,2-trichloroethane	1.80	1.956	3	3.610	1	0.527	0.403	16	18	2.029	0.000	1.561	0.000	0.000	0.000
0010	1,1-dichloroethane	1.49	1.251	2	2.129	0	1.814	0.096	12	9	1.810	0.000	1.500	0.000	0.000	0.000
0012	1,1-difluoroethylene	2.05	1.114	2	0.886	0	2.856	0.554	12	9	1.397	0.000	1.585	0.000	0.000	0.000
0014	1,1-dimethyl-3-(4-fluorophenyl) urea	1.43	1.358	2	2.844	3	4.090	-7.228	60	268	1.919	0.000	1.727	0.000	0.000	0.000
0015	1,1-dimethyl-3-(4-methoxy-phenyl) urea	1.72	1.136	2	3.476	4	3.892	-13.44	64	337	1.789	0.000	1.574	0.000	0.000	0.000
0017	1,2,3,4-tetrahydronaphthalene	3.28	3.343	0	1.462	0	0.855	-3.029	50	109	2.565	0.000	0.994	0.000	0.000	0.000
0019	1,2,3,4-tetramethylbenzene	3.55	3.775	0	1.797	0	0.686	-7.630	48	109	2.920	0.000	0.980	0.000	0.000	0.000
0020	1,2,3,5-tetrachlorobenzene	3.52	4.488	4	2.700	0	0.789	-6.285	48	110	4.300	0.000	1.459	0.000	0.000	0.000
0021	1,2,3,5-tetramethylbenzene	3.61	3.775	0	1.797	0	0.381	-8.035	48	110	2.920	0.000	0.980	0.000	0.000	0.000
0022	1,2,3-trichlorobenzene	3.23	3.823	3	2.226	0	2.050	-7.911	42	82	3.647	0.000	1.500	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0022	1,2,3-trichlorobenzene	3.23	3.823	3	2.226	0	2.050	-7.911	42	82	3.647	0.000	1.500	0.000	0.000	0.000
0025	1,2,4,5-tetrachlorobenzene	3.72	4.488	4	2.700	0	0.001	-5.760	48	111	4.300	0.000	1.459	0.000	0.000	0.000
0027	1,2,4-trichlorobenzene	3.11	3.823	3	2.226	0	1.049	-5.581	42	84	3.647	0.000	1.500	0.000	0.000	0.000
0029	1,2-dibromoethane	2.44	1.801	2	4.910	1	0.000	0.517	10	10	1.776	0.000	1.500	0.000	0.000	0.000
0031	1,2-dichloro-4-nitrobenzene	2.53	3.053	4	2.439	0	5.297	6.560	52	152	2.902	0.500	2.074	0.000	0.000	0.000
0032	1,2-dichloroethane	1.65	1.512	2	4.099	1	0.000	1.442	10	10	1.464	0.000	1.500	0.000	0.000	0.000
0036	1,2-dimethoxybenzene	2.51	1.797	2	2.424	2	1.775	-7.904	44	117	1.704	0.000	1.361	0.000	0.000	0.000
0037	1,2-dimethoxyethane	1.26	-0.080	2	4.854	3	0.000	-3.032	18	35	0.279	0.000	1.299	0.000	0.000	0.000
0038	1,2-dimethylnaphthalene	3.72	3.711	0	1.613	0	0.712	2.027	62	178	3.457	0.000	1.000	0.000	0.000	0.000
0039	1,2-diphenylethane	3.94	4.261	0	2.970	3	0.366	-6.966	66	343	3.472	0.000	1.000	0.000	0.000	0.000
0041	1,2-propylene oxide	1.39	0.247	1	0.256	0	2.152	0.111	18	8	0.405	0.000	1.295	1.000	0.000	0.000
0044	1,3,5-trichlorobenzene	2.85	3.823	3	2.226	0	0.000	-4.767	42	84	3.647	0.000	1.500	0.000	0.000	0.000
0045	1,3,5-trinitrobenzene	2.02	1.513	6	2.897	0	0.002	29.213	72	354	1.411	3.114	1.918	0.000	0.000	0.000
0046	1,3-benzodioxole	2.51	1.598	2	1.008	0	0.801	-5.088	46	79	1.415	0.000	1.429	1.000	0.000	0.000
0047	1,3-dichloropropene	1.51	1.518	2	4.596	1	1.362	-0.731	14	20	1.978	0.000	1.530	0.000	0.000	0.000
0048	1,3-dimethylnaphthalene	3.78	3.711	0	1.613	0	0.441	3.361	62	179	3.457	0.000	1.000	0.000	0.000	0.000
0050	1,3-propylene oxide	1.30	-0.069	1	0.401	0	2.113	-0.612	16	8	0.407	0.000	1.295	1.000	0.000	0.000
0052	1,4-cyclohexadiene	2.72	1.848	0	1.103	0	0.016	-2.075	24	27	1.893	0.000	0.985	0.000	0.000	0.000
0053	1,4-dimethylnaphthalene	3.75	3.711	0	1.613	0	0.047	4.821	62	176	3.457	0.000	1.000	0.000	0.000	0.000
0054	1,4-dioxane	1.15	-0.262	2	1.470	0	0.000	-0.611	24	27	0.033	0.000	1.379	1.000	0.000	0.000
0058	1,5-hexadiene	2.90	2.327	0	4.092	3	0.000	-2.779	18	35	2.139	0.000	0.954	0.000	0.000	0.000
0059	1,7-dimethylnaphthalene	3.79	3.711	0	1.613	0	0.776	2.484	62	180	3.457	0.000	1.000	0.000	0.000	0.000
0060	11H-benzo[a]fluorene	4.32	4.401	0	1.698	0	0.447	-17.20	98	461	4.411	0.000	0.978	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0061	11H-benzo[b]fluorene	4.51	4.401	0	1.698	0	0.333	-16.19	98	471	4.411	0.000	0.978	0.000	0.000	0.000
0062	13H-dibenzo[a,i]carbazole	6.10	5.140	0	2.008	0	0.879	-25.19	124	831	5.628	0.000	1.130	1.000	0.000	0.000
0064	1-bromo-2-chlorobenzene	2.60	3.243	2	1.921	0	1.900	-8.366	36	60	3.103	0.000	1.626	0.000	0.000	0.000
0066	1-bromo-3-chlorobenzene	2.60	3.243	2	1.921	0	1.208	-6.260	36	61	3.103	0.000	1.626	0.000	0.000	0.000
0067	1-bromo-3-nitrobenzene	2.42	2.473	3	2.134	0	6.006	4.320	46	117	2.357	0.500	1.985	0.000	0.000	0.000
0069	1-bromo-4-nitrobenzene	2.42	2.473	3	2.134	0	5.600	9.180	46	120	2.357	0.500	1.985	0.000	0.000	0.000
0070	1-bromobutane	2.87	2.320	1	4.910	2	1.811	-2.047	14	20	2.181	0.000	1.198	0.000	0.000	0.000
0072	1-bromohexane	3.44	3.232	1	6.924	4	1.863	-1.177	22	56	2.962	0.000	1.141	0.000	0.000	0.000
0073	1-bromooctane	4.04	4.145	1	8.932	6	1.886	-0.075	30	120	3.742	0.000	1.105	0.000	0.000	0.000
0076	1-butanol	1.83	0.971	1	3.928	3	1.496	-1.323	14	20	0.779	0.000	1.159	0.000	0.000	0.000
0078	1-chloro-2,4-dinitrobenzene	2.56	2.283	5	2.664	0	6.196	15.774	62	240	2.156	1.442	2.108	0.000	0.000	0.000
0079	1-chlorobutane	2.81	2.175	1	4.539	2	1.850	-0.273	14	20	2.025	0.000	1.198	0.000	0.000	0.000
0080	1-chloroheptane	3.64	3.544	1	7.554	5	1.953	1.744	26	84	3.196	0.000	1.121	0.000	0.000	0.000
0082	1-chloropentane	2.86	2.632	1	5.546	3	1.928	0.375	18	35	2.415	0.000	1.166	0.000	0.000	0.000
0086	1-ethylnaphthalene	3.77	3.681	0	1.826	1	0.532	2.302	60	182	3.402	0.000	1.000	0.000	0.000	0.000
0088	1-fluoropentane	2.65	2.367	1	4.872	3	1.926	2.454	18	35	2.146	0.000	1.166	0.000	0.000	0.000
0089	1H-benzimidazole	2.11	1.346	1	0.803	0	3.194	-8.105	46	79	1.563	0.000	1.429	1.000	0.000	0.000
0091	1-heptene	3.55	3.174	0	5.527	4	0.380	-2.160	22	56	2.753	0.000	0.918	0.000	0.000	0.000
0092	1-hexanol	2.48	1.883	1	5.926	5	1.509	-1.322	22	56	1.559	0.000	1.116	0.000	0.000	0.000
0097	1-iodobutane	3.01	2.851	1	5.421	2	1.534	-2.944	14	20	2.222	0.000	1.198	0.000	0.000	0.000
0098	1-iodopropane	2.74	2.395	1	4.411	1	1.559	-3.052	10	10	1.831	0.000	1.241	0.000	0.000	0.000
0099	1-methylfluorene	4.08	3.979	0	1.513	0	0.764	3.467	78	267	3.566	0.000	0.996	0.000	0.000	0.000
0100	1-methylnaphthalene	3.48	3.225	0	1.392	0	0.427	3.127	56	140	3.148	0.000	0.998	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0101	1-methylphenanthrene	4.17	4.133	0	1.751	0	0.282	-16.04	82	326	4.301	0.000	0.991	0.000	0.000	0.000
0102	1-Naphthaleneacetamide	2.00	1.775	1	2.188	2	3.579	-4.077	70	292	1.868	0.000	1.401	0.000	0.000	0.000
0105	1-naphthylamine	3.58	1.992	0	1.287	0	2.331	6.119	56	140	2.422	0.000	1.234	0.000	0.000	0.000
0106	1-nitrobutane	2.18	1.620	2	3.505	2	5.297	7.583	24	52	1.063	0.500	1.592	0.000	0.000	0.000
0107	1-nitropentane	2.47	2.076	2	4.453	3	5.420	9.879	28	79	1.453	0.500	1.529	0.000	0.000	0.000
0109	1-nonanol	3.56	3.252	1	8.924	8	1.598	-1.188	34	165	2.729	0.000	1.075	0.000	0.000	0.000
0110	1-nonene	4.18	4.087	0	7.516	6	0.384	-2.296	30	120	3.533	0.000	0.918	0.000	0.000	0.000
0111	1-octanol	3.05	2.796	1	7.925	7	1.512	-1.282	30	120	2.339	0.000	1.086	0.000	0.000	0.000
0112	1-octene	3.86	3.630	0	6.521	5	0.386	-2.228	26	84	3.143	0.000	0.918	0.000	0.000	0.000
0113	1-pentanol	2.20	1.427	1	4.927	4	1.595	-1.226	18	35	1.169	0.000	1.135	0.000	0.000	0.000
0114	1-pentyne	2.45	2.837	0	3.247	2	0.587	-1.985	14	20	1.420	0.000	0.961	0.000	0.000	0.000
0119	1-tetradecanol	4.66	5.533	1	13.923	13	1.514	-1.094	54	560	4.680	0.000	1.036	0.000	0.000	0.000
0122	1α,2β,3α,4β,5α,6β-hexachlorocyclohexane	3.12	4.163	6	4.436	0	0.000	0.973	60	174	3.644	0.000	1.585	0.000	0.000	0.000
0125	2-(2-ethoxyethoxy)ethanol	1.08	-0.271	3	7.775	7	1.467	-4.442	30	120	0.032	0.000	1.325	0.000	0.000	0.000
0126	2-(2-furyl)benzimidazole	2.55	2.666	2	1.442	1	2.379	-6.979	76	293	2.823	0.000	1.548	2.000	0.000	0.000
0127	2-(trifluoromethoxy)aniline	2.36	3.203	4	2.232	1	2.767	-9.098	58	197	2.167	0.000	1.952	0.000	0.000	0.000
0128	2-(trifluoromethyl)aniline	2.36	2.026	3	1.762	0	2.005	-8.144	54	144	2.288	0.000	1.739	0.000	0.000	0.000
0129	2,2,2-trichloroacetamide	1.94	0.846	4	2.173	0	3.102	-1.376	30	42	0.842	0.000	2.197	0.000	0.000	0.000
0131	2,2,2-trifluoroethanol	1.60	0.649	4	1.405	1	3.120	-2.474	24	28	0.541	0.000	1.891	0.000	0.000	0.000
0132	2,2',3,3',4,4',6-heptachlorobiphenyl	5.02	7.999	7	5.065	1	1.540	-10.15	100	642	7.927	0.000	1.395	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0134	2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	5.24	9.328	9	6.032	1	1.627	-13.16	112	800	9.234	0.000	1.207	0.000	0.000	0.000
0135	2,2',3,3',5,5',6,6'-octachlorobiphenyl	5.00	8.664	8	5.546	1	0.866	-12.76	106	702	8.581	0.000	1.322	0.000	0.000	0.000
0136	2,2',3,3',6,6'-hexachlorobiphenyl	4.11	7.335	6	4.590	1	0.973	-14.14	94	537	7.274	0.000	1.435	0.000	0.000	0.000
0137	2,2',3,3'-tetrachlorobiphenyl	6.00	6.006	4	3.657	1	0.360	-11.50	82	408	5.967	0.000	1.435	0.000	0.000	0.000
0138	2,2,3,3-tetramethylhexane	4.50	4.025	0	2.939	3	0.041	0.155	46	115	3.859	0.000	0.896	0.000	0.000	0.000
0139	2,2',3,4,5,5',6-heptachlorobiphenyl	3.83	7.999	7	5.065	1	2.273	-12.60	100	628	7.927	0.000	1.395	0.000	0.000	0.000
0140	2,2',3,4,5'-pentachlorobiphenyl	5.60	6.670	5	4.120	1	2.310	-11.43	88	486	6.621	0.000	1.449	0.000	0.000	0.000
0141	2,2',4,4',5,5'-hexachlorobiphenyl	3.83	7.335	6	4.590	1	0.350	-7.777	94	573	7.274	0.000	1.435	0.000	0.000	0.000
0144	2,2',4',5-tetrachlorobiphenyl	5.37	6.006	4	3.657	1	1.013	-9.151	82	419	5.967	0.000	1.435	0.000	0.000	0.000
0134	2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	5.24	9.328	9	6.032	1	1.627	-13.16	112	800	9.234	0.000	1.207	0.000	0.000	0.000
0135	2,2',3,3',5,5',6,6'-octachlorobiphenyl	5.00	8.664	8	5.546	1	0.866	-12.76	106	702	8.581	0.000	1.322	0.000	0.000	0.000
0136	2,2',3,3',6,6'-hexachlorobiphenyl	4.11	7.335	6	4.590	1	0.973	-14.14	94	537	7.274	0.000	1.435	0.000	0.000	0.000
0137	2,2',3,3'-tetrachlorobiphenyl	6.00	6.006	4	3.657	1	0.360	-11.50	82	408	5.967	0.000	1.435	0.000	0.000	0.000
0138	2,2,3,3-tetramethylhexane	4.50	4.025	0	2.939	3	0.041	0.155	46	115	3.859	0.000	0.896	0.000	0.000	0.000
0139	2,2',3,4,5,5',6-heptachlorobiphenyl	3.83	7.999	7	5.065	1	2.273	-12.60	100	628	7.927	0.000	1.395	0.000	0.000	0.000
0140	2,2',3,4,5'-pentachlorobiphenyl	5.60	6.670	5	4.120	1	2.310	-11.43	88	486	6.621	0.000	1.449	0.000	0.000	0.000
0141	2,2',4,4',5,5'-hexachlorobiphenyl	3.83	7.335	6	4.590	1	0.350	-7.777	94	573	7.274	0.000	1.435	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0145	2,2',4-trichlorobiphenyl	5.21	5.342	3	3.202	1	1.704	-11.40	76	352	5.314	0.000	1.395	0.000	0.000	0.000
0146	2,2',5,5'-tetrachlorobiphenyl	5.37	6.006	4	3.657	1	0.609	-9.779	82	412	5.967	0.000	1.435	0.000	0.000	0.000
0147	2,2',5-trichlorobiphenyl	5.21	5.342	3	3.202	1	1.531	-11.99	76	346	5.314	0.000	1.395	0.000	0.000	0.000
0150	2,2'-dichlorobiphenyl	4.70	4.677	2	2.758	1	0.449	-12.77	70	287	4.660	0.000	1.322	0.000	0.000	0.000
0152	2,2-dimethylbutane	3.46	2.654	0	1.633	1	0.135	-0.206	24	28	2.443	0.000	0.881	0.000	0.000	0.000
0154	2,3,4,5,6-pentachlorobiphenyl	4.80	6.670	5	4.120	1	1.292	-14.16	88	470	6.621	0.000	1.449	0.000	0.000	0.000
0156	2,3,4,5-tetrachlorobiphenyl	5.64	6.006	4	3.657	1	2.105	-13.37	82	412	5.967	0.000	1.435	0.000	0.000	0.000
0157	2,3',4',5-tetrachlorobiphenyl	4.85	6.006	4	3.657	1	2.144	-9.141	82	426	5.967	0.000	1.435	0.000	0.000	0.000
0158	2,3,4,5-tetrachloro-nitrobenzene	4.23	4.382	6	3.376	0	5.262	3.047	64	226	4.208	0.500	1.985	0.000	0.000	0.000
0159	2,3,4,5-tetrachlorophenol	2.88	4.246	5	2.896	1	1.813	-7.213	54	140	4.006	0.000	1.738	0.000	0.000	0.000
0160	2,3,4,6-tetrachloroaniline	3.94	3.741	4	2.761	0	2.866	-10.63	54	140	3.882	0.000	1.788	0.000	0.000	0.000
0161	2,3,4,6-tetrachlorophenol	2.88	4.246	5	2.896	1	1.545	-6.602	54	140	4.006	0.000	1.738	0.000	0.000	0.000
0162	2,3,4-trichloroaniline	2.60	3.077	3	2.292	0	4.048	-12.25	48	109	3.229	0.000	1.788	0.000	0.000	0.000
0165	2,3,4-trimethylphenol	3.76	3.047	1	1.769	1	1.179	-6.732	48	109	2.317	0.000	1.207	0.000	0.000	0.000
0168	2,3,5-trichlorobiphenyl	5.21	5.342	3	3.202	1	1.285	-11.72	76	348	5.314	0.000	1.395	0.000	0.000	0.000
0169	2,3,5-trichlorophenol	1.96	3.581	4	2.421	1	1.720	-5.79	48	110	3.352	0.000	1.776	0.000	0.000	0.000
0158	2,3,4,5-tetrachloro-nitrobenzene	4.23	4.382	6	3.376	0	5.262	3.047	64	226	4.208	0.500	1.985	0.000	0.000	0.000
0159	2,3,4,5-tetrachlorophenol	2.88	4.246	5	2.896	1	1.813	-7.213	54	140	4.006	0.000	1.738	0.000	0.000	0.000
0170	2,3,5-trimethylphenol	3.76	3.047	1	1.769	1	1.266	-7.052	48	110	2.317	0.000	1.207	0.000	0.000	0.000
0171	2,3,6-trichlorophenol	1.96	3.581	4	2.421	1	2.132	-6.519	48	109	3.352	0.000	1.776	0.000	0.000	0.000
0173	2,3-dichloroaniline	0.67	2.412	2	1.836	0	3.114	-10.91	42	82	2.576	0.000	1.727	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0175	2,3-dihydro-1H-inden-1-ol	4.06	1.785	1	1.243	1	1.802	-4.519	52	106	1.666	0.000	1.234	0.000	0.000	0.000
0176	2,3-dihydro-1H-inden-5-ol	4.06	2.645	1	1.243	1	1.472	-3.246	52	108	1.881	0.000	1.234	0.000	0.000	0.000
0177	2,3-dihydrobenzofuran	2.54	1.888	1	1.028	0	1.688	-4.332	46	79	1.621	0.000	1.264	1.000	0.000	0.000
0178	2,3-dimethylbutane	3.47	2.700	0	2.222	1	0.225	0.006	22	29	2.298	0.000	0.881	0.000	0.000	2.000
0180	2,3-xylenol	2.66	2.560	1	1.536	1	0.831	-6.300	42	82	2.009	0.000	1.236	0.000	0.000	0.000
0181	2,4,4′-trichlorobiphenyl	5.21	5.342	3	3.202	1	1.244	-7.205	76	368	5.314	0.000	1.395	0.000	0.000	0.000
0182	2,4,4-trimethyl-1-pentene	3.85	3.166	0	2.265	2	0.340	-2.132	34	66	2.999	0.000	0.918	0.000	0.000	0.000
0184	2,4',5-trichlorobiphenyl	5.21	5.342	3	3.202	1	1.232	-8.084	76	362	5.314	0.000	1.395	0.000	0.000	0.000
0187	2,4,5-trimethylphenol	3.76	3.047	1	1.769	1	1.621	-6.652	48	111	2.317	0.000	1.207	0.000	0.000	0.000
0188	2,4,6-trichlorobiphenyl	5.21	5.342	3	3.202	1	0.456	-11.28	76	348	5.314	0.000	1.395	0.000	0.000	0.000
0189	2,4,6-trichlorophenol	1.96	3.581	4	2.421	1	1.025	-4.782	48	110	3.352	0.000	1.776	0.000	0.000	0.000
0190	2,4,6-trimethylphenol	3.76	3.047	1	1.769	1	1.404	-6.822	48	110	2.317	0.000	1.207	0.000	0.000	0.000
0191	2,4,6-trimethylpyridine	2.40	1.731	1	1.516	0	1.937	-5.918	42	84	2.007	0.000	1.219	1.000	0.000	0.000
0192	2,4,6-trinitrotoluene	2.25	1.999	6	3.129	0	1.232	28.336	78	408	1.720	3.114	1.939	0.000	0.000	0.000
0193	2,4’-dichlorobiphenyl	4.55	4.677	2	2.758	1	2.340	-11.19	70	301	4.660	0.000	1.322	0.000	0.000	0.000
0194	2,4-DB	2.70	4.047	6	8.815	10	1.043	-7.855	88	1071	3.732	0.000	1.607	0.000	0.000	0.000
0196	2,4-dichlorophenol	2.55	2.917	3	1.958	1	2.006	-5.299	42	84	2.699	0.000	1.738	0.000	0.000	0.000
0197	2,4-dichlorophenoxyacetic acid	2.11	2.624	5	3.687	4	1.196	-0.699	60	266	2.457	0.500	1.813	0.000	0.000	0.000
0198	2,4-dichlorotoluene	3.68	3.645	2	1.990	0	1.505	-5.653	42	84	3.302	0.000	1.429	0.000	0.000	0.000
0199	2,4-dimethyl-3-pentanone	2.39	2.155	1	2.735	2	2.638	2.430	32	65	1.868	0.000	1.143	0.000	0.000	2.000
0202	2,5-dichloroaniline	0.67	2.412	2	1.836	0	2.180	-8.141	42	84	2.576	0.000	1.727	0.000	0.000	0.000
0204	2,5-dichlorophenol	2.55	2.917	3	1.958	1	1.170	-4.292	42	84	2.699	0.000	1.738	0.000	0.000	0.000
0205	2,5-dihydrofuran	1.63	0.337	1	0.711	0	1.771	-1.876	20	15	0.573	0.000	1.322	1.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0206	2,5-dimethyl-2,4-hexadiene	3.28	3.112	0	3.252	1	0.033	-6.129	30	74	2.919	0.000	0.946	0.000	0.000	0.000
0207	2,5-xylenol	2.66	2.560	1	1.536	1	1.400	-6.251	42	84	2.009	0.000	1.236	0.000	0.000	0.000
0209	2,6-dichloroaniline	0.67	2.412	2	1.836	0	0.844	-8.225	42	82	2.576	0.000	1.727	0.000	0.000	0.000
0211	2,6-dichlorobenzonitrile	2.60	3.038	3	2.158	1	4.381	-3.482	46	112	2.865	0.000	1.669	0.000	0.000	0.000
0212	2,6-dichlorobiphenyl	4.70	4.677	2	2.758	1	1.520	-12.94	70	286	4.660	0.000	1.322	0.000	0.000	0.000
0214	2,6-dimethyl-4-heptanol	3.05	2.832	1	4.707	5	1.803	2.388	40	135	2.440	0.000	1.075	0.000	0.000	2.000
0215	2,6-dimethylnaphthalene	3.72	3.711	0	1.613	0	0.000	-0.292	62	186	3.457	0.000	1.000	0.000	0.000	0.000
0216	2,6-dimethylpyridine	2.29	1.245	1	1.288	0	1.420	-5.484	36	61	1.698	0.000	1.253	1.000	0.000	0.000
0218	2,6-dinitrotoluene	2.52	2.105	4	2.450	0	5.201	13.712	62	234	1.811	1.442	1.871	0.000	0.000	0.000
0219	2,6-dinitro-trifluoro-p-toluidine	2.56	1.815	7	3.109	0	1.482	17.648	86	474	2.104	1.442	2.242	0.000	0.000	0.000
0220	2,6-di-tert-butyl-p-cresol	4.15	4.875	1	3.216	3	1.372	-7.324	84	392	4.296	0.000	1.106	0.000	0.000	0.000
0221	2,6-xylenol	2.66	2.560	1	1.536	1	1.246	-6.104	42	82	2.009	0.000	1.236	0.000	0.000	0.000
0224	2-bromo-4-methylaniline	1.96	2.318	1	1.762	0	1.828	-10.51	42	84	2.340	0.000	1.520	0.000	0.000	0.000
0226	2-bromobenzoic acid	2.57	2.208	3	2.189	2	2.675	-5.542	46	114	2.147	0.500	1.689	0.000	0.000	0.000
0227	2-bromopropane	2.41	1.717	1	1.979	0	1.743	0.966	12	9	1.790	0.000	1.241	0.000	0.000	0.000
0228	2-butoxyethanol	1.83	0.840	2	6.851	6	0.588	-2.978	26	84	0.795	0.000	1.241	0.000	0.000	0.000
0229	2-chloro-1-propene	2.47	1.516	1	1.370	0	1.301	-3.164	12	9	1.759	0.000	1.352	0.000	0.000	0.000
0232	2-chlorobiphenyl	3.84	4.013	1	2.327	1	1.181	-12.50	64	240	4.007	0.000	1.207	0.000	0.000	0.000
0233	2-chlorobutane	2.65	2.097	1	2.669	1	1.797	-0.383	16	18	2.024	0.000	1.198	0.000	0.000	0.000
0234	2-chloroethanol	1.39	0.307	2	3.453	2	1.351	-0.444	10	10	0.217	0.000	1.658	0.000	0.000	0.000
0235	2-chloronaphthalene	3.54	3.403	1	1.552	0	1.547	3.638	56	144	3.493	0.000	1.233	0.000	0.000	0.000
0236	2-chlorophenol	2.60	2.252	2	1.512	1	2.422	-6.717	36	60	2.046	0.000	1.614	0.000	0.000	0.000
0238	2-chloropropane	2.41	1.573	1	1.710	0	1.794	-0.035	12	9	1.634	0.000	1.241	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0239	2-cyclohexen-1-one	1.71	1.291	1	1.250	0	3.389	2.025	30	42	1.296	0.000	1.273	0.000	0.000	0.000
0240	2-decanone	3.43	3.300	1	7.540	7	3.065	9.053	40	212	3.326	0.000	1.094	0.000	0.000	0.000
0241	2-ethoxyethanol	1.20	-0.140	2	4.854	4	0.490	-2.648	18	35	0.015	0.000	1.299	0.000	0.000	0.000
0243	2-ethylfuran	2.68	1.746	1	1.157	1	0.713	-1.158	30	43	1.842	0.000	1.273	1.000	0.000	0.000
0246	2-ethyl-p-xylene	3.79	3.745	0	2.103	1	1.121	-7.420	46	115	2.866	0.000	0.980	0.000	0.000	0.000
0250	2-heptanone	2.45	1.931	1	4.621	4	2.998	5.168	28	79	2.156	0.000	1.143	0.000	0.000	0.000
0251	2-hexanol	2.33	1.804	1	4.104	4	1.601	-3.044	24	52	1.557	0.000	1.116	0.000	0.000	0.000
0252	2-hexanone	2.13	1.475	1	3.665	3	3.017	4.103	24	52	1.766	0.000	1.167	0.000	0.000	0.000
0253	2-hydroxy-1,4-naphthalenedione	2.17	1.220	3	1.601	1	1.177	-0.759	68	218	1.508	0.766	1.433	0.000	0.000	0.000
0255	2-hydroxybenzimidazole	1.99	1.645	2	0.987	1	1.845	-4.027	52	108	1.268	0.000	1.677	1.000	0.000	0.000
0256	2-hydroxyethyl acrylate	1.26	0.179	3	4.112	5	3.871	-2.900	28	76	-0.292	0.200	1.477	0.000	0.000	0.000
0257	2-iodopropane	2.95	2.249	1	2.363	0	1.623	1.529	12	9	1.830	0.000	1.241	0.000	0.000	0.000
0258	2-methoxy-1,4-naphthalenedione	2.11	1.446	3	2.018	1	0.634	-2.798	72	273	1.596	0.200	1.423	0.000	0.000	0.000
0262	2-methyl-1-butanol	2.08	1.290	1	3.141	3	1.394	-2.440	20	31	1.025	0.000	1.135	0.000	0.000	1.000
0263	2-methyl-3-nitrophenol	2.61	1.969	3	1.977	1	6.742	0.645	52	146	1.609	0.814	1.722	0.000	0.000	0.000
0264	2-methylanisole	2.87	2.300	1	1.853	1	0.985	-6.375	40	86	2.004	0.000	1.236	0.000	0.000	0.000
0266	2-methylbenzaldehyde	2.61	2.076	1	1.634	1	3.066	-2.674	40	86	1.808	0.000	1.264	0.000	0.000	0.000
0267	2-methylbenzofuran	3.13	2.279	1	1.037	0	0.919	-3.553	52	108	2.741	0.000	1.252	1.000	0.000	0.000
0268	2-methylfuran	2.38	1.079	1	0.675	0	0.469	-1.179	26	26	1.588	0.000	1.325	1.000	0.000	0.000
0269	2-methylnaphthalene	3.55	3.225	0	1.392	0	0.486	1.113	56	144	3.148	0.000	0.998	0.000	0.000	0.000
0270	2-methylpyridine	1.98	0.962	1	1.069	0	1.771	-4.162	30	42	1.390	0.000	1.296	1.000	0.000	0.000
0271	2-methylquinoline	2.79	2.299	1	1.354	0	1.672	-7.857	56	144	2.543	0.000	1.234	1.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0272	2-methyltetrahydrofuran	2.38	0.889	1	1.105	0	1.960	-4.064	26	26	1.185	0.000	1.198	1.000	0.000	0.000
0274	2-naphthalenemethanol	2.22	2.134	1	1.801	2	1.515	-1.297	60	190	2.332	0.000	1.220	0.000	0.000	0.000
0275	2-naphthol	2.85	2.496	1	1.370	1	1.117	7.022	56	144	2.545	0.000	1.236	0.000	0.000	0.000
0276	2-naphthylamine	3.58	1.992	0	1.287	0	2.598	-2.262	56	144	2.422	0.000	1.234	0.000	0.000	0.000
0277	2-nitrobenzamide	1.45	0.727	3	2.157	1	4.751	-6.849	56	188	0.694	0.814	1.841	0.000	0.000	0.000
0278	2-nitropropane	1.88	1.018	2	1.732	0	4.981	-0.313	22	29	0.672	0.500	1.669	0.000	0.000	0.000
0279	2-nonanone	3.10	2.844	1	6.561	6	3.023	7.674	36	158	2.936	0.000	1.108	0.000	0.000	0.000
0280	2-octanol	2.96	2.717	1	6.059	6	1.617	-3.288	32	114	2.338	0.000	1.086	0.000	0.000	0.000
0281	2-octanone	2.67	2.388	1	5.588	5	3.049	6.481	32	114	2.546	0.000	1.124	0.000	0.000	0.000
0282	2-pentanol	2.06	1.348	1	3.141	3	1.566	-3.297	20	32	1.167	0.000	1.135	0.000	0.000	0.000
0285	2-phenylethanol	2.12	1.547	1	2.279	3	1.226	-5.060	38	94	1.221	0.000	1.236	0.000	0.000	0.000
0286	2-propenophenone	2.40	2.268	1	2.002	2	2.583	-5.677	44	121	2.055	0.000	1.252	0.000	0.000	0.000
0287	2-propylphenol	2.97	2.987	1	2.459	3	0.776	-6.803	44	121	2.345	0.000	1.207	0.000	0.000	0.000
0288	2-pyrrolidone	0.92	-0.371	1	0.783	0	3.141	-4.410	26	26	-0.104	0.000	1.573	1.000	0.000	0.000
0289	2-undecanone	3.60	3.756	1	8.523	8	3.035	10.320	44	277	3.716	0.000	1.083	0.000	0.000	0.000
0290	3-(3,4-dichlorophenyl)-1-methylurea	2.46	2.275	3	3.395	3	4.616	-13.02	60	262	2.745	0.000	1.916	0.000	0.000	0.000
0291	3-(3,5-dimethyl-4-bromophenyl)-1,1-dimethylurea	2.53	2.873	2	3.741	3	3.750	-15.59	72	378	3.159	0.000	1.618	0.000	0.000	0.000
0292	3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.73	2.125	1	3.121	3	3.327	-14.11	66	316	2.397	0.000	1.438	0.000	0.000	0.000
0285	2-phenylethanol	2.12	1.547	1	2.279	3	1.226	-5.060	38	94	1.221	0.000	1.236	0.000	0.000	0.000
0286	2-propenophenone	2.40	2.268	1	2.002	2	2.583	-5.677	44	121	2.055	0.000	1.252	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0293	3-(3-chloro-4-methoxyphenyl)-1-methylurea	1.84	1.594	3	3.734	4	4.797	-15.03	64	326	2.100	0.000	1.821	0.000	0.000	0.000
0294	3-(3-chloro-4-methylphenyl)-1-methylurea	2.10	2.097	2	3.142	3	4.034	-13.51	60	262	2.400	0.000	1.727	0.000	0.000	0.000
0295	3-(3-chlorophenyl)-1,1-dimethylurea	1.79	1.817	2	3.142	3	3.989	-12.95	60	262	2.434	0.000	1.727	0.000	0.000	0.000
0297	3-(3-fluorophenyl)-1,1-dimethylurea	1.73	1.358	2	2.844	3	4.136	-9.903	60	262	1.919	0.000	1.727	0.000	0.000	0.000
0298	3-(3-methoxyphenyl)-1,1-dimethylurea	1.72	1.136	2	3.476	4	3.640	-15.52	64	325	1.789	0.000	1.574	0.000	0.000	0.000
0300	3-(4-fluorophenyl)-1,1-dimethylurea	1.43	1.358	2	2.844	3	4.090	-7.228	60	268	1.919	0.000	1.727	0.000	0.000	0.000
0301	3-(4-methoxyphenyl)-1,1-dimethylurea	1.40	1.136	2	3.476	4	3.892	-13.44	64	337	1.789	0.000	1.574	0.000	0.000	0.000
0302	3-(4-methylphenyl)-1,1-dimethylurea	1.51	1.638	1	2.901	3	3.351	-13.01	60	268	2.089	0.000	1.476	0.000	0.000	0.000
0303	3-(trifluoromethoxy)aniline	2.36	3.203	4	2.232	1	3.583	-10.05	58	202	2.167	0.000	1.952	0.000	0.000	0.000
0305	3-(trifluoromethylthio)aniline	3.83	3.762	4	2.419	1	3.111	-11.44	58	202	2.881	0.000	1.952	0.000	0.000	0.000
0312	3,4-dichloro-1,1'-biphenyl	4.70	4.677	2	2.758	1	2.365	-11.48	70	303	4.660	0.000	1.322	0.000	0.000	0.000
0313	3,4-dichloroacetanilide	2.34	2.279	3	2.952	2	4.046	-13.17	56	205	2.952	0.000	1.845	0.000	0.000	0.000
0315	3,4-dichlorobenzyltriazole	2.33	3.117	4	2.701	2	3.382	-0.531	70	318	2.702	0.000	1.776	1.000	0.000	0.000
0316	3,4-dichloronitrobenzene	2.53	3.053	4	2.439	0	5.298	6.014	52	152	2.902	0.500	2.074	0.000	0.000	0.000
0317	3,4-dichlorophenol	2.55	2.917	3	1.958	1	2.305	-6.119	42	84	2.699	0.000	1.738	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0318	3,4-dichlorophenylurea	2.49	2.069	3	2.785	2	4.569	-2.579	56	205	2.484	0.000	1.994	0.000	0.000	0.000
0319	3,4-dinitrobenzoic acid	1.53	1.249	6	2.948	2	7.452	7.229	72	354	1.201	3.138	1.871	0.000	0.000	0.000
0322	3,5-dichloroaniline	0.67	2.412	2	1.836	0	3.542	-10.39	42	84	2.576	0.000	1.727	0.000	0.000	0.000
0323	3,5-dichlorophenol	2.55	2.917	3	1.958	1	1.163	-4.304	42	84	2.699	0.000	1.738	0.000	0.000	0.000
0324	3,5-dimethylphenol	2.83	2.560	1	1.536	1	1.588	-6.083	42	84	2.009	0.000	1.236	0.000	0.000	0.000
0326	3,5-dinitrobenzamide	2.31	0.621	5	2.831	1	5.319	17.938	72	354	0.602	2.076	1.941	0.000	0.000	0.000
0327	3,5-xylenol	2.66	2.560	1	1.536	1	1.588	-6.083	42	84	2.009	0.000	1.236	0.000	0.000	0.000
0328	3,6-dichloro-2-methoxybenzoic acid	0.99	2.772	5	3.275	3	2.903	-5.058	62	226	2.700	0.500	1.813	0.000	0.000	0.000
0329	3,6-dichlorosalicylic acid	2.30	2.547	5	2.693	3	2.833	-4.964	58	181	2.397	0.945	1.850	0.000	0.000	0.000
0330	3-amino-1-propanol	0.77	-1.125	2	3.857	3	2.710	-1.212	14	20	-0.672	0.000	1.430	0.000	0.000	0.000
0332	3-bromo-1-propene	2.35	1.608	1	3.397	1	1.486	-3.393	10	10	1.567	0.000	1.352	0.000	0.000	0.000
0333	3-bromo-2-methylaniline	1.96	2.318	1	1.762	0	3.082	-11.78	42	82	2.340	0.000	1.520	0.000	0.000	0.000
0334	3-bromo-4-methylaniline	1.96	2.318	1	1.762	0	2.898	-12.69	42	84	2.340	0.000	1.520	0.000	0.000	0.000
0335	3-bromo-5-chlorophenol	2.69	3.001	3	2.110	1	1.075	-5.461	42	84	2.808	0.000	1.892	0.000	0.000	0.000
0338	3-bromophenylcarbamate	1.89	0.642	3	2.619	1	10.768	-4.407	50	162	1.204	0.500	1.921	0.000	0.000	0.000
0339	3-bromophenylurea	2.12	1.489	2	2.485	2	4.035	-3.125	50	162	1.940	0.000	1.875	0.000	0.000	0.000
0340	3-chloro-4-bromo-nitrobenzene	2.60	3.137	4	2.592	0	5.210	8.339	52	152	3.011	0.500	2.217	0.000	0.000	0.000
0342	3-chloro-4-methoxyphenylurea	2.00	1.388	3	3.108	3	4.740	-4.953	60	260	1.839	0.000	1.890	0.000	0.000	0.000
0344	3-chloroanisidine	1.93	1.731	2	2.142	1	4.009	-13.36	46	116	1.931	0.000	1.745	0.000	0.000	0.000
0345	3-chlorobiphenyl	3.87	4.013	1	2.327	1	1.450	-11.02	64	246	4.007	0.000	1.207	0.000	0.000	0.000
0347	3-chlorophenyl urea	2.01	1.405	2	2.332	2	4.084	-3.328	50	162	1.831	0.000	1.875	0.000	0.000	0.000
0348	3-ethyl-o-xylene	3.74	3.745	0	2.103	1	0.959	-5.894	46	113	2.866	0.000	0.980	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0349	3-ethylphenylcarbamate	1.66	0.836	2	2.824	2	10.616	-6.510	54	209	1.004	0.500	1.562	0.000	0.000	0.000
0350	3-fluoroacetanilide	1.57	1.156	2	2.207	2	3.696	-8.991	50	162	1.784	0.000	1.722	0.000	0.000	0.000
0351	3-fluorophenyl urea	1.77	0.946	2	2.056	2	4.236	-1.886	50	162	1.316	0.000	1.875	0.000	0.000	0.000
0352	3-heptanol	2.60	2.328	1	5.078	5	1.789	0.874	28	76	1.948	0.000	1.099	0.000	0.000	0.000
0354	3-hydroxyphenol	0.98	1.346	2	1.282	2	2.596	-5.073	36	61	1.098	0.250	1.449	0.000	0.000	0.000
0355	3-mercaptopropionic acid	1.61	0.343	3	3.170	4	2.429	2.172	20	32	0.391	0.500	1.730	0.000	0.000	0.000
0356	3-methoxyphenol	1.55	1.572	2	1.822	2	2.613	-5.915	40	88	1.401	0.000	1.402	0.000	0.000	0.000
0358	3-methyl-1-butanol	2.07	1.223	1	3.141	3	1.563	-0.568	20	32	1.025	0.000	1.135	0.000	0.000	1.000
0362	3-methyl-4-bromoaniline	2.26	2.318	1	1.762	0	3.559	-14.17	42	84	2.340	0.000	1.520	0.000	0.000	0.000
0363	3-methyl-4-bromophenylurea	2.37	1.975	2	2.703	2	3.848	-2.472	56	205	2.248	0.000	1.796	0.000	0.000	0.000
0365	3-methyl-4-nitrophenol	2.61	1.969	3	1.977	1	6.034	3.479	52	150	1.609	0.721	1.722	0.000	0.000	0.000
0366	3-methylacetanilide	1.45	1.437	1	2.261	2	2.617	-11.32	50	162	1.953	0.000	1.433	0.000	0.000	0.000
0368	3-methylanisole	2.82	2.300	1	1.853	1	1.040	-6.567	40	88	2.004	0.000	1.236	0.000	0.000	0.000
0369	3-methylbenzenemethanol	2.25	1.712	1	1.853	2	1.090	-8.119	40	88	1.487	0.000	1.236	0.000	0.000	0.000
0370	3-methylbutanoic acid	2.01	1.170	2	2.601	3	1.856	2.635	26	48	1.117	0.500	1.333	0.000	0.000	1.000
0371	3-methylpentane	3.34	2.904	0	3.200	2	0.099	-1.140	20	31	2.443	0.000	0.881	0.000	0.000	1.000
0372	3-methylphenylcarbamate	1.48	0.380	2	2.230	1	10.898	-5.649	50	162	0.750	0.500	1.616	0.000	0.000	0.000
0373	3-methylphenylurea	1.56	1.227	1	2.108	2	3.404	-4.327	50	162	1.486	0.000	1.572	0.000	0.000	0.000
0374	3-methylpyridine	2.03	1.166	1	1.069	0	2.271	-3.242	30	42	1.390	0.000	1.296	1.000	0.000	0.000
0375	3-methylthiophene	2.65	1.614	1	0.926	0	0.258	-2.298	26	26	2.057	0.000	1.325	1.000	0.000	0.000
0377	3-nitrobenzamide	1.95	0.727	3	2.157	1	3.145	5.074	56	197	0.694	0.721	1.841	0.000	0.000	0.000
0378	3-nitrobenzotrifluoride	2.80	2.667	5	2.329	0	5.545	5.940	64	240	2.614	0.500	2.064	0.000	0.000	0.000
0380	3-phenyl-1-cycloheptylurea	2.37	3.261	1	4.419	4	3.667	-1.417	80	582	3.531	0.000	1.379	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0381	3-phenyl-1-cyclohexylurea	2.07	2.805	1	3.805	4	4.425	-10.25	76	495	3.141	0.000	1.406	0.000	0.000	0.000
0382	3-Phenyl-1-cyclopentylurea	1.93	2.348	1	3.223	4	3.854	-13.31	72	411	2.751	0.000	1.437	0.000	0.000	0.000
0383	3-phenyl-1-cyclopropyl urea	1.72	1.436	1	2.166	4	3.397	-11.49	64	275	1.971	0.000	1.514	0.000	0.000	0.000
0385	3-trifluoromethylacetanilide	1.75	1.893	4	2.785	2	4.433	-13.04	68	309	2.664	0.000	1.856	0.000	0.000	0.000
0386	3-trifluoromethylaniline	2.36	2.026	3	1.762	0	4.221	-10.70	54	148	2.288	0.000	1.739	0.000	0.000	0.000
0381	3-phenyl-1-cyclohexylurea	2.07	2.805	1	3.805	4	4.425	-10.25	76	495	3.141	0.000	1.406	0.000	0.000	0.000
0387	3-trifluoromethylphenylurea	1.98	1.683	4	2.640	2	4.863	-1.807	68	309	2.196	0.000	1.992	0.000	0.000	0.000
0388	4-(trifluoromethoxy)aniline	2.36	3.203	4	2.232	1	4.566	-12.82	58	207	2.167	0.000	1.952	0.000	0.000	0.000
0390	4-(trifluoromethylthio)aniline	2.36	3.762	4	2.419	1	4.398	-15.02	58	207	2.881	0.000	1.952	0.000	0.000	0.000
0391	4,4'-dichloro-1,1'-biphenyl	5.27	4.677	2	2.758	1	0.100	-5.670	70	315	4.660	0.000	1.322	0.000	0.000	0.000
0393	4,5,6-trichloroguaiacol	2.99	3.565	5	3.207	2	1.470	-6.523	58	182	3.361	0.000	1.851	0.000	0.000	0.000
0394	4-aminonitrobenzene	1.88	0.978	2	1.639	0	10.342	-3.302	46	120	1.177	0.500	1.811	0.000	0.000	0.000
0395	4-biphenylmethanol	2.69	2.744	1	2.611	3	1.539	-15.68	68	319	2.846	0.000	1.196	0.000	0.000	0.000
0397	4-bromo-2-methylaniline	1.96	2.318	1	1.762	0	3.912	-13.68	42	84	2.340	0.000	1.520	0.000	0.000	0.000
0398	4-bromo-3-methylaniline	1.96	2.318	1	1.762	0	3.559	-14.17	42	84	2.340	0.000	1.520	0.000	0.000	0.000
0399	4-bromoacetanilde	1.95	1.699	2	2.653	2	3.423	-13.22	50	166	2.407	0.000	1.722	0.000	0.000	0.000
0403	4-bromo-N-(1,1-dimethyl-2-propynyl)benzamide	2.01	3.561	2	3.541	4	2.356	-5.990	72	388	2.591	0.000	1.568	0.000	0.000	1.000
0404	4-bromophenol	2.41	2.336	2	1.655	1	1.274	-5.168	36	62	2.155	0.000	1.614	0.000	0.000	0.000
0405	4-bromophenylurea	2.12	1.489	2	2.485	2	4.052	-2.277	50	166	1.940	0.000	1.875	0.000	0.000	0.000
0406	4-butylphenol	3.36	3.443	1	3.116	4	1.477	-5.150	48	174	2.735	0.000	1.183	0.000	0.000	0.000
0407	4-chloroaniline	1.96	1.748	1	1.398	0	3.880	-10.87	36	62	1.922	0.000	1.592	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0408	4-chlorobenzaldoxime-N-methylcarbamate	2.19	2.327	4	4.095	4	3.802	-11.46	62	365	2.030	0.000	1.869	0.000	0.000	0.000
0409	4-chlorobenzyltriazole	1.98	2.453	3	2.272	2	3.351	-0.332	64	265	2.049	0.000	1.664	1.000	0.000	0.000
0410	4-chlorobiphenyl	3.89	4.013	1	2.327	1	1.579	-9.841	64	252	4.007	0.000	1.207	0.000	0.000	0.000
0411	4-chloro-N-(1,1-dimethyl-2-propynyl)benzamide	1.90	3.477	2	3.386	4	2.314	-5.397	72	388	2.482	0.000	1.568	0.000	0.000	1.000
0414	4-fluoroacetanilide	1.48	1.156	2	2.207	2	3.537	-6.870	50	166	1.784	0.000	1.722	0.000	0.000	0.000
0415	4-fluorobenzyltriazole	1.87	1.994	3	2.037	2	3.330	1.018	64	265	1.535	0.000	1.664	1.000	0.000	0.000
0416	4-fluoro-N-(1,1-dimethyl-2-propynyl)benzamide	1.68	3.018	2	3.105	4	2.277	-3.031	72	388	1.967	0.000	1.568	0.000	0.000	1.000
0417	4-fluorophenylurea	1.52	0.946	2	2.056	2	4.138	0.058	50	166	1.316	0.000	1.875	0.000	0.000	0.000
0418	4-heptanol	2.59	2.328	1	5.078	5	1.658	0.274	28	75	1.948	0.000	1.099	0.000	0.000	0.000
0420	4-iso-propyl-N-(1,1-dimethyl-2-propynyl)benzamide	2.17	4.007	1	3.958	5	3.568	-9.207	82	564	2.952	0.000	1.300	0.000	0.000	2.000
0421	4-isopropylphenylcarbamate	1.94	1.088	2	3.033	2	11.998	1.650	60	270	1.565	0.500	1.514	0.000	0.000	1.000
0423	4-methoxybenzyltriazole	1.80	1.772	3	2.554	3	3.640	-4.486	68	334	1.404	0.000	1.603	1.000	0.000	0.000
0424	4-methoxy-N-(1,1-dimethyl-2-propynyl)benzamide	1.83	2.796	2	3.701	5	2.116	-9.660	76	475	1.837	0.000	1.447	0.000	0.000	1.000
0425	4-methoxyphenylcarbamate	1.40	-0.122	3	2.790	2	12.697	-0.760	54	217	0.450	0.500	1.684	0.000	0.000	0.000
0426	4-methyl-1-pentene	2.74	2.514	0	2.823	2	0.371	-1.651	20	32	2.218	0.000	0.918	0.000	0.000	1.000
0427	4-methyl-2-pentanone	0.63	1.271	1	2.648	2	2.947	3.953	26	48	1.622	0.000	1.167	0.000	0.000	1.000
0428	4-methyl-3-nitrophenol	2.61	1.969	3	1.977	1	6.654	1.449	52	148	1.609	0.814	1.722	0.000	0.000	0.000
0429	4-methylacetophenone	2.57	2.056	1	1.855	1	3.291	-3.344	46	120	2.198	0.000	1.234	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0430	4-methylaniline	1.60	1.570	0	1.203	0	1.963	-10.33	36	62	1.577	0.000	1.253	0.000	0.000	0.000
0431	4-methylanisole	2.91	2.300	1	1.853	1	1.461	-6.212	40	90	2.004	0.000	1.236	0.000	0.000	0.000
0432	4-methylbenzamide	1.78	1.318	1	1.714	1	3.796	-6.768	46	120	1.094	0.000	1.483	0.000	0.000	0.000
0434	4-methylbenzoic acid	1.77	1.946	2	1.826	2	3.015	-4.346	46	120	1.693	0.500	1.392	0.000	0.000	0.000
0437	4-methylphenol	2.70	2.074	1	1.308	1	1.534	-5.150	36	62	1.701	0.000	1.272	0.000	0.000	0.000
0438	4-methylphenyl acetate	2.53	2.084	2	2.387	2	3.304	-9.128	50	166	1.920	0.000	1.357	0.000	0.000	0.000
0440	4-n-butylbenzyltriazole	2.16	3.513	2	3.697	5	3.723	4.062	76	479	2.738	0.000	1.337	1.000	0.000	0.000
0441	4-nitrobenzamide	1.93	0.727	3	2.157	1	5.471	6.469	56	206	0.694	0.651	1.841	0.000	0.000	0.000
0446	4-phenylcyclohexanone	2.71	2.598	1	2.438	1	2.666	-2.243	64	252	2.913	0.000	1.187	0.000	0.000	1.000
0449	4-t-butylphenylcarbamate	2.07	1.294	2	2.911	2	12.331	4.611	68	325	1.739	0.500	1.473	0.000	0.000	0.000
0451	5-bromo-2-methylaniline	1.96	2.318	1	1.762	0	3.360	-12.91	42	84	2.340	0.000	1.520	0.000	0.000	0.000
0452	5-ethyl-m-xylene	3.85	3.745	0	2.103	1	0.216	-7.701	46	116	2.866	0.000	0.980	0.000	0.000	0.000
0453	5-hexen-2-one	1.93	1.085	1	3.292	3	2.690	3.185	24	52	1.542	0.000	1.221	0.000	0.000	0.000
0454	5-hexyn-2-one	1.69	1.660	1	3.045	3	2.547	2.526	24	52	0.989	0.000	1.273	0.000	0.000	0.000
0458	6-chloropicolinic acid	1.37	1.611	4	1.988	2	4.591	-3.695	46	117	1.433	0.500	1.985	1.000	0.000	0.000
0459	6-chrysenamine	5.58	3.809	0	2.037	0	2.945	-25.39	108	620	4.728	0.000	1.151	0.000	0.000	0.000
0460	7,12-dimethylbenz[a]anthracene	1.82	5.528	0	2.340	0	0.379	-21.23	114	696	5.763	0.000	0.991	0.000	0.000	0.000
0462	9,10-dimethylphenanthrene	2.48	4.619	0	1.967	0	0.424	-16.83	88	376	4.610	0.000	0.997	0.000	0.000	0.000
0463	9-anthracenecarboxylic acid	4.47	3.277	2	2.165	2	5.169	-3.804	92	452	3.691	0.500	1.280	0.000	0.000	0.000
0464	9-anthracenemethanol	2.54	3.042	1	2.118	2	1.554	-3.310	86	388	3.485	0.000	1.178	0.000	0.000	0.000
0469	acetal	0.30	0.778	2	5.014	4	1.890	-1.712	28	75	1.405	0.000	1.241	0.000	0.000	0.000
0471	acetamide	1.62	-0.832	1	0.759	0	3.561	-1.641	12	9	-0.508	0.000	1.658	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0478	acetylacetone	2.26	-0.193	2	2.266	2	2.466	9.362	26	48	0.555	0.250	1.400	0.000	0.000	0.000
0479	acetylene	1.60	1.975	0	0.000	0	0.000	-0.007	2	1	0.249	0.000	1.000	0.000	0.000	0.000
0481	acridine	2.05	3.353	1	1.506	0	1.915	-8.250	76	279	3.388	0.000	1.192	1.000	0.000	0.000
0482	acrolein	3.23	0.515	1	2.055	1	1.013	1.606	10	10	0.371	0.000	1.406	0.000	0.000	0.000
0484	acrylic acid	0.95	0.493	2	1.457	2	0.804	1.422	16	18	0.257	0.500	1.530	0.000	0.000	0.000
0486	adipic acid	1.51	0.553	4	4.702	7	0.001	11.735	38	151	0.716	1.301	1.485	0.000	0.000	0.000
0488	alachlor	1.20	3.425	3	6.159	7	4.707	5.905	82	569	2.987	0.000	1.518	0.000	0.000	0.000
0489	aldicarb	2.48	1.168	4	4.922	5	4.149	-14.36	50	233	1.470	0.000	1.741	0.000	0.000	1.000
0491	aldicarb sulfoxide	0.42	-0.576	5	5.176	6	4.756	14.599	60	341	-0.336	0.516	1.905	0.000	0.000	1.000
0492	aldrin	0.56	4.264	6	2.398	0	1.776	-2.540	120	448	5.270	0.000	1.526	0.000	0.000	6.000
0494	allyl acetate	2.17	0.638	2	3.236	3	1.544	-1.669	24	52	0.736	0.000	1.400	0.000	0.000	0.000
0496	allylamine	1.47	-0.031	1	2.498	1	1.603	-2.148	10	10	0.131	0.000	1.241	0.000	0.000	0.000
0497	alpha-chlordane	1.39	4.788	8	3.390	0	0.757	5.417	114	459	5.683	0.000	1.555	0.000	0.000	4.000
0498	alpha-hexachlorocyclohexane	5.15	4.163	6	4.436	0	1.871	-0.52	60	174	3.644	0.000	1.585	0.000	0.000	0.000
0499	ametryn	3.30	2.743	4	4.482	5	2.957	-12.74	68	384	1.846	0.000	1.574	1.000	0.000	0.000
0500	amitraz	2.13	5.350	2	5.100	4	4.171	-22.77	108	1261	4.872	0.000	1.281	0.000	0.000	0.000
0501	amitrole	3.00	-0.615	2	0.506	0	3.959	-5.286	26	26	-0.613	0.000	1.522	1.000	0.000	0.000
0503	ancymidol	2.33	1.719	4	3.045	5	3.650	-2.831	102	673	2.131	0.000	1.512	1.000	0.000	2.000
0504	anilazine	2.08	4.392	6	3.432	2	2.754	0.445	80	449	3.575	0.000	1.874	1.000	0.000	0.000
0505	aniline	3.00	1.083	0	0.984	0	2.297	-8.794	30	42	1.269	0.000	1.296	0.000	0.000	0.000
0506	anisole	1.87	1.814	1	1.648	1	1.286	-5.479	34	64	1.695	0.000	1.272	0.000	0.000	0.000
0507	anthracene	2.25	3.647	0	1.539	0	0.001	-5.440	76	279	3.993	0.000	0.980	0.000	0.000	0.000
0510	ascorbic acid	3.22	-1.709	6	2.554	6	5.135	5.276	58	188	-1.41	2.350	1.571	1.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0478	acetylacetone	2.26	-0.193	2	2.266	2	2.466	9.362	26	48	0.555	0.250	1.400	0.000	0.000	0.000
0479	acetylene	1.60	1.975	0	0.000	0	0.000	-0.007	2	1	0.249	0.000	1.000	0.000	0.000	0.000
0481	acridine	2.05	3.353	1	1.506	0	1.915	-8.250	76	279	3.388	0.000	1.192	1.000	0.000	0.000
0482	acrolein	3.23	0.515	1	2.055	1	1.013	1.606	10	10	0.371	0.000	1.406	0.000	0.000	0.000
0484	acrylic acid	0.95	0.493	2	1.457	2	0.804	1.422	16	18	0.257	0.500	1.530	0.000	0.000	0.000
0486	adipic acid	1.51	0.553	4	4.702	7	0.001	11.735	38	151	0.716	1.301	1.485	0.000	0.000	0.000
0488	alachlor	1.20	3.425	3	6.159	7	4.707	5.905	82	569	2.987	0.000	1.518	0.000	0.000	0.000
0489	aldicarb	2.48	1.168	4	4.922	5	4.149	-14.36	50	233	1.470	0.000	1.741	0.000	0.000	1.000
0491	aldicarb sulfoxide	0.42	-0.576	5	5.176	6	4.756	14.599	60	341	-0.336	0.516	1.905	0.000	0.000	1.000
0492	aldrin	0.56	4.264	6	2.398	0	1.776	-2.540	120	448	5.270	0.000	1.526	0.000	0.000	6.000
0494	allyl acetate	2.17	0.638	2	3.236	3	1.544	-1.669	24	52	0.736	0.000	1.400	0.000	0.000	0.000
0496	allylamine	1.47	-0.031	1	2.498	1	1.603	-2.148	10	10	0.131	0.000	1.241	0.000	0.000	0.000
0497	alpha-chlordane	1.39	4.788	8	3.390	0	0.757	5.417	114	459	5.683	0.000	1.555	0.000	0.000	4.000
0498	alpha-hexachlorocyclohexane	5.15	4.163	6	4.436	0	1.871	-0.52	60	174	3.644	0.000	1.585	0.000	0.000	0.000
0499	ametryn	3.30	2.743	4	4.482	5	2.957	-12.74	68	384	1.846	0.000	1.574	1.000	0.000	0.000
0500	amitraz	2.13	5.350	2	5.100	4	4.171	-22.77	108	1261	4.872	0.000	1.281	0.000	0.000	0.000
0501	amitrole	3.00	-0.615	2	0.506	0	3.959	-5.286	26	26	-0.613	0.000	1.522	1.000	0.000	0.000
0503	ancymidol	2.33	1.719	4	3.045	5	3.650	-2.831	102	673	2.131	0.000	1.512	1.000	0.000	2.000
0504	anilazine	2.08	4.392	6	3.432	2	2.754	0.445	80	449	3.575	0.000	1.874	1.000	0.000	0.000
0505	aniline	3.00	1.083	0	0.984	0	2.297	-8.794	30	42	1.269	0.000	1.296	0.000	0.000	0.000
0506	anisole	1.87	1.814	1	1.648	1	1.286	-5.479	34	64	1.695	0.000	1.272	0.000	0.000	0.000
0507	anthracene	2.25	3.647	0	1.539	0	0.001	-5.440	76	279	3.993	0.000	0.980	0.000	0.000	0.000
0510	ascorbic acid	3.22	-1.709	6	2.554	6	5.135	5.276	58	188	-1.41	2.350	1.571	1.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0511	asulam	0.49	0.422	4	3.275	4	7.037	-30.00	72	378	0.313	0.945	1.955	0.000	0.000	0.000
0513	azelaic acid	2.24	1.922	4	7.437	10	0.850	18.296	50	344	1.886	1.026	1.391	0.000	0.000	0.000
0514	azinophos methyl	2.23	3.299	7	4.698	5	8.902	-11.41	96	728	1.999	0.000	2.124	1.000	0.000	0.000
0517	azulene	3.13	2.738	0	1.175	0	1.252	-9.257	50	107	2.791	0.000	0.991	0.000	0.000	0.000
0518	benazolin	3.13	2.250	5	2.600	3	4.021	-10.08	78	339	1.801	0.814	2.069	1.000	0.000	0.000
0521	benomyl	3.99	2.965	4	4.887	8	5.285	-2.235	102	944	2.572	0.167	1.667	1.000	0.000	0.000
0523	bensulide	2.60	3.678	7	8.723	10	6.817	-0.637	110	1358	3.773	0.500	1.808	0.000	0.000	0.000
0526	benzalacetone	4.59	2.028	1	2.612	2	3.244	-3.694	48	174	2.289	0.000	1.229	0.000	0.000	0.000
0530	benzene	1.46	1.830	0	0.913	0	0.000	-5.000	24	27	1.687	0.000	1.000	0.000	0.000	0.000
0531	benzeneacetaldehyde	1.87	1.517	1	2.022	2	2.335	1.345	38	94	1.428	0.000	1.264	0.000	0.000	0.000
0532	benzeneacetic acid	2.35	1.495	2	2.179	3	1.579	-10.14	44	126	1.314	0.500	1.392	0.000	0.000	0.000
0533	benzeneacetonitrile	2.14	1.744	1	1.871	2	2.954	0.304	38	94	1.753	0.000	1.272	0.000	0.000	0.000
0534	benzeneethanamine	2.23	1.257	1	2.279	2	1.414	-2.520	38	94	1.188	0.000	1.219	0.000	0.000	0.000
0537	benzo[a]pyrene	2.40	4.854	0	1.781	0	0.210	-23.20	120	680	5.737	0.000	0.954	0.000	0.000	0.000
0542	benzophenone	2.23	3.234	1	2.410	2	3.071	-6.274	68	307	2.918	0.000	1.196	0.000	0.000	0.000
0543	benzothiazole	2.64	2.265	2	0.993	0	1.486	-5.291	46	79	2.296	0.000	1.574	1.000	0.000	0.000
0545	benzotriazole	1.97	1.435	2	0.773	0	3.437	-2.500	46	79	0.958	0.000	1.531	1.000	0.000	0.000
0546	benzotrifluoride	3.07	2.772	3	1.656	0	2.530	-5.792	48	114	2.705	0.000	1.506	0.000	0.000	0.000
0547	benzyl acetate	3.04	1.605	2	2.807	3	1.571	-5.387	48	174	1.750	0.000	1.357	0.000	0.000	0.000
0548	benzyl alcohol	2.44	1.226	1	1.648	2	1.532	-6.948	34	64	1.179	0.000	1.272	0.000	0.000	0.000
0549	benzyl benzoate	1.95	3.269	2	3.463	4	2.299	-12.26	76	496	3.044	0.000	1.296	0.000	0.000	0.000
0550	benzyl chloride	3.54	2.430	1	1.925	1	1.315	-4.940	34	64	2.425	0.000	1.287	0.000	0.000	0.000
0551	benzyl ethyl ether	2.63	1.983	1	2.966	3	1.431	-8.032	42	133	2.223	0.000	1.207	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0552	benzyl methyl ether	2.55	1.634	1	2.279	2	1.517	-7.483	38	94	1.833	0.000	1.236	0.000	0.000	0.000
0553	benzyl phenyl ether	2.11	3.397	1	2.939	3	1.103	-11.26	66	343	3.266	0.000	1.196	0.000	0.000	0.000
0554	benzylamine	3.44	0.936	1	1.648	1	1.730	-7.022	34	64	1.145	0.000	1.253	0.000	0.000	0.000
0556	biphenox	5.38	4.469	7	5.227	4	4.022	8.666	110	1089	4.481	0.814	1.875	0.000	0.000	0.000
0557	biphenyl	3.04	3.348	0	1.910	1	0.470	-11.09	58	198	3.354	0.000	0.994	0.000	0.000	0.000
0558	bis(2-chloroethyl) ether	3.30	1.381	3	7.045	4	0.160	4.250	22	56	1.481	0.000	1.640	0.000	0.000	0.000
0560	BPMC	3.18	3.244	2	4.307	5	3.372	-8.425	68	374	2.918	0.000	1.422	0.000	0.000	1.000
0561	bromacil	1.71	1.935	3	3.311	2	4.566	-2.329	68	280	1.579	0.250	1.768	1.000	0.000	0.000
0563	bromobenzene	1.60	2.578	1	1.471	0	1.213	-6.882	30	42	2.449	0.000	1.325	0.000	0.000	0.000
0564	bromochloromethane	3.00	1.284	2	3.481	0	1.473	-1.476	6	4	1.578	0.000	1.922	0.000	0.000	0.000
0565	bromocyclohexane	2.14	2.849	1	2.170	0	1.888	0.985	30	42	2.714	0.000	1.194	0.000	0.000	0.000
0566	bromoethane	3.12	1.340	1	2.877	0	1.664	-2.512	6	4	1.401	0.000	1.299	0.000	0.000	0.000
0570	bromoxynil octanoate	2.39	5.921	5	8.047	9	3.202	-0.276	90	974	5.349	0.000	1.639	0.000	0.000	0.000
0571	bromoxynil	4.00	2.964	4	2.658	2	2.304	1.528	52	148	2.789	0.000	1.921	0.000	0.000	0.000
0573	butanamide	2.86	0.291	1	2.456	2	3.762	0.653	20	32	0.272	0.000	1.472	0.000	0.000	0.000
0576	butyl acetate	3.98	1.350	2	4.560	4	1.694	-1.030	28	79	1.350	0.000	1.295	0.000	0.000	0.000
0577	butyl acrylate	2.37	2.047	2	5.120	5	2.478	-3.460	32	110	1.516	0.000	1.313	0.000	0.000	0.000
0579	butyl mercaptan	3.47	1.942	1	4.655	3	2.072	-2.708	14	20	1.716	0.000	1.159	0.000	0.000	0.000
0580	butyl methacrylate	2.62	2.494	2	4.852	5	1.659	-5.084	38	143	1.906	0.000	1.281	0.000	0.000	0.000
0581	butylamine	2.94	0.681	1	3.928	2	1.497	-1.123	14	20	0.745	0.000	1.122	0.000	0.000	0.000
0582	butylate	1.85	3.514	2	6.888	7	2.378	-4.332	58	326	3.474	0.000	1.369	0.000	0.000	2.000
0583	butylbenzene	2.11	3.685	0	3.006	3	0.610	-5.907	42	133	3.029	0.000	0.980	0.000	0.000	0.000
0584	butyl-n-phenylcarbamate	3.69	2.922	2	4.718	6	2.002	-14.83	60	364	3.035	0.000	1.456	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0585	butyraldehyde	2.26	0.941	1	3.428	2	2.640	3.667	14	20	0.985	0.000	1.239	0.000	0.000	0.000
0588	butyronitrile	1.81	1.168	1	3.134	2	3.313	4.249	14	20	1.310	0.000	1.281	0.000	0.000	0.000
0589	captafol	1.70	4.023	7	4.444	3	2.395	-1.931	96	567	3.521	0.250	2.098	1.000	0.000	2.000
0590	Captan	3.32	4.533	6	3.458	1	3.417	-0.642	86	405	2.914	0.250	2.115	1.000	0.000	2.000
0592	carbendazym (MBC)	2.02	1.651	3	2.157	3	2.665	-4.659	70	314	1.741	0.000	1.749	1.000	0.000	0.000
0593	carbetamide	2.35	1.486	3	5.157	7	6.351	2.540	76	600	1.760	0.200	1.597	0.000	0.000	0.000
0594	carbofuran	1.95	2.234	3	2.695	3	4.513	7.949	84	425	2.118	0.000	1.523	1.000	0.000	1.000
0595	carbon disulfide	1.79	1.651	2	2.383	0	0.000	2.665	6	4	1.018	0.000	0.918	0.000	0.000	0.000
0596	carbon tetrabromide	2.54	4.021	4	3.162	0	0.001	0.004	20	16	3.177	0.000	0.722	0.000	0.000	0.000
0598	carbon tetrafluoride	2.27	2.437	4	0.794	0	0.002	-0.002	20	16	1.476	0.000	0.722	0.000	0.000	0.000
0601	carboxin	4.67	1.600	3	3.536	3	4.219	6.573	78	459	2.620	0.000	1.647	1.000	0.000	0.000
0602	chinomethionate	2.41	4.133	5	1.835	0	4.607	-7.792	84	341	2.575	0.000	1.881	2.000	0.000	0.000
0603	chloramben methyl	3.36	2.268	4	3.140	2	4.235	-9.192	62	234	2.362	0.000	1.939	0.000	0.000	0.000
0605	chloramphenicol	2.74	1.025	7	6.310	8	7.122	7.879	94	880	0.909	1.622	1.979	0.000	0.000	0.000
0606	chlorbromuron	2.00	2.411	4	4.379	4	5.542	-12.22	70	394	3.128	0.000	2.014	0.000	0.000	0.000
0607	chlorbufam	2.58	3.828	3	4.165	5	4.849	-4.722	68	412	2.910	0.000	1.713	0.000	0.000	0.000
0608	chlorfenvinphos (cis)	2.47	4.122	7	7.555	7	4.580	2.922	94	818	5.728	0.000	1.879	0.000	0.000	0.000
0609	chlorfenvinphos (trans)	2.47	4.122	7	7.555	7	7.937	9.011	94	818	5.728	0.000	1.879	0.000	0.000	0.000
0610	chloridazon (Pyrazon)	2.04	0.650	3	2.430	1	5.638	-19.26	76	352	1.468	0.000	1.829	1.000	0.000	0.000
0614	chlorobenzene	2.22	2.494	1	1.324	0	1.320	-5.662	30	42	2.340	0.000	1.325	0.000	0.000	0.000
0616	chlorodifluoromethane	1.97	1.224	3	1.522	0	1.564	3.823	12	9	1.448	0.000	1.922	0.000	0.000	0.000
0618	chloroform	1.65	1.617	3	2.591	0	1.003	0.651	12	9	1.986	0.000	1.371	0.000	0.000	0.000
0619	chloroneb	3.22	3.126	4	3.349	2	0.001	-6.929	56	192	3.011	0.000	1.722	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0620	chloropicrin	1.79	3.288	5	2.263	0	3.671	8.351	30	42	1.591	0.500	1.842	0.000	0.000	0.000
0621	chlorothalonil	2.98	4.245	6	3.476	2	2.382	2.691	68	272	4.044	0.000	1.379	0.000	0.000	0.000
0623	chlorotrifluoromethane	2.28	2.724	4	1.064	0	0.556	1.109	20	16	1.745	0.000	1.371	0.000	0.000	0.000
0624	chloroxuron	3.55	3.377	3	4.606	5	3.924	-5.177	98	962	4.226	0.000	1.666	0.000	0.000	0.000
0625	chlorpropham	2.53	2.984	3	3.919	4	4.742	-2.471	64	335	3.297	0.000	1.691	0.000	0.000	0.000
0626	chlorpyrifos ethyl	3.79	4.972	8	6.792	6	5.635	-17.41	86	612	4.718	0.000	2.234	1.000	0.000	0.000
0627	chlorpyrifos methyl	3.52	4.275	8	5.420	4	4.062	-9.779	78	434	3.938	0.000	2.401	1.000	0.000	0.000
0628	chlorsulfuron	1.60	1.859	8	5.085	6	6.189	4.645	116	1268	1.352	0.945	2.111	1.000	0.000	0.000
0631	cinnamamide	2.14	1.300	1	2.440	2	4.514	-4.391	48	174	1.185	0.000	1.469	0.000	0.000	0.000
0632	cinnamic acid	2.54	1.928	2	2.577	3	3.548	-3.198	48	174	1.784	0.500	1.378	0.000	0.000	0.000
0633	cinnamonitrile	2.44	2.177	1	2.280	2	4.223	1.125	42	133	2.223	0.000	1.253	0.000	0.000	0.000
0634	ciprofloxacin	4.79	1.436	5	3.618	4	10.139	18.178	134	1234	1.583	0.945	1.724	2.000	0.000	0.000
0636	cis-1,2-dichloropropene	2.48	1.571	2	2.715	0	1.916	-4.249	16	18	2.325	0.000	1.530	0.000	0.000	0.000
0637	cis-1,3-pentadiene	2.68	1.817	0	3.118	1	0.345	-3.598	14	20	1.749	0.000	0.961	0.000	0.000	0.000
0638	cis-2,trans-4-hexadiene	2.90	2.220	0	4.092	1	0.413	-4.231	18	35	2.139	0.000	0.954	0.000	0.000	0.000
0639	cis-2-butene	2.65	1.752	0	2.562	0	0.335	-2.018	10	10	1.582	0.000	0.918	0.000	0.000	0.000
0640	cis-2-methylcyclohexanol	2.38	1.820	1	1.896	1	1.354	-0.193	36	60	1.557	0.000	1.143	0.000	0.000	1.000
0641	cis-permethrin	3.19	5.439	5	5.832	7	7.334	-1.594	136	1945	6.113	0.000	1.492	0.000	0.000	2.000
0643	coronene	4.67	5.450	0	1.674	0	0.019	-30.67	156	1002	6.919	0.000	0.918	0.000	0.000	0.000
0644	crotoxyphos (trans)	2.00	2.539	6	6.946	8	7.530	32.808	98	1066	3.612	0.167	1.584	0.000	0.000	0.000
0645	cumene	3.37	3.024	0	1.884	1	0.607	-5.919	40	88	2.810	0.000	0.985	0.000	0.000	1.000
0646	cyanazine	2.26	2.336	5	3.850	5	4.838	3.909	76	456	1.671	0.000	1.681	1.000	0.000	1.000
0647	cyanogen	1.42	0.069	2	1.475	1	0.000	3.631	10	10	0.034	0.000	1.000	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0648	cycloate	2.54	3.337	2	5.231	5	3.052	3.725	62	312	3.514	0.000	1.407	0.000	0.000	0.000
0649	cyclododecanone	3.61	4.052	1	5.879	0	2.711	-3.723	54	264	3.860	0.000	1.097	0.000	0.000	0.000
0651	cyclohexane	3.25	2.737	0	1.543	0	0.006	0.309	24	27	2.341	0.000	0.918	0.000	0.000	0.000
0652	cyclohexanol	2.05	1.500	1	1.687	1	1.586	-6.325	30	42	1.311	0.000	1.167	0.000	0.000	0.000
0653	cyclohexanone	1.82	1.314	1	1.447	0	2.950	-0.059	30	42	1.520	0.000	1.221	0.000	0.000	0.000
0654	cyclohexanone oxime	1.83	1.401	2	2.032	1	1.030	-2.275	34	64	1.781	0.000	1.429	0.000	0.000	0.000
0655	cyclohexene	2.93	2.293	0	1.313	0	0.326	-1.881	24	27	2.117	0.000	0.954	0.000	0.000	0.000
0656	cyclohexylamine	2.19	1.211	1	1.687	0	1.480	-2.417	30	42	1.278	0.000	1.141	0.000	0.000	0.000
0657	cyclooctane	3.80	3.650	0	3.015	0	0.034	-0.483	32	64	3.121	0.000	0.918	0.000	0.000	0.000
0659	cyclopropane	2.31	1.369	0	0.099	0	0.037	-0.443	12	3	1.170	0.000	0.918	0.000	0.000	0.000
0660	cyfluthrin	5.00	5.510	7	6.402	8	4.687	-15.06	152	2425	6.317	0.000	1.726	0.000	0.000	2.000
0662	cypermethrin	5.00	5.305	6	6.219	8	5.767	-19.10	146	2244	6.178	0.000	1.606	0.000	0.000	2.000
0663	cyromazine	2.30	0.314	3	1.458	2	0.303	-13.26	62	201	-0.390	0.000	1.539	1.000	0.000	0.000
0664	dalapon	0.40	0.924	4	2.047	2	2.614	0.808	30	42	1.265	0.500	1.936	0.000	0.000	0.000
0665	DBCP	1.85	2.495	3	5.329	2	1.430	2.287	20	31	2.384	0.000	1.790	0.000	0.000	0.000
0671	dementon-S-methyl	1.49	1.729	5	7.788	7	7.244	4.671	48	234	2.874	0.000	1.760	0.000	0.000	0.000
0672	desmedipham	3.18	3.283	4	5.645	8	3.333	-42.22	104	1241	3.866	0.125	1.616	0.000	0.000	0.000
0674	diallate (cis)	3.28	3.274	4	7.316	6	1.548	-3.790	64	400	4.277	0.000	1.728	0.000	0.000	0.000
0675	diallate (trans)	3.28	3.274	4	7.316	6	2.318	-5.587	64	400	4.277	0.000	1.728	0.000	0.000	0.000
0676	diazinon	2.36	3.818	6	6.497	7	6.949	-11.89	90	720	3.585	0.000	1.772	1.000	0.000	1.000
0677	dibenz[a,h]anthracene	6.07	5.464	0	2.307	0	0.000	-24.71	128	971	6.299	0.000	0.964	0.000	0.000	0.000
0678	dibenzofuran	3.62	3.333	1	1.221	0	1.420	-5.081	72	219	3.586	0.000	1.201	1.000	0.000	0.000
0679	dibenzopyrrole	3.40	3.323	0	1.221	0	0.941	-8.734	72	219	3.321	0.000	1.207	1.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0681	dibromomethane	2.63	1.496	2	3.907	0	1.526	-2.143	6	4	1.734	0.000	1.522	0.000	0.000	0.000
0682	dibutyl ether	3.12	2.708	2	3.907	0	1.478	-1.963	6	4	2.603	0.000	1.086	0.000	0.000	0.000
0683	dibutyl phthalate	3.95	4.198	2	3.907	0	1.478	-1.963	6	4	3.600	0.200	1.342	0.000	0.000	0.000
0684	dibutylamine	2.92	2.442	2	3.907	0	1.478	-1.963	6	4	2.176	0.000	1.068	0.000	0.000	0.000
0686	dichlobenil	2.33	3.038	2	3.907	0	1.478	-1.963	6	4	2.865	0.000	1.669	0.000	0.000	0.000
0687	dichloroacetic acid	1.88	0.991	2	3.907	0	1.478	-1.963	6	4	0.875	0.500	2.000	0.000	0.000	0.000
0688	dichlorodifluoromethane	2.55	3.011	2	3.907	0	1.478	-1.962	6	4	2.014	0.000	1.522	0.000	0.000	0.000
0689	dichlorofluoromethane	2.22	1.421	2	3.907	0	1.478	-1.962	6	4	1.717	0.000	1.922	0.000	0.000	0.000
0691	dichloroprop butoxyethyl ester	3.00	4.532	6	8.883	10	2.746	-21.34	94	1170	4.121	0.000	1.576	0.000	0.000	0.000
0692	dichlorprop	3.00	3.108	5	3.892	4	2.122	-13.37	66	316	2.845	0.500	1.765	0.000	0.000	0.000
0694	diclofop	4.20	4.668	6	5.334	6	2.600	-4.873	104	1076	4.638	0.500	1.662	0.000	0.000	0.000
0695	diclofop-methyl	4.20	4.894	6	5.940	6	2.547	-6.643	108	1236	4.726	0.000	1.634	0.000	0.000	0.000
0696	dicofol	3.70	5.620	6	4.803	3	1.139	-6.582	106	744	5.600	0.000	1.636	0.000	0.000	1.000
0698	dicrotophos (cis)	1.66	0.136	5	5.751	6	11.501	16.310	66	400	1.396	0.167	1.741	0.000	0.000	0.000
0700	dieldrin	4.11	3.407	7	2.179	0	1.407	-5.670	134	520	4.481	0.000	1.698	1.000	1.000	6.000
0701	diethanolamine	0.60	-1.295	3	5.779	6	2.354	-1.774	22	56	-1.439	0.167	1.500	0.000	0.000	0.000
0702	diethathyl-ethyl	3.15	3.630	4	7.400	9	2.497	-13.66	96	888	2.946	0.200	1.546	0.000	0.000	0.000
0703	diethyl carbonate	2.04	1.362	3	4.499	4	3.342	-0.747	28	75	1.179	0.000	1.415	0.000	0.000	0.000
0704	diethyl ether	1.86	0.748	1	3.928	2	1.160	-2.464	14	20	1.043	0.000	1.159	0.000	0.000	0.000
0706	diethyl malonate	1.90	0.755	4	5.598	6	2.228	4.042	42	184	0.503	0.250	1.451	0.000	0.000	0.000
0708	diethyl phthalate	2.72	2.238	4	4.822	6	2.375	-12.95	72	446	2.040	0.200	1.429	0.000	0.000	0.000
0709	diethyl succinate	2.03	0.790	4	6.511	7	0.001	2.296	46	244	0.893	0.200	1.420	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0710	diethyl sulfate	2.00	0.169	4	3.758	4	6.875	11.530	36	96	0.304	0.500	1.657	0.000	0.000	0.000
0711	diethyl sulfide	2.44	1.493	1	4.655	2	1.876	-4.189	14	20	1.759	0.000	1.159	0.000	0.000	0.000
0712	diethylacetamide	1.84	0.277	1	3.239	3	3.263	0.045	30	67	0.875	0.000	1.363	0.000	0.000	0.000
0714	diethylene glycol dibutyl ether	2.42	2.446	3	13.769	12	1.125	-9.781	54	560	2.636	0.000	1.212	0.000	0.000	0.000
0715	diethylene glycol diethyl ether	1.59	0.486	3	9.772	8	1.148	-7.290	38	220	1.076	0.000	1.278	0.000	0.000	0.000
0717	diethylene glycol monobutyl ether	1.68	0.709	3	9.772	9	1.492	-4.930	38	220	0.812	0.000	1.278	0.000	0.000	0.000
0721	di-isobutyl phthalate	3.14	3.924	4	6.549	8	2.463	-14.13	92	878	3.312	0.200	1.342	0.000	0.000	2.000
0722	diisopropanolamine	0.93	-0.540	3	4.667	6	2.667	0.433	34	108	-0.662	0.167	1.414	0.000	0.000	0.000
0725	dimethipin	0.48	-0.374	4	2.078	0	0.742	-10.14	64	172	0.081	1.629	1.790	1.000	0.000	0.000
0726	dimethoate	2.56	0.725	5	6.131	6	3.252	13.573	50	218	0.983	0.000	2.027	0.000	0.000	0.000
0727	dimethyl disulfide	2.34	1.386	2	4.347	1	0.000	-7.809	10	10	1.627	0.000	1.371	0.000	0.000	0.000
0728	dimethyl ether	1.43	0.051	1	1.934	0	1.532	-1.160	6	4	0.263	0.000	1.224	0.000	0.000	0.000
0729	dimethyl phthalate	1.63	1.541	4	3.502	4	2.485	-11.67	64	295	1.260	0.200	1.483	0.000	0.000	0.000
0730	dimethyl sulfate	2.01	-0.529	4	2.206	2	6.592	5.569	28	44	-0.476	0.500	1.738	0.000	0.000	0.000
0731	dimethyl sulfone	0.61	-0.221	2	0.961	0	5.314	8.115	20	16	-0.339	0.500	1.686	0.000	0.000	0.000
0734	dimethylacetylene	2.17	1.874	0	2.278	0	0.000	-2.840	10	10	1.030	0.000	0.971	0.000	0.000	0.000
0735	dimethylamine	2.72	-0.216	1	1.934	0	1.465	-0.907	6	4	-0.164	0.000	1.157	0.000	0.000	0.000
0737	di-n-hexyl phthalate	4.72	6.023	4	10.988	14	2.291	-17.68	104	1650	5.161	0.200	1.280	0.000	0.000	0.000
0738	dinitramine	3.63	2.674	7	5.039	3	3.704	17.480	110	914	2.950	1.442	2.075	0.000	0.000	0.000
0739	dinoseb	1.59	3.027	5	3.999	3	5.184	19.434	82	486	2.722	2.252	1.760	0.000	0.000	1.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0740	dioctyl phthalate	5.51	7.848	4	14.392	18	2.284	-19.75	120	2724	6.721	0.200	1.234	0.000	0.000	0.000
0741	diphenamide	2.08	2.774	1	3.777	4	3.086	1.600	88	575	2.907	0.000	1.315	0.000	0.000	1.000
0744	diphenylacetylene	3.98	3.939	0	2.637	2	0.444	-15.26	66	343	3.086	0.000	0.980	0.000	0.000	0.000
0745	diphenylamine	2.78	3.380	0	2.278	2	1.415	-5.493	62	264	3.430	0.000	1.207	0.000	0.000	0.000
0747	diphenylmethanol	2.83	2.838	1	2.611	3	1.336	-1.113	68	307	2.768	0.000	1.196	0.000	0.000	0.000
0750	dipropyl sulfone	1.59	1.524	2	3.857	4	5.538	14.635	36	96	1.221	0.500	1.445	0.000	0.000	0.000
0751	di-propylamine	2.29	1.529	1	5.926	4	1.231	-2.542	22	56	1.396	0.000	1.091	0.000	0.000	0.000
0752	diquat	6.00	1.927	0	1.596	0	3.351	-13.89	76	271	0.942	0.000	1.314	3.000	1.000	0.000
0753	disulfoton	3.22	3.326	5	10.354	9	4.681	-8.105	56	356	3.770	0.000	1.667	0.000	0.000	0.000
0754	diuron	2.82	2.481	3	3.607	3	4.536	-13.53	66	321	3.087	0.000	1.845	0.000	0.000	0.000
0756	dodecane	4.97	5.846	0	11.000	9	0.000	-3.293	42	286	4.927	0.000	0.900	0.000	0.000	0.000
0757	dodecanoic acid	3.88	4.568	2	10.426	11	2.015	8.458	52	444	3.992	0.500	1.167	0.000	0.000	0.000
0758	dodecylbenzene	6.08	7.334	0	9.607	11	0.632	-5.636	74	889	6.150	0.000	0.954	0.000	0.000	0.000
0760	dyfonate	3.44	3.600	3	5.036	5	3.988	-15.01	64	316	4.145	0.000	1.623	0.000	0.000	0.000
0756	dodecane	4.97	5.846	0	11.000	9	0.000	-3.293	42	286	4.927	0.000	0.900	0.000	0.000	0.000
0757	dodecanoic acid	3.88	4.568	2	10.426	11	2.015	8.458	52	444	3.992	0.500	1.167	0.000	0.000	0.000
0761	eicosanoic acid	6.43	8.218	2	18.364	19	2.024	15.674	84	1752	7.113	0.500	1.094	0.000	0.000	0.000
0762	endosulfan	4.13	2.143	9	3.680	0	2.084	6.030	116	552	3.690	0.000	2.072	1.000	1.000	4.000
0763	endothall	2.14	-0.331	5	1.941	4	5.285	8.967	70	219	-0.051	1.629	1.531	2.000	0.000	2.000
0765	enrofloxacin	4.85	2.320	5	4.282	5	10.521	21.339	144	1601	2.316	0.945	1.661	2.000	0.000	0.000
0767	epsilon-caprolactam	1.27	0.542	1	1.890	0	3.359	-0.882	34	61	0.677	0.000	1.429	1.000	0.000	0.000
0768	EPTC	2.38	2.875	2	7.155	7	1.645	-8.497	46	220	2.982	0.000	1.430	0.000	0.000	0.000
0769	esfenvalerate	3.72	6.565	5	7.372	9	3.909	-10.72	150	2659	6.680	0.000	1.490	0.000	0.000	2.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0770	ethalfluralin	3.60	4.135	7	5.563	4	2.414	-1.310	114	1078	3.924	1.442	1.995	0.000	0.000	0.000
0772	ethion	3.94	4.527	8	12.518	12	4.538	28.271	82	792	5.005	0.000	1.830	0.000	0.000	0.000
0773	ethofumesate	2.17	2.457	5	3.701	4	5.447	0.250	102	691	2.058	0.500	1.567	1.000	0.000	0.000
0774	ethoprofos	1.80	3.418	4	8.782	8	6.309	-5.747	52	276	4.417	0.000	1.603	0.000	0.000	0.000
0777	ethyl acrylate	2.10	1.068	2	3.236	3	2.464	-2.523	24	50	0.735	0.000	1.400	0.000	0.000	0.000
0778	ethyl alcohol	1.21	-0.009	1	1.934	1	1.481	-1.252	6	4	-0.001	0.000	1.224	0.000	0.000	0.000
0779	ethyl benzoate	2.81	2.034	2	2.807	3	2.135	-7.007	48	164	1.863	0.000	1.357	0.000	0.000	0.000
0780	ethyl butyl ether	2.48	1.728	1	5.926	4	1.151	-3.140	22	56	1.823	0.000	1.116	0.000	0.000	0.000
0781	ethyl chloride	2.16	1.195	1	2.511	0	1.730	-1.334	6	4	1.245	0.000	1.299	0.000	0.000	0.000
0782	ethyl formate	1.50	0.291	2	3.361	2	4.138	2.475	14	20	0.179	0.000	1.435	0.000	0.000	0.000
0783	ethyl heptanoate	2.61	2.862	2	7.474	7	1.993	1.128	40	202	2.520	0.000	1.217	0.000	0.000	0.000
0785	ethyl iodide	2.47	1.871	1	3.394	0	1.387	-2.891	6	4	1.441	0.000	1.299	0.000	0.000	0.000
0787	ethyl octanoate	3.02	3.318	2	8.455	8	1.952	1.531	44	265	2.910	0.000	1.198	0.000	0.000	0.000
0788	ethyl pentanoate	1.97	1.949	2	5.524	5	1.965	0.310	32	108	1.740	0.000	1.265	0.000	0.000	0.000
0789	ethyl phenylacetate	1.89	2.069	2	3.482	4	1.616	-12.06	52	221	1.792	0.000	1.325	0.000	0.000	0.000
0790	ethyl propanoate	2.31	1.037	2	3.606	3	1.882	-0.044	24	50	0.960	0.000	1.333	0.000	0.000	0.000
0791	ethyl vanillin	2.24	1.680	3	2.962	4	2.963	-1.440	54	202	1.603	0.167	1.437	0.000	0.000	0.000
0793	ethyl-3,5-dinitrobenzoate	2.74	1.823	6	4.098	3	5.612	20.015	80	516	1.680	2.076	1.842	0.000	0.000	0.000
0794	ethyl-4-hydroxybenzoate	2.21	1.792	3	2.962	4	1.230	-6.581	54	211	1.569	0.167	1.437	0.000	0.000	0.000
0795	ethyl-4-methylbenzoate	2.59	2.520	2	2.997	3	2.604	-8.147	54	211	2.172	0.000	1.325	0.000	0.000	0.000
0796	ethyl-4-nitrobenzoate	2.48	1.929	4	3.441	3	5.362	9.603	64	331	1.772	0.651	1.695	0.000	0.000	0.000
0797	ethylamine	1.31	-0.299	1	1.934	0	1.500	-0.869	6	4	-0.035	0.000	1.157	0.000	0.000	0.000
0799	ethylene	1.99	0.947	0	0.000	0	0.000	0.111	2	1	0.802	0.000	0.918	0.000	0.000	0.000

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0800	ethylene glycol	0.64	-0.897	2	2.862	3	0.000	-1.479	10	10	-1.029	0.333	1.371	0.000	0.000	0.000
0801	ethylene oxide	1.21	-0.131	1	0.089	0	2.049	0.342	12	3	0.017	0.000	1.379	1.000	0.000	0.000
0803	Ethyl-n-phenylcarbamate	1.82	1.942	2	3.288	4	1.887	-13.67	52	221	2.255	0.000	1.542	0.000	0.000	0.000
0806	fenac	1.80	3.488	5	3.563	3	2.531	-11.67	62	238	3.274	0.500	1.816	0.000	0.000	0.000
0807	fenamiphos	2.52	3.241	5	6.435	7	3.755	1.474	90	738	4.238	0.000	1.675	0.000	0.000	0.000
0808	fenamiphos sulfone	1.64	2.225	6	6.133	7	3.168	21.97	104	966	2.920	0.595	1.756	0.000	0.000	0.000
0809	fenamiphos sulfoxide	1.57	2.129	5	6.554	7	5.007	29.80	96	851	3.254	0.125	1.721	0.000	0.000	0.000
0811	fenitrothion	3.51	3.065	6	4.878	4	9.575	5.496	82	540	2.799	0.500	1.990	0.000	0.000	0.000
0812	fenobucarb	1.71	5.391	0	4.610	5	1.086	-1.817	68	374	4.709	0.000	0.974	0.000	0.000	1.000
0813	fenoxaprop-ethyl	3.98	4.646	7	5.450	7	2.974	-3.109	128	1795	4.604	0.000	1.683	1.000	0.000	0.000
0815	fenoxycarb	3.00	3.558	4	6.570	9	1.196	16.544	102	1386	3.604	0.000	1.499	0.000	0.000	0.000
0816	fenpropimorph	3.40	4.843	2	5.679	5	1.005	-1.902	112	1212	4.272	0.000	1.183	1.000	0.000	1.000
0819	fensulfothion sulfone	2.17	2.908	6	6.106	7	10.946	-6.875	92	762	2.766	0.500	1.805	0.000	0.000	0.000
0820	fenthion	3.18	3.712	5	5.309	5	3.036	-6.559	76	457	3.613	0.000	1.774	0.000	0.000	0.000
0821	fenuron	1.40	1.152	1	2.689	3	3.415	-10.98	54	212	1.780	0.000	1.520	0.000	0.000	0.000
0824	fluazifop-p-butyl	3.76	5.225	8	7.464	9	3.871	-11.33	132	2356	5.003	0.000	1.727	1.000	0.000	0.000
0829	fluoranthene	4.14	3.945	0	1.386	0	0.180	-18.00	94	364	4.487	0.000	0.961	0.000	0.000	0.000
0830	fluorene	3.66	3.493	0	1.307	0	0.390	3.984	72	219	3.258	0.000	0.988	0.000	0.000	0.000
0831	fluorobenzene	2.61	2.036	1	1.069	0	1.543	-3.546	30	42	1.826	0.000	1.325	0.000	0.000	0.000
0832	fluoroform	1.73	1.027	3	1.088	0	1.720	1.799	12	9	1.178	0.000	1.371	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0833	fluoroxypyr	1.53	1.853	7	3.809	4	5.064	-2.745	72	372	1.573	0.500	2.321	1.000	0.000	0.000
0834	fluridone	3.01	3.785	4	4.012	2	8.000	-17.31	128	1293	4.738	0.000	1.596	1.000	0.000	0.000
0836	folpet	3.27	4.961	6	3.094	1	4.933	-9.192	86	405	3.259	0.250	2.158	1.000	0.000	0.000
0837	fomesaten	1.78	3.674	10	6.085	5	8.668	29.296	146	2154	3.749	2.196	2.246	0.000	0.000	0.000
0838	formaldehyde	1.57	-0.884	1	0.000	0	0.937	2.191	2	1	-0.185	0.000	1.500	0.000	0.000	0.000
0839	formamide	0.56	-0.911	1	1.210	0	0.891	1.014	6	4	-0.899	0.000	1.792	0.000	0.000	0.000
0840	formanilide	2.00	0.872	1	1.855	2	2.607	-0.948	38	94	1.255	0.000	1.544	0.000	0.000	0.000
0845	furfuryl alcohol	1.53	0.407	2	1.130	2	1.073	-1.499	30	43	0.772	0.000	1.460	1.000	0.000	0.000
0847	glufosinate	2.00	-1.059	5	3.891	6	5.469	13.475	48	172	-0.311	1.442	1.801	0.000	0.000	0.000
0848	glutaric acid	1.22	0.097	4	3.827	6	0.884	10.104	34	108	0.326	1.442	1.522	0.000	0.000	0.000
0849	glutaronitrile	0.99	0.595	2	4.254	4	3.279	2.708	22	56	1.204	0.000	1.460	0.000	0.000	0.000
0850	glycerol	0.42	-1.408	3	3.023	5	2.975	-7.951	20	31	-1.668	0.909	1.414	0.000	0.000	0.000
0851	glyceryl triacetate	1.51	-0.271	6	6.683	8	4.250	24.963	62	424	0.044	0.410	1.501	0.000	0.000	0.000
0853	GS-38946	3.17	3.431	8	5.701	4	3.228	5.830	128	1373	3.527	1.442	1.981	1.000	0.000	0.000
0856	heptane	3.83	3.565	0	6.000	4	0.090	-1.800	22	56	2.977	0.000	0.887	0.000	0.000	0.000
0857	heptanoic acid	2.69	2.287	2	5.524	6	2.008	4.297	32	114	2.041	0.500	1.265	0.000	0.000	0.000
0858	heptylamine	2.78	2.050	1	6.925	5	1.555	-1.419	26	84	1.916	0.000	1.078	0.000	0.000	0.000
0859	hexachloro-1,3-butadiene	4.00	3.634	6	5.578	1	0.771	-2.109	42	121	4.757	0.000	0.971	0.000	0.000	0.000
0860	hexachlorobenzene	4.49	5.816	6	3.676	0	0.001	-9.000	60	174	5.607	0.000	1.000	0.000	0.000	0.000
0862	hexachloroethane	3.55	3.376	6	3.377	0	0.000	1.644	38	58	3.727	0.000	0.811	0.000	0.000	0.000
0863	hexachlorophene	3.52	7.307	8	5.563	4	1.188	-8.461	110	860	6.609	0.167	1.750	0.000	0.000	0.000
0864	hexadecanoic acid	5.28	6.393	2	14.388	15	2.021	12.038	68	954	5.552	0.500	1.124	0.000	0.000	0.000
0866	hexafluorobenzene	2.76	3.063	6	1.993	0	0.001	7.523	60	174	2.521	0.000	1.000	0.000	0.000	0.000

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0868	hexamethyl phosphoramide	1.53	-1.116	4	3.712	3	4.038	3.939	50	142	0.779	0.000	1.571	0.000	0.000	0.000
0869	hexamethylbenzene	3.93	4.747	0	2.273	0	0.014	-9.315	60	174	3.537	0.000	0.971	0.000	0.000	0.000
0870	hexamethyldisiloxane	3.66	3.497	1	2.286	2	0.361	-1.704	42	88	2.673	0.000	1.326	0.000	0.000	0.000
0871	hexanal	2.35	1.853	1	5.403	4	2.701	6.131	22	56	1.766	0.000	1.167	0.000	0.000	0.000
0872	hexane	3.55	3.109	0	5.000	3	0.000	-1.511	18	35	2.587	0.000	0.881	0.000	0.000	0.000
0873	hexanenitrile	2.25	2.080	1	5.090	4	3.387	6.761	22	56	2.090	0.000	1.194	0.000	0.000	0.000
0875	hexazinone	1.73	2.601	3	3.540	2	7.063	18.181	92	571	0.513	0.250	1.578	1.000	0.000	0.000
0877	hexylbenzene	4.38	4.597	0	4.513	5	0.623	-5.902	50	242	3.809	0.000	0.971	0.000	0.000	0.000
0879	hydramethylnon	5.86	6.464	8	7.719	5	4.623	-3.122	182	4426	6.382	0.000	1.651	1.000	0.000	0.000
0880	hydrazobenzene	2.98	3.402	0	2.666	3	0.233	-9.634	66	343	3.126	0.000	1.314	0.000	0.000	0.000
0883	imazamethabenz	2.04	2.524	4	3.478	4	4.596	-2.657	106	756	1.984	0.651	1.553	1.000	0.000	2.000
0884	imazapyr	2.35	1.315	5	3.195	4	6.092	-4.977	100	661	1.071	0.651	1.669	2.000	0.000	2.000
0885	imidacloprid	2.64	1.048	5	3.501	3	5.599	-3.416	84	559	0.688	0.500	1.964	2.000	0.000	0.000
0886	imidazole	1.33	-0.283	1	0.433	0	3.889	-4.681	20	15	0.410	0.000	1.530	1.000	0.000	0.000
0887	indane	3.19	2.887	0	1.048	0	0.754	0.747	46	79	2.175	0.000	0.998	0.000	0.000	0.000
0888	indene	2.97	2.442	0	0.922	0	0.646	-6.314	46	79	2.256	0.000	0.998	0.000	0.000	0.000
0890	iodobenzene	3.16	2.408	1	1.679	0	1.348	-7.767	30	42	2.291	0.000	1.325	0.000	0.000	0.000
0891	ioxynil	2.30	2.623	4	3.092	2	2.128	2.080	52	148	2.473	0.000	1.921	0.000	0.000	0.000
0892	ipazine	3.39	3.238	4	4.734	5	2.958	-10.15	74	448	2.191	0.000	1.561	1.000	0.000	0.000
0893	iprobenfos	2.40	3.803	4	6.436	7	6.611	-2.079	84	651	4.878	0.000	1.565	0.000	0.000	0.000
0896	isobutanol	1.79	0.834	1	2.195	2	1.428	-1.420	16	18	0.635	0.000	1.159	0.000	0.000	1.000
0897	isobutene	2.66	1.796	0	1.033	0	0.571	-2.120	12	9	1.582	0.000	0.918	0.000	0.000	0.000
0900	isobutylamine	1.77	0.544	1	2.195	1	1.590	-1.663	16	18	0.601	0.000	1.122	0.000	0.000	1.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0902	isobutyric acid	1.89	0.925	2	1.806	2	1.650	1.462	22	29	0.727	0.500	1.379	0.000	0.000	1.000
0903	isobutyronitrile	1.63	1.174	1	1.595	1	3.242	3.372	16	18	1.166	0.000	1.281	0.000	0.000	1.000
0904	isofenphos	2.78	3.693	6	7.830	9	9.560	-1.796	104	1066	3.890	0.000	1.684	0.000	0.000	0.000
0905	isopentane	2.63	2.448	0	2.250	1	0.103	-0.643	16	18	2.052	0.000	0.874	0.000	0.000	1.000
0907	isophthalic acid	2.28	1.090	4	2.323	4	0.291	1.009	56	197	1.083	1.442	1.530	0.000	0.000	0.000
0908	isoprene	2.69	1.861	0	1.584	1	0.387	-3.592	16	18	1.749	0.000	0.961	0.000	0.000	0.000
0909	isopropalin	4.00	4.720	4	6.576	6	1.442	-11.63	104	968	4.253	1.442	1.594	0.000	0.000	1.000
0911	isopropyl benzoate	3.11	2.412	2	2.997	3	2.070	-5.798	54	209	2.252	0.000	1.325	0.000	0.000	0.000
0912	isopropyl phenylcarbamate	1.95	2.320	2	3.461	4	3.880	-3.832	58	276	2.644	0.000	1.496	0.000	0.000	0.000
0915	isoquinoline	2.51	1.588	1	1.139	0	2.244	-5.272	50	109	2.235	0.000	1.253	1.000	0.000	0.000
0919	lactonitrile	0.87	-0.143	2	1.548	2	4.079	0.266	16	18	-0.109	0.000	1.685	0.000	0.000	0.000
0920	leptofos	4.50	5.998	6	5.661	4	3.093	8.603	102	792	5.416	0.000	2.063	0.000	0.000	0.000
0921	levulinic acid	1.11	-0.259	3	3.030	4	1.128	8.744	30	74	0.440	0.814	1.477	0.000	0.000	0.000
0924	linolenic acid	4.89	5.972	2	14.991	14	1.257	8.019	76	1313	5.661	0.500	1.159	0.000	0.000	0.000
0925	linuron	2.43	2.327	4	4.201	4	5.597	-10.08	70	394	3.019	0.000	1.934	0.000	0.000	0.000
0927	Malathion	3.07	2.161	8	10.081	11	8.918	-19.33	82	738	2.122	0.200	1.789	0.000	0.000	0.000
0928	maleic acid	1.12	0.039	4	2.679	4	2.161	-5.218	30	74	-0.288	1.629	1.585	0.000	0.000	0.000
0929	maleic hydrazide	0.45	-2.200	4	3.849	4	4.907	-1.842	38	141	-2.478	0.200	1.837	0.000	0.000	0.000
0930	malononitrile	1.05	0.104	2	2.372	2	3.252	6.608	14	20	0.424	0.000	1.557	0.000	0.000	0.000
0931	m-bromoaniline	1.96	1.832	1	1.534	0	3.154	-12.05	36	61	2.031	0.000	1.592	0.000	0.000	0.000
0932	m-bromophenol	2.41	2.336	2	1.655	1	2.120	-7.137	36	61	2.155	0.000	1.614	0.000	0.000	0.000
0933	m-chloroaniline	3.13	1.748	1	1.398	0	3.189	-10.18	36	61	1.922	0.000	1.592	0.000	0.000	0.000
0934	m-chloronitrobenzene	2.72	2.389	3	1.988	0	6.027	3.252	46	117	2.248	0.500	1.985	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0935	m-chlorophenol	1.82	2.252	2	1.512	1	2.227	-5.661	36	61	2.046	0.000	1.614	0.000	0.000	0.000
0936	MCPA	1.73	2.446	4	3.422	4	0.460	0.118	60	266	2.112	0.500	1.650	0.000	0.000	0.000
0937	m-cresol	1.54	2.074	1	1.308	1	1.148	-5.578	36	61	1.701	0.000	1.272	0.000	0.000	0.000
0938	m-cymene	3.83	3.510	0	2.103	1	0.607	-6.884	46	117	3.118	0.000	0.980	0.000	0.000	1.000
0939	m-dibromobenzene	3.42	3.327	2	2.085	0	1.127	-6.923	36	61	3.212	0.000	1.459	0.000	0.000	0.000
0940	m-dichlorobenzene	2.78	3.159	2	1.765	0	1.299	-5.492	36	61	2.993	0.000	1.459	0.000	0.000	0.000
0941	m-diethylbenzene	3.86	3.715	0	2.494	2	0.844	-6.569	44	121	2.811	0.000	0.980	0.000	0.000	0.000
0943	m-dinitrobenzene	2.19	1.619	4	2.221	0	5.991	12.892	56	197	1.503	1.442	1.906	0.000	0.000	0.000
0944	mecoprop	2.10	2.930	4	3.633	4	3.072	-9.191	66	316	2.500	0.500	1.603	0.000	0.000	0.000
0945	meobal	1.71	2.566	2	3.033	3	4.161	-10.96	60	262	2.022	0.000	1.496	0.000	0.000	0.000
0946	mesitylene	3.24	3.289	0	1.563	0	0.042	-7.433	42	84	2.612	0.000	0.985	0.000	0.000	0.000
0947	Metalaxyl	1.66	2.057	4	5.853	7	5.098	16.437	94	754	1.844	0.200	1.483	0.000	0.000	0.000
0950	methabenzthiazuron	2.72	2.108	3	2.552	3	3.562	-13.08	76	365	2.072	0.000	1.776	1.000	0.000	0.000
0952	methacrylonitrile	1.75	1.189	1	1.303	1	3.193	5.002	16	18	1.086	0.000	1.361	0.000	0.000	0.000
0954	methane	1.97	1.376	0	0.000	0	0.001	0.001	0	0	0.636	0.000	0.722	0.000	0.000	0.000
0956	methidathion	1.53	2.731	8	5.585	6	7.335	-8.471	76	471	1.521	0.000	2.225	1.000	0.000	0.000
0958	methomyl	1.86	0.652	4	4.783	4	3.091	-7.707	38	141	1.039	0.000	1.880	0.000	0.000	0.000
0959	methoxychlor	4.90	4.970	5	5.527	4	2.300	8.240	106	932	5.206	0.000	1.577	0.000	0.000	1.000
0960	methoxypropazine	2.43	2.562	4	4.422	5	3.107	-6.746	74	458	1.521	0.000	1.542	1.000	0.000	0.000
0961	methyl acetate	1.48	0.021	2	1.764	1	1.523	0.194	16	18	0.179	0.000	1.435	0.000	0.000	0.000
0962	methyl acrylate	1.81	0.719	2	2.326	2	2.360	-1.799	20	31	0.345	0.000	1.459	0.000	0.000	0.000
0964	methyl benzoate	2.57	1.685	2	2.179	2	2.164	-5.565	44	121	1.473	0.000	1.392	0.000	0.000	0.000
0965	methyl bromide	0.79	0.991	1	0.000	0	1.658	-2.668	2	1	1.011	0.000	1.371	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
0967	methyl chloride	1.87	0.847	1	0.000	0	1.662	-1.640	2	1	0.855	0.000	1.371	0.000	0.000	0.000
0968	methyl cinnamate	2.80	2.153	2	3.231	3	3.246	-5.396	52	226	1.873	0.000	1.349	0.000	0.000	0.000
0970	methyl decanoate	3.78	3.881	2	9.439	9	1.842	4.121	48	346	3.300	0.000	1.182	0.000	0.000	0.000
0971	methyl ethyl ketone	1.54	0.563	1	1.814	1	2.907	2.062	16	18	0.985	0.000	1.239	0.000	0.000	0.000
0972	methyl ethyl sulfide	2.22	1.144	1	3.643	1	2.009	-3.859	10	10	1.369	0.000	1.189	0.000	0.000	0.000
0973	methyl fluoride	1.65	0.582	1	0.000	0	1.680	0.132	2	1	0.586	0.000	1.371	0.000	0.000	0.000
0974	methyl formate	1.39	-0.058	2	2.387	1	4.062	1.573	10	10	-0.211	0.000	1.500	0.000	0.000	0.000
0975	methyl iodide	1.04	1.522	1	0.000	0	1.272	-2.656	2	1	1.051	0.000	1.371	0.000	0.000	0.000
0976	methyl isopropyl ketone	1.68	1.025	1	1.849	1	2.722	1.582	22	29	1.231	0.000	1.198	0.000	0.000	1.000
0980	methyl propanoate	1.83	0.688	2	2.670	2	1.730	0.619	20	31	0.569	0.000	1.379	0.000	0.000	0.000
0981	methyl propyl ether	2.04	0.923	1	3.928	2	1.460	-1.892	14	20	1.043	0.000	1.159	0.000	0.000	0.000
0983	methyl salicylate	2.76	1.443	3	2.355	3	3.265	-6.654	50	152	1.179	0.250	1.471	0.000	0.000	0.000
0984	methyl tert-butyl ether	1.89	0.982	1	1.595	1	1.686	0.008	24	28	1.431	0.000	1.135	0.000	0.000	1.000
0986	methylamine	1.07	-0.648	1	0.000	0	1.661	-0.542	2	1	-0.425	0.000	1.149	0.000	0.000	0.000
0987	methylcyclohexane	3.49	2.989	0	1.722	0	0.094	0.845	30	42	2.587	0.000	0.918	0.000	0.000	1.000
0988	methylcyclopentane	3.21	2.533	0	1.134	0	0.104	-0.744	26	26	2.197	0.000	0.918	0.000	0.000	1.000
0989	methylethanolamine	0.87	-0.755	2	3.857	3	1.221	-1.729	14	20	-0.802	0.000	1.430	0.000	0.000	0.000
0990	methylethylamine	1.46	0.133	1	2.930	1	1.292	-1.375	10	10	0.226	0.000	1.140	0.000	0.000	0.000
0993	methyl-n-phenylcarbamate	1.73	1.594	2	2.629	3	1.606	-13.33	48	168	1.865	0.000	1.595	0.000	0.000	0.000
0994	m-ethylphenol	2.74	2.530	1	1.853	2	0.915	-6.087	40	88	1.955	0.000	1.236	0.000	0.000	0.000
0996	metobromuron	2.02	1.747	3	3.910	4	5.082	-9.775	64	333	2.474	0.000	1.821	0.000	0.000	0.000
0997	metolachlor	2.20	3.364	3	6.323	7	3.651	-6.476	88	656	3.164	0.000	1.487	0.000	0.000	0.000
1000	metsulfuron methyl	1.54	1.050	9	5.919	8	10.057	-16.63	130	1753	0.486	1.424	1.967	1.000	0.000	0.000

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1001	mevinphos (cis)	2.30	0.578	6	5.831	6	6.168	6.276	60	332	1.481	0.167	1.671	0.000	0.000	0.000
1003	m-nitroaniline	2.12	0.978	2	1.639	0	7.963	-3.132	46	117	1.177	0.500	1.811	0.000	0.000	0.000
1004	m-nitrophenol	1.72	1.482	3	1.749	1	7.148	1.639	46	117	1.300	0.814	1.782	0.000	0.000	0.000
1006	molinate	1.92	2.503	2	4.363	3	1.887	-2.376	52	206	2.736	0.000	1.478	1.000	0.000	0.000
1007	monocrotophos	0.00	-0.070	5	5.639	6	6.661	8.434	60	332	1.054	0.167	1.787	0.000	0.000	0.000
1008	monoethanolamine	0.66	-1.187	2	2.862	2	1.306	-1.193	10	10	-1.063	0.000	1.491	0.000	0.000	0.000
1010	monuron	1.70	1.817	2	3.142	3	4.041	-10.54	60	268	2.434	0.000	1.727	0.000	0.000	0.000
1011	morphine	1.83	1.412	4	2.212	2	2.627	-0.844	132	712	1.198	0.167	1.448	2.000	1.000	1.000
1012	morpholine	0.40	-0.528	2	1.470	0	1.146	-5.263	24	27	-0.394	0.000	1.472	1.000	0.000	0.000
1013	m-phenylenediamine	1.20	0.337	0	1.079	0	2.198	-13.39	36	61	0.851	0.000	1.406	0.000	0.000	0.000
1014	m-toluenediamine	1.45	0.823	0	1.304	0	0.321	-14.15	42	84	1.159	0.000	1.360	0.000	0.000	0.000
1015	m-toluic acid	2.67	1.946	2	1.826	2	2.881	-3.988	46	117	1.693	0.500	1.392	0.000	0.000	0.000
1017	m-xylene	2.46	2.802	0	1.335	0	0.417	-6.372	36	61	2.303	0.000	0.991	0.000	0.000	0.000
1018	N-(1,1-dimethyl-2-propynyl)benzamide	1.54	2.813	1	2.931	4	2.960	-8.483	66	316	1.828	0.000	1.380	0.000	0.000	1.000
1019	N,N-diethylaniline	3.18	2.690	0	2.964	3	3.132	-6.056	48	158	2.533	0.000	1.169	0.000	0.000	0.000
1020	N,N-dimethylacetamide	0.96	-0.420	1	1.640	1	3.354	-0.819	22	29	0.095	0.000	1.472	0.000	0.000	0.000
1021	N,N-dimethylaniline	2.63	1.992	0	1.730	1	2.432	-8.266	40	88	1.753	0.000	1.219	0.000	0.000	0.000
1023	N,N-dimethylbenzylamine	2.45	1.904	1	2.459	2	1.471	-6.549	44	126	1.748	0.000	1.192	0.000	0.000	0.000
1024	N,N-dimethylformamide	0.83	-0.499	1	1.572	1	3.259	0.044	16	18	-0.296	0.000	1.551	0.000	0.000	0.000
1025	NAA ethyl ester	2.48	2.977	2	3.320	4	1.690	-1.667	78	447	2.945	0.000	1.287	0.000	0.000	0.000
1026	naled	2.26	2.875	8	6.375	5	8.308	13.704	60	248	3.651	0.000	2.339	0.000	0.000	0.000
1027	naphthacene	4.51	4.555	0	1.920	0	0.001	-19.99	102	569	5.146	0.000	0.971	0.000	0.000	0.000

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1028	naphthalene	3.00	2.738	0	1.175	0	0.000	2.194	50	109	2.840	0.000	0.991	0.000	0.000	0.000
1030	n-butyl benzyl phthalate	3.21	4.453	4	6.660	9	2.454	-20.26	108	1340	4.001	0.200	1.353	0.000	0.000	0.000
1031	neburon	3.40	3.810	3	5.586	6	4.264	-10.39	78	586	4.257	0.000	1.680	0.000	0.000	0.000
1032	neopentane	3.07	2.198	0	1.000	0	0.022	-0.013	20	16	2.052	0.000	0.874	0.000	0.000	0.000
1033	NIA 23486	1.70	2.644	4	2.562	2	4.487	-1.322	92	482	2.332	0.000	1.580	2.000	0.000	1.000
1034	nicosulfuron	2.26	0.688	9	6.559	9	8.998	-34.77	140	2142	0.101	1.424	1.944	2.000	0.000	0.000
1035	nitralin	2.92	0.688	9	6.559	9	6.094	-35.54	140	2142	0.101	1.424	1.944	2.000	0.000	0.000
1037	nitrobenzene	2.01	1.724	2	1.555	0	6.512	0.848	40	88	1.595	0.500	1.727	0.000	0.000	0.000
1041	N-methyl-2-pyrrolidone	1.17	-0.165	1	1.006	0	2.967	-4.542	32	40	0.239	0.000	1.491	1.000	0.000	0.000
1042	N-methylacetamide	0.81	-0.626	1	1.572	1	3.371	-1.826	16	18	-0.248	0.000	1.551	0.000	0.000	0.000
1044	N-methylbenzamide	1.42	1.038	1	2.050	2	3.281	-6.778	44	121	1.046	0.000	1.483	0.000	0.000	0.000
1045	N-methylformamide	0.85	-0.705	1	2.143	1	3.482	0.438	10	10	-0.638	0.000	1.658	0.000	0.000	0.000
1048	3-(4-Chlorophenyl)-1,1-dimethylurea	2.50	2.873	2	3.741	3	3.750	-15.59	72	378	3.159	0.000	1.618	0.000	0.000	0.000
1050	nonanoic acid	3.24	3.200	2	7.474	8	2.024	5.913	40	212	2.822	0.500	1.217	0.000	0.000	0.000
1051	nonylbenzene	5.25	5.966	0	6.983	8	0.660	-5.769	62	498	4.980	0.000	0.961	0.000	0.000	0.000
1052	norflurazon	2.66	2.024	6	3.715	2	6.835	-22.97	104	797	2.946	0.000	2.063	1.000	0.000	0.000
1054	N-phenyl-n'-cycloheptylurea	2.37	3.261	1	4.419	4	3.063	-2.386	80	582	3.531	0.000	1.379	0.000	0.000	0.000
1055	N-phenyl-n'-cyclohexylurea	2.07	2.805	1	3.805	4	3.123	6.114	76	495	3.141	0.000	1.406	0.000	0.000	0.000
1056	N-phenyl-n'-cyclopentylurea	1.93	2.348	1	3.223	4	3.508	-11.47	72	411	2.751	0.000	1.437	0.000	0.000	0.000
1057	N-phenyl-n'-cyclopropylurea	1.74	1.436	1	2.166	4	3.390	-8.207	64	275	1.971	0.000	1.514	0.000	0.000	0.000
1058	N-phenyl-n'-methylurea	1.29	0.946	1	2.491	3	3.394	-6.069	48	168	1.438	0.000	1.572	0.000	0.000	0.000
1059	N-phenyl-N-methylurea	1.29	0.946	1	2.108	2	3.504	9.263	50	156	1.202	0.000	1.572	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1060	o-bromoaniline	1.96	1.832	1	1.534	0	2.076	-9.300	36	60	2.031	0.000	1.592	0.000	0.000	0.000
1061	o-bromophenol	2.41	2.336	2	1.655	1	2.472	-8.707	36	60	2.155	0.000	1.614	0.000	0.000	0.000
1063	o-chlorobenzoic acid	2.49	2.124	3	2.041	2	2.690	-4.961	46	114	2.038	0.500	1.689	0.000	0.000	0.000
1065	o-chlorophenol	1.71	2.252	2	1.512	1	2.422	-6.717	36	60	2.046	0.000	1.614	0.000	0.000	0.000
1067	o-cresol	1.34	2.981	1	1.542	0	1.208	-6.282	36	60	2.648	0.000	1.287	0.000	0.000	0.000
1068	octadecanoic acid	5.85	7.305	2	16.375	17	2.023	13.853	76	1313	6.333	0.500	1.108	0.000	0.000	0.000
1069	octamethylcyclotetrasiloxane	4.15	6.277	4	3.187	0	0.023	-6.701	88	376	2.874	0.000	1.571	1.000	0.000	0.000
1070	octane	4.18	4.021	0	7.000	5	0.000	-2.104	26	84	3.367	0.000	0.890	0.000	0.000	0.000
1072	octanoic acid	3.04	2.743	2	6.496	7	1.998	5.047	36	158	2.431	0.500	1.239	0.000	0.000	0.000
1073	octylamine	2.96	2.506	1	7.925	6	1.496	-1.587	30	120	2.306	0.000	1.068	0.000	0.000	0.000
1074	octylbenzene	4.80	5.510	0	6.138	7	0.628	-5.840	58	399	4.590	0.000	0.964	0.000	0.000	0.000
1075	o-cymene	3.76	3.510	0	2.103	1	1.443	-5.867	46	114	3.118	0.000	0.980	0.000	0.000	1.000
1078	o-difluorobenzene	2.67	2.241	2	1.242	0	2.663	-2.348	36	60	1.965	0.000	1.459	0.000	0.000	0.000
1079	o-dinitrobenzene	2.30	1.619	4	2.221	0	9.411	-2.476	56	188	1.503	1.629	1.906	0.000	0.000	0.000
1082	o-ethyltoluene	3.30	3.259	0	1.884	1	1.413	-5.991	40	86	2.557	0.000	0.985	0.000	0.000	0.000
1086	o-nitrophenol	2.06	1.482	3	1.749	1	7.738	-0.037	46	114	1.300	0.945	1.782	0.000	0.000	0.000
1087	o-nitrotoluene	2.63	2.211	2	1.777	0	5.966	0.834	46	114	1.903	0.500	1.658	0.000	0.000	0.000
1088	o-phenylenediamine	1.46	0.337	0	1.079	0	3.460	-11.65	36	60	0.851	0.000	1.406	0.000	0.000	0.000
1089	oryzalin	3.40	2.231	7	6.267	6	3.883	39.938	112	1082	1.777	3.114	1.904	0.000	0.000	0.000
1091	o-toluidine	1.74	1.570	0	1.203	0	2.350	-8.838	36	60	1.577	0.000	1.253	0.000	0.000	0.000
1092	oxadiazole	3.51	-0.183	3	0.400	0	1.344	-0.686	20	15	0.070	0.000	1.950	1.000	0.000	0.000
1094	oxamyl	0.90	0.212	5	5.733	6	6.137	-7.964	58	337	0.107	0.167	1.893	0.000	0.000	0.000
1095	oxazole	1.44	-0.273	2	0.433	0	1.555	0.098	20	15	0.675	0.000	1.811	1.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1098	oxyfluorfen	5.00	5.224	8	5.553	4	1.137	17.618	122	1442	5.458	0.500	2.003	0.000	0.000	0.000
1102	p,p-ddt	5.31	6.331	5	4.918	2	1.177	-3.390	98	678	6.496	0.000	1.470	0.000	0.000	1.000
1103	p-aminoazobenzene	3.23	3.453	2	2.739	2	4.567	-22.82	72	420	3.684	0.000	1.399	0.000	0.000	0.000
1104	p-aminobiphenyl	2.93	2.602	0	2.006	1	3.050	-18.99	64	252	2.936	0.000	1.207	0.000	0.000	0.000
1105	paraldehyde	1.74	0.088	3	2.053	0	1.829	-2.899	42	84	1.088	0.000	1.379	1.000	0.000	0.000
1106	parathion ethyl	3.02	3.276	6	6.007	6	7.602	7.789	84	661	3.271	0.500	1.933	0.000	0.000	0.000
1110	p-bromotoluene	3.23	3.065	1	1.686	0	1.739	-7.860	36	62	2.758	0.000	1.287	0.000	0.000	0.000
1111	p-chloroaniline	3.13	1.748	1	1.398	0	3.880	-10.87	36	62	1.922	0.000	1.592	0.000	0.000	0.000
1112	p-chloronitrobenzene	2.68	2.389	3	1.988	0	5.561	6.082	46	120	2.248	0.500	1.985	0.000	0.000	0.000
1113	p-chlorophenol	1.85	2.252	2	1.512	1	1.305	-4.259	36	62	2.046	0.000	1.614	0.000	0.000	0.000
1115	p-cresol	1.69	2.074	1	1.308	1	1.534	-5.150	36	62	1.701	0.000	1.272	0.000	0.000	0.000
1116	p-cymene	3.61	3.510	0	2.103	1	0.224	-6.903	46	120	3.118	0.000	0.980	0.000	0.000	1.000
1117	p-dichlorobenzene	2.78	3.159	2	1.765	0	0.001	-4.372	36	62	2.993	0.000	1.459	0.000	0.000	0.000
1118	p-diethylbenzene	3.87	3.715	0	2.494	2	0.384	-7.137	44	125	2.811	0.000	0.980	0.000	0.000	0.000
1119	p-difluorobenzene	2.54	2.241	2	1.242	0	0.001	-0.734	36	62	1.965	0.000	1.459	0.000	0.000	0.000
1120	p-dimethylamino benzaldehyde	2.36	1.752	1	2.261	2	6.057	-5.159	50	162	1.565	0.000	1.433	0.000	0.000	0.000
1121	p-dinitrobenzene	2.17	1.619	4	2.221	0	0.001	17.365	56	206	1.503	1.301	1.906	0.000	0.000	0.000
1122	pebulate	2.80	3.331	2	8.098	8	1.372	-9.888	50	288	3.372	0.000	1.398	0.000	0.000	0.000
1123	pencycuron	3.33	4.802	2	5.187	6	3.971	-14.35	116	1237	5.317	0.000	1.483	0.000	0.000	0.000
1124	pendimethalin	3.70	4.174	4	5.291	4	7.168	3.516	96	747	3.720	1.442	1.655	0.000	0.000	0.000
1127	pentachloroethane	2.95	2.888	5	3.426	0	0.948	1.653	30	42	3.160	0.000	1.299	0.000	0.000	0.000
1129	pentachlorophenol	3.73	4.910	6	3.379	1	0.830	-7.500	60	174	4.659	0.000	1.614	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1130	pentaerythritol	0.46	-2.165	4	3.721	8	2.122	3.412	36	88	-2.058	1.500	1.410	0.000	0.000	0.000
1131	pentamethylbenzene	3.86	4.261	0	2.034	0	0.366	-8.667	54	140	3.229	0.000	0.975	0.000	0.000	0.000
1133	pentanoic acid	2.13	1.375	2	3.606	4	1.970	2.847	24	52	1.261	0.500	1.333	0.000	0.000	0.000
1135	pentylbenzene	4.04	4.141	0	3.742	4	0.649	-5.914	46	182	3.419	0.000	0.975	0.000	0.000	0.000
1136	pentyl-n-phenylcarbamate	2.61	3.379	2	5.479	7	1.960	-16.18	64	456	3.425	0.000	1.422	0.000	0.000	0.000
1137	permethrin	5.00	5.439	5	5.832	7	7.334	-1.594	136	1945	6.113	0.000	1.492	0.000	0.000	2.000
1138	perylene	4.78	4.854	0	1.781	0	0.001	-22.81	120	654	5.737	0.000	0.954	0.000	0.000	0.000
1139	p-ethylphenol	2.74	2.530	1	1.853	2	1.445	-5.184	40	90	1.955	0.000	1.236	0.000	0.000	0.000
1140	p-ethyltoluene	3.35	3.259	0	1.884	1	0.180	-6.796	40	90	2.557	0.000	0.985	0.000	0.000	0.000
1141	p-fluorotoluene	2.78	2.522	1	1.288	0	2.011	-3.750	36	62	2.134	0.000	1.287	0.000	0.000	0.000
1142	phenanthrene	3.77	3.647	0	1.539	0	0.221	-14.97	76	271	3.993	0.000	0.980	0.000	0.000	0.000
1143	phenazine	2.92	3.060	2	1.473	0	0.009	-12.94	76	279	2.783	0.000	1.322	1.000	0.000	0.000
1144	phenetole	2.74	2.162	1	2.279	2	1.237	-6.290	38	94	2.085	0.000	1.236	0.000	0.000	0.000
1147	phenyl acetate	2.19	1.598	2	2.179	2	3.060	-7.871	44	126	1.612	0.000	1.392	0.000	0.000	0.000
1148	phenyl benzoate	3.33	3.262	2	2.905	3	2.137	-9.529	72	394	2.906	0.000	1.311	0.000	0.000	0.000
1150	phenyl mercaptan	2.75	2.190	1	1.272	1	1.523	-6.752	30	42	1.975	0.000	1.314	0.000	0.000	0.000
1152	phenylhydrazine	2.06	1.106	1	1.491	1	2.750	-11.08	34	64	0.972	0.000	1.406	0.000	0.000	0.000
1153	phenyloxirane	2.25	1.481	1	1.028	1	2.052	-9.133	46	87	1.758	0.000	1.264	1.000	0.000	0.000
1154	phenylurea	1.35	0.740	1	1.894	2	3.520	-4.214	44	126	1.177	0.000	1.634	0.000	0.000	0.000
1155	phorate	2.82	3.308	5	9.405	8	8.030	-4.666	52	280	3.728	0.000	1.710	0.000	0.000	0.000
1156	phosalone	2.93	4.375	7	6.082	7	7.395	19.757	106	959	4.236	0.000	2.069	1.000	0.000	0.000
1158	phosphamidon	0.85	1.203	6	7.746	8	9.719	12.662	80	636	2.743	0.167	1.816	0.000	0.000	0.000
1159	phthalic acid	1.77	1.090	4	2.323	4	3.062	-9.193	56	188	1.083	1.629	1.530	0.000	0.000	0.000

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1160	phthalic anhydride	2.25	1.304	3	1.135	0	5.377	1.869	58	137	0.997	0.250	1.457	1.000	0.000	0.000
1161	p-hydroquinone	1.70	1.346	2	1.282	2	2.147	-4.478	36	62	1.098	0.200	1.449	0.000	0.000	0.000
1164	piperalin	3.70	4.510	5	6.491	6	0.980	-7.155	102	1118	4.415	0.000	1.577	1.000	0.000	0.000
1165	piperazine	0.74	-0.794	2	1.470	0	0.005	3.981	24	27	-0.821	0.000	1.299	1.000	0.000	0.000
1166	piperidine	1.83	0.701	1	1.506	0	1.296	2.223	24	27	0.760	0.000	1.166	1.000	0.000	0.000
1170	p-methoxyphenol	1.75	1.572	2	1.822	2	2.324	-5.083	40	90	1.401	0.000	1.402	0.000	0.000	0.000
1171	p-nitroaniline	2.13	0.978	2	1.639	0	10.342	-3.302	46	120	1.177	0.500	1.811	0.000	0.000	0.000
1174	p-phenylenediamine	1.21	0.337	0	1.079	0	0.001	-13.64	36	62	0.851	0.000	1.406	0.000	0.000	0.000
1175	prochloraz	4.13	4.407	6	6.715	8	3.662	-6.409	112	1313	4.602	0.000	1.847	1.000	0.000	0.000
1176	profenofos	3.30	4.977	6	7.288	7	6.294	-0.231	84	633	5.769	0.000	1.971	0.000	0.000	0.000
1178	prometryn	2.80	3.121	4	4.667	5	2.549	-9.723	74	458	2.234	0.000	1.542	1.000	0.000	0.000
1180	propachlor	2.42	2.415	2	3.956	4	4.904	-9.805	64	296	2.667	0.000	1.545	0.000	0.000	0.000
1181	propane	2.66	1.740	0	2.000	0	0.091	-0.613	6	4	1.416	0.000	0.845	0.000	0.000	0.000
1182	propanil	2.48	2.946	3	3.576	3	4.097	-12.07	60	262	3.342	0.000	1.775	0.000	0.000	0.000
1183	propanoic acid	1.56	0.462	2	1.764	2	1.854	1.727	16	18	0.481	0.500	1.435	0.000	0.000	0.000
1184	propargite	3.60	5.281	4	6.081	7	4.596	7.195	122	1458	3.654	0.500	1.425	0.000	0.000	0.000
1185	propargyl alcohol	1.17	0.834	1	2.218	2	1.631	-3.517	10	10	-0.388	0.000	1.406	0.000	0.000	0.000
1187	propham	1.83	2.320	2	3.461	4	3.978	-3.444	58	276	2.644	0.000	1.496	0.000	0.000	0.000
1189	propionaldehyde	1.70	0.484	1	2.450	1	2.616	2.568	10	10	0.595	0.000	1.295	0.000	0.000	0.000
1190	propionitrile	1.46	0.712	1	2.173	1	3.151	2.423	10	10	0.920	0.000	1.352	0.000	0.000	0.000
1191	propoxur	1.67	2.304	3	4.269	5	4.539	-10.66	68	384	2.192	0.000	1.526	0.000	0.000	0.000
1193	propyl alcohol	1.51	0.515	1	2.930	2	1.588	-1.153	10	10	0.389	0.000	1.189	0.000	0.000	0.000

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1195	propyl mercaptan	2.36	1.486	1	3.643	2	2.151	-2.795	10	10	1.326	0.000	1.189	0.000	0.000	0.000
1196	propylamine	1.64	0.225	1	2.930	1	1.564	-0.905	10	10	0.355	0.000	1.140	0.000	0.000	0.000
1197	propylbenzene	3.38	3.229	0	2.315	2	0.631	-5.901	38	94	2.639	0.000	0.985	0.000	0.000	0.000
1198	propylene glycol	0.36	-0.520	2	2.140	3	1.553	-6.732	16	18	-0.641	0.333	1.335	0.000	0.000	0.000
1200	Propyl-n-phenylcarbamate	2.06	2.466	2	3.986	5	1.887	-14.94	56	286	2.645	0.000	1.496	0.000	0.000	0.000
1201	p-terphenyl	4.66	4.867	0	2.930	2	0.496	-13.44	92	657	5.021	0.000	0.989	0.000	0.000	0.000
1203	p-toluidine	1.90	1.570	0	1.203	0	1.963	-10.32	36	62	1.577	0.000	1.253	0.000	0.000	0.000
1205	pyrene	4.38	3.945	0	1.386	0	0.001	-18.21	94	362	4.584	0.000	0.961	0.000	0.000	0.000
1206	pyridine	1.73	0.679	1	0.865	0	2.059	-3.008	24	27	1.082	0.000	1.349	1.000	0.000	0.000
1208	pyrocatechol	2.07	1.346	2	1.282	2	2.223	-5.482	36	60	1.098	0.333	1.449	0.000	0.000	0.000
1210	pyrrolidine	1.63	0.245	1	0.892	0	1.677	-1.316	20	15	0.370	0.000	1.198	1.000	0.000	0.000
1211	quinoline	2.48	2.016	1	1.139	0	1.988	-6.213	50	109	2.235	0.000	1.253	1.000	0.000	0.000
1213	quizalofop-ethyl	2.71	4.582	7	5.901	7	3.396	-1.709	132	2011	4.406	0.000	1.701	1.000	0.000	0.000
1214	R-40244	2.55	3.307	6	3.968	2	3.114	-1.997	100	684	3.514	0.000	1.996	1.000	0.000	1.000
1215	resorcinol	1.02	1.346	2	1.282	2	2.596	-5.073	36	61	1.098	0.250	1.449	0.000	0.000	0.000
1217	salicylic acid	2.57	1.218	3	1.798	3	3.573	-4.773	46	114	1.090	0.945	1.505	0.000	0.000	0.000
1218	SD11830	2.37	1.307	6	3.980	2	4.613	7.397	96	630	0.972	3.114	2.012	0.000	0.000	0.000
1219	SD12030	3.10	3.401	6	6.935	7	5.368	7.244	116	1219	2.923	3.114	1.807	0.000	0.000	0.000
1220	SD12346	3.30	2.180	6	5.097	4	4.792	6.796	104	848	1.753	3.114	1.922	0.000	0.000	0.000
1221	SD12639	2.56	2.005	6	5.097	4	5.280	7.898	104	830	1.753	3.114	1.922	0.000	0.000	0.000
1222	SD13207	2.71	2.353	6	5.689	5	5.209	7.217	108	947	2.143	3.114	1.881	0.000	0.000	0.000
1223	sec-bumeton	2.78	2.709	4	4.911	6	3.087	-10.12	72	465	1.522	0.000	1.542	1.000	0.000	0.000
1224	sec-butanol	1.73	0.892	1	2.195	2	1.586	-3.732	16	18	0.777	0.000	1.159	0.000	0.000	0.000

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1225	sec-butyl acetate	2.31	1.271	2	3.443	3	4.701	6.683	30	71	1.348	0.000	1.295	0.000	0.000	0.000
1228	siduron	2.31	3.124	1	4.017	4	3.945	-14.30	82	572	3.387	0.000	1.379	0.000	0.000	1.000
1229	silvex	3.28	3.773	6	4.371	4	2.596	-10.89	72	374	3.499	0.500	1.837	0.000	0.000	0.000
1230	simazine	2.08	2.158	4	3.696	4	3.956	-12.42	58	260	1.389	0.000	1.673	1.000	0.000	0.000
1231	sorbitol	0.18	-2.940	6	5.305	11	4.037	3.195	50	206	-3.585	3.603	1.457	0.000	0.000	0.000
1232	strychnine	4.14	1.146	3	2.266	0	2.312	7.056	164	1096	2.093	0.000	1.420	5.000	1.000	2.000
1233	styrene	3.04	2.382	0	1.476	1	0.103	-6.722	34	64	2.330	0.000	1.000	0.000	0.000	0.000
1235	succinonitrile	0.84	0.139	2	3.303	3	0.000	11.560	18	35	0.814	0.000	1.522	0.000	0.000	0.000
1236	sulfolane	0.96	0.240	2	1.072	0	6.120	-1.400	34	39	0.195	0.500	1.640	1.000	0.000	0.000
1239	Sulprofos	4.08	5.005	5	7.765	8	5.919	-15.20	82	666	5.192	0.000	1.683	0.000	0.000	0.000
1240	tebuconazole	2.67	3.632	4	4.690	7	4.866	-14.31	108	963	3.342	0.000	1.546	1.000	0.000	1.000
1241	tebuthiuron	1.83	1.900	4	3.284	4	4.382	-20.82	74	375	1.611	0.000	1.711	1.000	0.000	0.000
1242	temephos	5.00	5.656	9	8.932	10	8.052	-4.852	134	2272	5.630	0.000	1.880	0.000	0.000	0.000
1243	terbacil	1.63	1.533	3	2.585	1	4.284	-0.048	72	269	1.253	0.250	1.768	1.000	0.000	1.000
1244	terbufos	2.50	3.891	5	8.209	8	7.807	-4.258	66	412	4.506	0.000	1.628	0.000	0.000	1.000
1246	terbufos sulfoxide	2.18	2.779	5	7.994	8	7.579	-18.39	72	474	3.522	0.000	1.688	0.000	0.000	1.000
1247	terbutryn	2.85	2.948	4	4.229	5	4.033	-12.21	76	452	2.236	0.000	1.542	1.000	0.000	1.000
1248	terbutylazine	2.32	2.741	4	3.682	4	2.809	-12.78	72	380	2.167	0.000	1.595	1.000	0.000	1.000
1249	terephthalic acid	2.47	1.090	4	2.323	4	2.041	1.971	56	206	1.083	1.301	1.530	0.000	0.000	0.000
1250	terpinolene	3.81	3.643	0	2.311	0	0.361	-4.145	46	120	3.453	0.000	0.961	0.000	0.000	0.000
1251	tert-butanol	1.57	0.573	1	0.969	1	1.795	-3.138	20	16	0.777	0.000	1.159	0.000	0.000	1.000
1253	tert-butylamine	1.60	0.284	1	0.969	0	1.684	0.552	20	16	0.744	0.000	1.122	0.000	0.000	1.000
1254	tert-butylbenzene	3.61	3.230	0	1.797	1	0.813	-5.206	48	114	2.984	0.000	0.980	0.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1255	tert-pentyl-alcohol	1.86	1.097	1	1.595	2	1.815	-3.146	24	28	1.167	0.000	1.135	0.000	0.000	1.000
1256	tetrachloroethylene	2.31	2.429	4	3.422	0	0.000	-3.924	22	29	3.068	0.000	0.918	0.000	0.000	0.000
1257	tetrachloroguaiacol	2.85	4.229	6	3.689	2	2.129	-7.987	64	220	4.014	0.000	1.873	0.000	0.000	0.000
1258	tetrachloromethane	1.80	3.585	4	2.146	0	0.002	0.001	20	16	2.553	0.000	0.722	0.000	0.000	0.000
1260	tetradecane	5.29	6.758	0	13.000	11	0.000	-3.890	50	455	5.707	0.000	0.902	0.000	0.000	0.000
1261	tetradecanoic acid	4.70	5.481	2	12.405	13	2.019	10.235	60	667	4.772	0.500	1.143	0.000	0.000	0.000
1262	tetrahydrofuran	1.63	0.512	1	0.892	0	2.069	-3.459	20	15	0.797	0.000	1.239	1.000	0.000	0.000
1264	thiabendazole	3.24	2.368	3	1.606	1	4.385	-6.420	76	293	2.686	0.000	1.648	2.000	0.000	0.000
1265	thiazole	1.62	0.499	2	0.667	0	1.904	-2.279	20	15	1.143	0.000	1.811	1.000	0.000	0.000
1266	thidiazuron	2.04	1.425	4	2.890	4	5.852	2.596	72	411	2.182	0.000	1.892	1.000	0.000	0.000
1267	thifensulfuron	1.65	0.550	10	5.181	8	10.144	10.975	122	1418	0.459	2.348	2.123	2.000	0.000	0.000
1268	thifensulfuron-methyl	1.60	0.776	10	5.734	8	10.475	10.518	126	1591	0.547	1.424	2.084	2.000	0.000	0.000
1270	thiodicarb	2.54	2.102	9	10.165	10	6.257	2.207	90	1140	3.079	0.167	1.977	0.000	0.000	0.000
1271	thiophanate-methyl	3.26	2.715	6	7.324	10	6.328	-24.59	100	1189	1.792	0.091	1.994	0.000	0.000	0.000
1272	thiophene	2.36	1.127	1	0.711	0	0.105	-2.198	20	15	1.748	0.000	1.392	1.000	0.000	0.000
1273	thiram	3.01	3.156	4	5.902	5	8.138	-10.45	50	226	2.061	0.000	1.730	0.000	0.000	0.000
1275	tralomethrin	5.00	6.927	8	7.640	8	5.327	-11.81	160	2661	7.461	0.000	1.705	0.000	0.000	2.000
1276	trans-1,2-dichloroethylene	2.43	1.057	2	3.586	0	0.000	-0.818	10	10	1.935	0.000	1.585	0.000	0.000	0.000
1277	trans-1,3-pentadiene	2.70	1.817	0	3.118	1	0.392	-3.804	14	20	1.749	0.000	0.961	0.000	0.000	0.000
1279	trans-2-butene	2.63	1.752	0	2.562	0	0.049	-2.311	10	10	1.582	0.000	0.918	0.000	0.000	0.000
1281	trans-chlordane	5.15	4.788	8	3.390	0	2.295	1.772	114	459	5.683	0.000	1.555	0.000	0.000	4.000
1282	trans-permethrin	3.19	5.439	5	5.832	7	7.145	7.140	136	1945	6.113	0.000	1.492	0.000	0.000	2.000
1284	triadimefon	2.71	3.639	5	4.204	5	2.224	-8.078	102	802	3.124	0.000	1.724	1.000	0.000	0.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1285	triadimenol	1.95	3.247	5	4.423	6	2.533	-6.842	102	802	2.916	0.000	1.692	1.000	0.000	0.000
1286	triallate	3.35	3.960	5	7.735	6	2.091	-6.376	70	478	4.844	0.000	1.813	0.000	0.000	0.000
1287	tribufos	3.70	5.869	4	13.248	12	7.117	-9.774	68	616	6.694	0.000	1.456	0.000	0.000	0.000
1288	trichlorfon	1.90	1.126	7	4.833	4	2.303	4.803	56	185	2.161	0.333	2.084	0.000	0.000	0.000
1289	trichloroacetaldehyde	1.92	1.496	4	2.189	0	1.721	2.989	24	28	1.556	0.000	1.842	0.000	0.000	0.000
1290	trichloroacetamide	0.99	0.846	4	2.173	0	3.036	-0.069	30	42	0.842	0.000	2.197	0.000	0.000	0.000
1291	trichloroethylene	2.15	1.743	3	3.172	0	2.576	-1.617	16	18	2.502	0.000	1.459	0.000	0.000	0.000
1292	trichlorofluoromethane	2.75	3.298	4	1.739	0	0.804	1.512	20	16	2.284	0.000	1.371	0.000	0.000	0.000
1293	triclopyr	1.43	2.886	7	4.096	4	2.596	-0.430	66	318	2.505	0.500	2.105	1.000	0.000	0.000
1294	tricyclazole	3.09	2.293	3	1.240	0	6.287	-2.019	74	213	2.252	0.000	1.675	2.000	0.000	0.000
1295	tridecylbenzene	6.47	7.791	0	10.505	12	0.662	-5.530	78	1054	6.540	0.000	0.953	0.000	0.000	0.000
1296	tridemorph	3.31	6.197	2	11.257	12	1.221	-4.800	90	1348	5.407	0.000	1.126	1.000	0.000	0.000
1297	tridiphane	3.75	3.976	6	3.580	2	1.915	-3.817	88	422	4.979	0.000	1.720	1.000	0.000	1.000
1298	trietazine	2.74	2.861	4	4.550	5	4.098	-10.80	68	374	1.803	0.000	1.595	1.000	0.000	0.000
1299	triethanolamine	0.83	-1.298	4	6.842	9	2.428	-7.650	36	138	-1.735	0.500	1.489	0.000	0.000	0.000
1302	trifluoroacetamide	1.44	0.256	4	1.251	0	3.481	-1.584	30	42	0.034	0.000	2.197	0.000	0.000	0.000
1303	trifluralin	4.49	4.468	7	6.160	5	2.247	-4.541	112	1082	4.148	1.442	1.962	0.000	0.000	0.000
1304	triforine	2.30	2.099	10	8.093	6	2.852	24.946	108	1093	1.489	0.091	2.058	1.000	0.000	0.000
1305	trimethacarb	2.60	3.052	2	3.251	3	4.227	-11.71	66	312	2.330	0.000	1.456	0.000	0.000	0.000
1306	trimethyl phosphate	1.02	0.208	4	3.242	3	8.688	3.383	32	64	1.034	0.000	1.659	0.000	0.000	0.000
1309	trioxane	1.14	-0.446	3	1.434	0	2.424	-1.118	24	27	-0.078	0.000	1.500	1.000	0.000	0.000
1312	triphenylene	4.36	4.555	0	1.920	0	0.001	-18.00	102	513	5.146	0.000	0.971	0.000	0.000	0.000
1313	triphenylmethanol	3.38	4.277	1	3.360	4	1.304	0.732	104	730	3.971	0.000	1.150	0.000	0.000	1.000

Code	name	log K_{oc}	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1314	triphenylphosphine	4.47	5.707	0	3.719	3	1.315	0.020	96	666	3.445	0.000	1.156	0.000	0.000	0.000
1315	tripropylamine	2.90	2.938	1	7.043	6	1.432	-4.150	36	138	2.518	0.000	1.058	0.000	0.000	0.000
1316	undecylbenzene	5.81	6.878	0	8.719	10	0.661	-5.657	70	742	5.760	0.000	0.956	0.000	0.000	0.000
1317	valeronitrile	1.86	1.624	1	4.108	3	3.303	5.216	18	35	1.700	0.000	1.231	0.000	0.000	0.000
1318	vanillin	2.04	1.331	3	2.355	3	2.791	-1.187	50	154	1.213	0.167	1.471	0.000	0.000	0.000
1319	VEL 3510	2.51	1.838	6	5.847	8	6.485	-34.04	96	916	1.918	0.000	1.728	1.000	0.000	0.000
1321	vinclozolin	2.43	4.282	5	3.189	2	3.632	-2.308	96	559	3.421	0.250	1.855	1.000	0.000	1.000
1323	vinyl bromide	2.23	1.086	1	2.383	0	0.918	-0.805	6	4	1.525	0.000	1.459	0.000	0.000	0.000
1324	vinyl chloride	2.13	1.002	1	2.050	0	2.011	-0.133	6	4	1.369	0.000	1.459	0.000	0.000	0.000
1326	vinylcyclohexene	3.52	2.610	0	1.899	1	0.116	-2.651	34	64	2.529	0.000	0.971	0.000	0.000	1.000
1328	α-methylstyrene	3.27	2.828	0	1.685	1	0.250	-7.281	40	88	2.720	0.000	0.998	0.000	0.000	0.000
1329	α-pinene	4.01	2.873	0	1.073	0	0.241	-0.420	58	102	2.999	0.000	0.961	0.000	0.000	2.000
1330	γ-butyrolactone	1.03	0.277	2	0.881	0	4.273	0.172	26	26	0.323	0.000	1.459	1.000	0.000	0.000

Table A-2 Chemicals list, values of exp log KOC and physicochemical properties in a test set

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
9	1,10-phenanthroline	2.37	2.203	2	1.392	0	3.119	-13.22	76	271	2.783	0.000	1.322	2.000	0.000	0.000
11	1,1-dichloroethylene	2.54	1.688	2	1.751	0	2.562	-3.573	12	9	1.935	0.000	1.585	0.000	0.000	0.000
13	1,1-dimethyl-3-(3-fluorophenyl) urea	1.73	1.358	2	2.844	3	4.136	-9.903	60	262	1.919	0.000	1.727	0.000	0.000	0.000
16	1,2,3,4-tetrachlorobenzene	3.52	4.488	4	2.700	0	1.582	-7.569	48	109	4.300	0.000	1.459	0.000	0.000	0.000
18	1,2,3,4-tetrahydroquinoline	2.62	2.170	0	1.347	0	1.595	0.256	50	109	2.045	0.000	1.222	1.000	0.000	0.000
23	1,2,3-trichloropropane	2.61	2.206	3	4.626	2	1.385	2.843	20	31	2.071	0.000	1.539	0.000	0.000	0.000
24	1,2,3-trimethylbenzene	3.34	3.289	0	1.563	0	0.832	-6.700	42	82	2.612	0.000	0.985	0.000	0.000	0.000
26	1,2,4,5-tetramethylbenzene	3.61	3.775	0	1.797	0	0.020	-8.190	48	111	2.920	0.000	0.980	0.000	0.000	0.000
28	1,2,4-trimethylbenzene	3.35	3.289	0	1.563	0	0.401	-7.266	42	84	2.612	0.000	0.985	0.000	0.000	0.000
30	1,2-dichloro-1,1,2,2-tetrafluoroethane	2.91	2.590	6	1.987	1	0.527	2.528	38	58	2.650	0.000	1.500	0.000	0.000	0.000
33	1,2-dichloropropane	2.47	1.889	2	3.123	1	0.299	1.654	16	18	1.853	0.000	1.435	0.000	0.000	0.000
34	1,2-dihydro-3-methylbenz[j]aceanthrylene	6.10	5.642	0	2.080	0	1.071	-23.60	126	804	5.553	0.000	0.987	0.000	0.000	0.000
35	1,2-diiodoethane	2.85	2.863	2	6.088	1	0.000	-0.597	10	10	1.856	0.000	1.500	0.000	0.000	0.000
40	1,2-propanediol	0.88	-0.520	2	2.140	3	0.350	-1.142	16	18	-0.641	0.333	1.335	0.000	0.000	0.000
42	1,3 butadiene	2.46	1.415	0	2.158	1	0.000	0.855	10	10	1.358	0.000	0.971	0.000	0.000	0.000
43	1,3,5,7-cyclooctatetraene	3.05	1.871	0	1.931	0	0.000	-2.878	32	64	2.225	0.000	1.000	0.000	0.000	0.000
49	1,3-propanediol	0.81	-0.835	2	3.857	4	2.936	-1.371	14	20	-0.639	0.250	1.335	0.000	0.000	0.000
51	1,4-butanediol	0.93	-0.255	2	4.854	5	0.000	-0.937	18	35	-0.249	0.200	1.299	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
56	1,5-cyclooctadiene	3.10	2.760	0	2.441	0	0.111	-1.772	32	64	2.673	0.000	0.971	0.000	0.000	0.000
57	1,5-dimethylnaphthalene	3.76	3.711	0	1.613	0	0.001	4.381	62	176	3.457	0.000	1.000	0.000	0.000	0.000
63	1-amino-2-propanol	0.86	-0.810	2	2.140	2	1.597	-1.348	16	18	-0.674	0.000	1.430	0.000	0.000	0.000
65	1-bromo-2-nitrobenzene	2.42	2.473	3	2.134	0	5.628	-9.488	46	114	2.357	0.500	1.985	0.000	0.000	0.000
68	1-bromo-4-chlorobenzene	2.60	3.243	2	1.921	0	0.089	-4.934	36	62	3.103	0.000	1.626	0.000	0.000	0.000
71	1-bromoheptane	3.75	3.688	1	7.929	5	1.921	-0.642	26	84	3.352	0.000	1.121	0.000	0.000	0.000
74	1-bromopentane	3.21	2.776	1	5.918	3	1.893	-1.654	18	35	2.572	0.000	1.166	0.000	0.000	0.000
75	1-bromopropane	2.52	1.864	1	3.898	1	1.831	-2.377	10	10	1.791	0.000	1.241	0.000	0.000	0.000
77	1-butene	2.68	1.806	0	2.562	1	0.354	-1.917	10	10	1.582	0.000	0.918	0.000	0.000	0.000
81	1-chloronaphthalene	3.50	3.403	1	1.552	0	1.389	2.094	56	140	3.493	0.000	1.233	0.000	0.000	0.000
83	1-chloropropane	2.49	1.719	1	3.529	1	1.864	-0.810	10	10	1.635	0.000	1.241	0.000	0.000	0.000
84	1-decanol	3.86	3.708	1	9.924	9	1.514	-1.224	38	220	3.119	0.000	1.065	0.000	0.000	0.000
85	1-dodecanol	4.17	4.620	1	11.923	11	1.514	-1.160	46	364	3.900	0.000	1.049	0.000	0.000	0.000
87	1-fluorobutane	2.78	1.911	1	3.875	2	1.857	1.716	14	20	1.756	0.000	1.198	0.000	0.000	0.000
90	1-heptanol	2.80	2.339	1	6.925	6	1.597	-1.223	26	84	1.949	0.000	1.099	0.000	0.000	0.000
93	1-hexene	3.23	2.718	0	4.535	3	0.379	-2.084	18	35	2.363	0.000	0.918	0.000	0.000	0.000
94	1-hexyne	2.86	3.294	0	4.226	3	0.581	-2.238	18	35	1.810	0.000	0.954	0.000	0.000	0.000
95	1H-indene-1,3(2H)-dione	1.71	1.325	2	1.154	0	2.704	-9.564	58	137	1.456	0.250	1.379	0.000	0.000	0.000
96	1H-pyrazole	1.45	0.274	1	0.433	0	2.309	0.318	20	15	0.410	0.000	1.530	1.000	0.000	0.000
103	1-naphthalenemethanol	2.22	2.134	1	1.801	2	1.391	9.560	60	182	2.332	0.000	1.220	0.000	0.000	0.000
104	1-naphthol	2.92	2.496	1	1.370	1	1.476	3.848	56	140	2.545	0.000	1.236	0.000	0.000	0.000
108	1-nitropropane	1.85	1.164	2	2.575	1	5.276	5.669	20	32	0.673	0.500	1.669	0.000	0.000	0.000
115	1-phenyl-1-propanone	2.57	2.237	1	2.212	2	2.774	-3.263	44	121	2.279	0.000	1.234	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
116	1-phenyl-2-propanone	2.16	1.595	1	2.212	2	2.701	-7.250	44	126	1.818	0.000	1.234	0.000	0.000	0.000
117	1-phenylethanol	1.57	1.603	1	1.853	2	1.425	-5.339	40	88	1.740	0.000	1.236	0.000	0.000	0.000
118	1-propanol	0.48	0.515	1	2.930	2	1.588	-1.153	10	10	0.389	0.000	1.189	0.000	0.000	0.000
120	1-tridecanol	4.54	5.077	1	12.923	12	1.599	-1.080	50	455	4.290	0.000	1.042	0.000	0.000	0.000
121	1-undecanol	3.95	4.164	1	10.923	10	1.599	-1.138	42	286	3.510	0.000	1.056	0.000	0.000	0.000
123	gamma-hexachlorocyclohexane	3.41	4.163	6	4.436	0	2.573	-1.684	60	174	3.644	0.000	1.585	0.000	0.000	0.000
124	delta-hexachlorocyclohexane	3.30	4.163	6	4.436	0	1.621	0.946	60	174	3.644	0.000	1.585	0.000	0.000	0.000
130	2,2,2-trichloroethanol	2.11	1.240	4	2.525	1	2.634	-2.190	24	28	1.349	0.000	1.891	0.000	0.000	0.000
133	2,2',3,3',4,4'-hexachlorobiphenyl	5.82	7.335	6	4.590	1	0.620	-9.009	94	569	7.274	0.000	1.435	0.000	0.000	0.000
142	2,2',4,4',6,6'-hexachlorobiphenyl	5.64	7.335	6	4.590	1	0.994	-10.82	94	555	7.274	0.000	1.435	0.000	0.000	0.000
143	2,2',4,5,5'-pentachlorobiphenyl	4.80	6.670	5	4.120	1	1.509	-9.521	88	488	6.621	0.000	1.449	0.000	0.000	0.000
148	2,2',6,6'-tetrachlorobiphenyl	4.89	6.006	4	3.657	1	1.012	-15.60	82	394	5.967	0.000	1.435	0.000	0.000	0.000
149	2,2'-biquinoline	4.26	4.578	2	2.458	1	1.369	-15.30	110	818	4.450	0.000	1.248	2.000	0.000	0.000
151	2,2-dimethyl-1-propanol	2.09	1.108	1	1.595	2	1.271	-1.303	24	28	1.025	0.000	1.135	0.000	0.000	0.000
153	2,3,3′,4,4′,5-hexachlorobiphenyl	3.83	7.335	6	4.590	1	0.558	-7.729	94	577	7.274	0.000	1.435	0.000	0.000	0.000
155	2,3,4,5-tetrachloroaniline	3.03	3.741	4	2.761	0	3.162	-12.12	54	140	3.882	0.000	1.788	0.000	0.000	0.000
163	2,3',4'-trichlorobiphenyl	5.21	5.342	3	3.202	1	2.797	-11.99	76	358	5.314	0.000	1.395	0.000	0.000	0.000
164	2,3,4-trichlorophenol	1.96	3.581	4	2.421	1	2.672	-7.828	48	109	3.352	0.000	1.776	0.000	0.000	0.000
166	2,3,5,6-tetrachloro-nitrobenzene	4.05	4.382	6	3.376	0	5.994	-0.183	64	222	4.208	0.500	1.985	0.000	0.000	0.000
167	2,3,5,6-tetrachlorophenol	2.88	4.246	5	2.896	1	1.100	-6.090	54	140	4.006	0.000	1.738	0.000	0.000	0.000
172	2,3,6-trimethylphenol	3.76	3.047	1	1.769	1	0.995	-7.005	48	109	2.317	0.000	1.207	0.000	0.000	0.000
174	2,3-dichlorophenol	2.55	2.917	3	1.958	1	2.922	-8.162	42	82	2.699	0.000	1.738	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
179	2,3-dimethylnaphthalene	3.77	3.711	0	1.613	0	0.855	1.277	62	182	3.457	0.000	1.000	0.000	0.000	0.000
183	2,4,5-trichlorobiphenyl	5.21	5.342	3	3.202	1	1.511	-11.20	76	354	5.314	0.000	1.395	0.000	0.000	0.000
185	2,4,5-trichlorophenol	1.96	3.581	4	2.421	1	1.085	-4.935	48	111	3.352	0.000	1.776	0.000	0.000	0.000
186	2,4,5-trichlorophenoxyacetic acid	1.72	3.288	6	4.162	4	0.656	-0.802	66	318	3.110	0.500	1.873	0.000	0.000	0.000
195	2,4-dichloroaniline	0.67	2.412	2	1.836	0	3.334	-9.415	42	84	2.576	0.000	1.727	0.000	0.000	0.000
200	2,4-dinitrotoluene	2.45	2.105	4	3.129	0	5.994	15.625	78	240	1.811	1.442	1.871	0.000	0.000	0.000
201	2,4-xylenol	2.66	2.560	1	1.536	1	1.207	-6.243	42	84	2.009	0.000	1.236	0.000	0.000	0.000
203	2,5-dichlorobiphenyl	4.70	4.677	2	2.758	1	0.563	-10.76	70	293	4.660	0.000	1.322	0.000	0.000	0.000
208	2,6-dichloro-4-nitroaniline	3.00	2.307	4	2.516	0	9.023	2.861	58	188	2.484	0.500	2.156	0.000	0.000	0.000
210	2,6-dichlorobenzamide	0.53	2.161	3	2.368	1	4.402	-7.677	52	144	2.092	0.000	1.921	0.000	0.000	0.000
213	2,6-dichlorophenol	2.55	2.917	3	1.958	1	2.077	-5.941	42	82	2.699	0.000	1.738	0.000	0.000	0.000
217	2,6-dinitro-N-propyl-4-(trifluoromethyl)aniline	3.61	3.242	7	4.735	3	2.033	5.822	98	760	3.344	1.442	2.109	0.000	0.000	0.000
222	2-anthracenamine	4.48	2.900	0	1.655	0	3.013	-13.64	82	342	3.575	0.000	1.187	0.000	0.000	0.000
223	2-bromo-4-chlorophenol	2.60	3.001	3	2.110	1	2.131	-6.840	42	84	2.808	0.000	1.892	0.000	0.000	0.000
225	2-bromo-5-methylaniline	1.96	2.318	1	1.762	0	2.168	-10.85	42	84	2.340	0.000	1.520	0.000	0.000	0.000
230	2-chloro-2-methylbutane	2.75	2.302	1	1.921	1	1.881	-0.481	24	28	2.414	0.000	1.166	0.000	0.000	1.000
231	2-chlorobenzamide	1.51	1.497	2	1.921	1	3.946	-5.170	46	114	1.439	0.000	1.802	0.000	0.000	0.000
237	2-chlorophenyl urea	1.61	1.405	2	2.332	2	3.905	-5.693	50	158	1.831	0.000	1.875	0.000	0.000	0.000
242	2-ethyl butyric acid	2.29	1.837	2	3.443	4	1.697	2.033	30	67	1.507	0.500	1.295	0.000	0.000	1.000
244	2-ethyl-m-xylene	3.71	3.745	0	2.103	1	1.548	-6.565	46	112	2.866	0.000	0.980	0.000	0.000	0.000
245	2-ethylnaphthalene	3.76	3.681	0	1.826	1	0.623	0.933	60	190	3.402	0.000	1.000	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
247	2-fluorophenyl urea	1.31	0.946	2	2.056	2	3.920	-3.780	50	158	1.316	0.000	1.875	0.000	0.000	0.000
248	2H-1-benzopyran-2-one	2.13	1.900	2	1.333	0	4.702	2.267	56	144	1.793	0.000	1.379	1.000	0.000	0.000
249	2-heptanol	2.63	2.261	1	5.078	5	1.593	-3.694	28	79	1.948	0.000	1.099	0.000	0.000	0.000
254	2-hydroxy-3-methyl-1,4-naphthalenedione	2.03	1.667	3	1.824	1	1.282	-1.759	74	263	1.898	0.766	1.423	0.000	0.000	0.000
259	2-methoxyethanol	0.96	-0.489	2	3.857	3	0.227	-2.145	14	20	-0.375	0.000	1.335	0.000	0.000	0.000
260	2-methoxyphenol or guaiacol	1.60	1.572	2	1.822	2	2.020	-6.790	40	86	1.401	0.000	1.402	0.000	0.000	0.000
261	2-methyl-1,4-naphthalenedione	2.57	2.204	2	1.621	0	0.704	-1.458	68	218	2.012	0.200	1.342	0.000	0.000	0.000
265	2-methylanthracene	4.18	4.133	0	1.751	0	0.520	-7.112	82	342	4.301	0.000	0.991	0.000	0.000	0.000
273	2-methylthiophene	2.65	1.410	1	0.926	0	0.361	-2.516	26	26	2.057	0.000	1.325	1.000	0.000	0.000
283	2-phenyl-1H-indene-1,3(2H)-dione	2.96	2.820	2	2.149	1	2.594	-17.69	92	473	2.849	0.250	1.280	0.000	0.000	1.000
284	2-phenylacetophenone	3.11	3.269	1	2.934	3	3.034	-8.915	72	394	3.112	0.000	1.187	0.000	0.000	0.000
296	3-(3-chlorophenyl)-1-methylurea	1.93	1.611	2	2.936	3	4.143	-12.13	54	211	2.091	0.000	1.796	0.000	0.000	0.000
299	3-(4-chlorophenyl)-1-methoxy-1-methylurea	1.84	1.663	3	3.734	4	5.095	-6.974	64	333	2.365	0.000	1.821	0.000	0.000	0.000
304	3-(trifluoromethyl)aniline	2.36	2.026	3	1.762	0	4.221	-10.70	54	148	2.288	0.000	1.739	0.000	0.000	0.000
307	3,3',4,4'-tetrachlorobiphenyl	5.00	6.006	4	3.657	1	0.603	-5.523	82	440	5.967	0.000	1.435	0.000	0.000	0.000
314	3,4-dichloroaniline	0.67	2.412	2	1.836	0	4.402	-12.54	42	84	2.576	0.000	1.727	0.000	0.000	0.000
320	3,4-dinitrotoluene	2.51	2.105	4	2.450	0	9.964	-1.038	62	234	1.811	1.629	1.871	0.000	0.000	0.000
321	3,4-xylenol	2.66	2.560	1	1.536	1	1.484	-5.850	42	84	2.009	0.000	1.236	0.000	0.000	0.000
325	3,5-dinitroaniline	2.55	0.872	4	2.309	0	8.476	10.044	62	240	1.085	1.442	1.955	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
331	3-aminonitrobenzene	1.73	0.978	2	1.639	0	7.964	-2.764	46	117	1.177	0.500	1.811	0.000	0.000	0.000
336	3-bromoacetanilide	2.01	1.699	2	2.653	2	3.446	-14.90	50	162	2.408	0.000	1.722	0.000	0.000	0.000
337	3-bromobenzoic acid	2.94	2.208	3	2.189	2	1.564	-2.526	46	117	2.147	0.500	1.689	0.000	0.000	0.000
341	3-chloro-4-methoxyacetanilde	1.95	2.101	2	3.280	2	3.375	-13.27	60	205	2.607	0.000	1.653	0.000	0.000	0.000
343	3-chloroacetanilide	1.86	1.615	2	2.493	2	3.503	-12.0	50	162	2.298	0.000	1.722	0.000	0.000	0.000
346	3-chlorophenol	2.54	2.252	2	1.512	1	2.227	-5.661	36	61	2.046	0.000	1.614	0.000	0.000	0.000
353	3-hexanol	2.28	1.872	1	4.104	4	1.755	0.756	24	50	1.557	0.000	1.116	0.000	0.000	0.000
357	3-methoxyphenylcarbamate	1.44	-0.122	3	2.790	2	12.157	-5.568	54	209	0.450	0.500	1.684	0.000	0.000	0.000
359	3-methyl-2-butanol	2.07	1.211	1	2.175	2	1.700	-2.685	22	29	1.023	0.000	1.135	0.000	0.000	1.000
360	3-methyl-2-nitrophenol	2.61	1.969	3	1.977	1	7.087	-0.539	52	144	1.609	0.945	1.722	0.000	0.000	0.000
364	3-methyl-4-fluorophenylurea	1.75	1.432	2	2.279	2	3.927	-0.318	56	205	1.625	0.000	1.796	0.000	0.000	0.000
367	3-methylaniline	1.65	1.570	0	1.203	0	2.037	-9.893	36	61	1.577	0.000	1.253	0.000	0.000	0.000
376	3-nitroacetanilide	1.94	0.845	3	2.709	2	7.953	-4.192	60	258	1.553	0.651	1.785	0.000	0.000	0.000
379	3-pentanol	2.04	1.416	1	3.141	3	1.759	-0.213	20	31	1.167	0.000	1.135	0.000	0.000	0.000
384	3-phenyl-1-methylurea	1.29	0.946	1	2.491	3	3.560	-9.936	48	168	1.438	0.000	1.572	0.000	0.000	0.000
389	4-(trifluoromethyl)aniline	2.36	2.026	3	1.762	0	5.171	-12.33	54	152	2.288	0.000	1.739	0.000	0.000	0.000
392	4,4'-dimethylbiphenyl	4.15	4.321	0	2.361	1	0.653	-14.69	70	315	3.970	0.000	1.000	0.000	0.000	0.000
396	4-bromo-2-chlorophenol	2.60	3.001	3	2.110	1	1.984	-5.498	42	84	2.808	0.000	1.892	0.000	0.000	0.000
400	4-bromoaminobenzene	2.42	2.296	1	1.916	1	1.618	-8.403	34	64	2.408	0.000	1.592	0.000	0.000	0.000
401	4-bromoaniline	1.96	1.832	1	1.534	0	3.846	-13.90	36	62	2.031	0.000	1.592	0.000	0.000	0.000
402	4-bromobenzoic acid	2.93	2.208	3	2.189	2	1.509	-1.823	46	120	2.147	0.500	1.689	0.000	0.000	0.000
413	4-ethyl-o-xylene	3.83	3.745	0	2.103	1	0.579	-7.458	46	117	2.866	0.000	0.980	0.000	0.000	0.000
419	4-hydroxybenzoic acid	1.43	1.218	3	1.798	3	1.816	-3.133	46	120	1.090	0.721	1.505	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
422	4-methoxyacetanilide	1.40	0.934	2	2.824	3	3.450	-12.08	54	217	1.654	0.000	1.542	0.000	0.000	0.000
433	4-methylbenzenemethanol	2.24	1.712	1	1.853	2	1.263	-8.282	40	90	1.487	0.000	1.236	0.000	0.000	0.000
435	4-methylbiphenyl	3.90	3.835	0	2.133	1	0.715	-12.66	64	252	3.662	0.000	0.999	0.000	0.000	0.000
436	4-methyl-N-(1,1-dimethyl-2-propynyl)benzamide	1.76	3.299	1	3.159	4	3.347	-9.938	72	388	2.137	0.000	1.350	0.000	0.000	1.000
439	4-methylpyridine	2.04	1.166	1	1.069	0	2.584	-2.867	30	42	1.390	0.000	1.296	1.000	0.000	0.000
442	4-nitrobenzoic acid	1.54	1.354	4	2.272	2	4.481	9.324	56	206	1.293	1.301	1.778	0.000	0.000	0.000
443	4-nitrophenol	2.37	1.482	3	1.749	1	6.548	4.186	46	120	1.300	0.721	1.782	0.000	0.000	0.000
444	4-octanol	2.84	2.784	1	6.059	6	1.691	0.247	32	108	2.338	0.000	1.086	0.000	0.000	0.000
445	4-phenoxyphenylurea	2.56	2.301	2	3.373	4	4.128	0.366	82	598	2.970	0.000	1.578	0.000	0.000	0.000
447	4-phenylpyridine	2.79	2.198	1	1.866	1	2.558	-4.895	58	198	2.749	0.000	1.222	1.000	0.000	0.000
448	4-propylphenol	3.12	2.987	1	2.459	3	1.563	-5.216	44	127	2.345	0.000	1.207	0.000	0.000	0.000
450	5,8,11,14-eicosatetraenoic acid	5.17	6.439	2	16.51	15	2.109	7.984	84	1752	6.217	0.500	1.154	0.000	0.000	0.000
455	5-methyl-2-hexanone	2.40	1.727	1	3.495	3	2.996	4.788	30	74	2.012	0.000	1.143	0.000	0.000	1.000
456	5-methyl-2-nitrophenol	2.61	1.969	3	1.977	1	8.483	1.246	52	150	1.609	0.945	1.722	0.000	0.000	0.000
457	5-methyl-2-octanone	2.97	2.639	1	5.275	5	2.988	4.811	38	143	2.792	0.000	1.108	0.000	0.000	1.000
461	8-hydroxyquinoline	5.29	1.774	2	1.333	1	2.708	-6.529	56	140	1.940	0.000	1.493	1.000	0.000	0.000
465	9H-fluoren-9-one	3.43	2.923	1	1.367	0	3.201	-5.439	78	262	2.898	0.000	1.182	0.000	0.000	0.000
466	9-methylanthracene	3.33	4.133	0	1.751	0	0.410	-5.148	82	326	4.301	0.000	0.991	0.000	0.000	0.000
467	acenaphthene	4.14	3.339	0	1.092	0	0.949	-11.16	68	166	2.938	0.000	0.994	0.000	0.000	0.000
468	acephate	3.53	-0.097	4	4.012	4	9.856	-0.949	42	122	1.240	0.250	2.023	0.000	0.000	0.000
470	acetaldehyde	1.83	-0.183	1	1.486	0	2.578	1.227	6	4	0.205	0.000	1.379	0.000	0.000	0.000
473	acetic acid	2.01	-0.205	2	0.917	1	1.667	1.135	12	9	0.091	0.500	1.500	0.000	0.000	0.000

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480	acifluorfen	1.58	4.521	9	4.994	4	3.999	16.94	124	1421	4.758	1.629	2.073	0.000	0.000	0.000
483	acrylamide	1.37	-0.135	1	1.281	1	0.827	0.654	16	18	-0.342	0.000	1.685	0.000	0.000	0.000
485	acrylonitrile	1.57	0.742	1	1.801	1	3.164	3.350	10	10	0.696	0.000	1.449	0.000	0.000	0.000
487	adiponitrile	1.42	1.051	2	5.218	5	0.000	18.035	26	84	1.594	0.000	1.406	0.000	0.000	0.000
490	aldicarb sulfone	1.30	0.152	5	4.210	5	4.420	14.661	64	337	0.151	0.651	1.845	0.000	0.000	1.000
493	allene	4.69	1.242	0	1.277	0	0.000	4.959	6	4	0.957	0.000	0.985	0.000	0.000	0.000
495	allyl alcohol	1.91	0.259	1	2.498	2	1.526	-2.502	10	10	0.165	0.000	1.295	0.000	0.000	0.000
502	amphetamine	2.00	1.635	1	2.459	2	2.050	-4.378	44	126	1.576	0.000	1.192	0.000	0.000	0.000
508	anthracene-9-carboxylic acid	3.86	3.277	2	2.165	2	5.169	-3.804	92	452	3.691	0.500	1.280	0.000	0.000	0.000
509	anthraquinone	2.74	2.808	2	1.772	0	1.590	-8.469	88	378	2.462	0.200	1.281	0.000	0.000	0.000
512	atrazine	2.48	2.536	4	3.882	4	3.346	-10.37	64	319	1.777	0.000	1.632	1.000	0.000	0.000
515	azinphos ethyl	3.17	3.996	7	5.523	7	10.297	-35.73	104	976	2.780	0.000	2.006	1.000	0.000	0.000
516	azobenzene	2.69	4.199	2	2.666	2	0.557	-12.94	66	343	4.102	0.000	1.325	0.000	0.000	0.000
519	bendiocarb	1.34	1.479	4	2.670	3	3.894	-7.896	84	425	1.912	0.000	1.611	1.000	0.000	0.000
520	benfluralin	2.76	4.401	7	6.160	5	2.226	-4.149	112	1098	4.148	1.442	1.962	0.000	0.000	0.000
522	bensulfuron-methyl	3.28	1.748	9	7.115	10	9.724	11.393	138	2240	0.932	1.310	1.899	1.000	0.000	0.000
524	bentazone	3.00	0.677	3	2.381	1	6.391	-10.84	86	382	1.207	0.945	1.843	1.000	0.000	0.000
525	benz[a]anthracene	1.53	4.555	0	1.920	0	0.264	-19.88	102	553	5.146	0.000	0.971	0.000	0.000	0.000
527	benzaldehyde	2.50	1.589	1	1.424	1	2.890	-2.313	34	64	1.499	0.000	1.296	0.000	0.000	0.000
528	benzaldoxime-N-methylcarbamate	2.18	1.662	3	3.657	4	3.125	-12.71	56	296	1.377	0.000	1.665	0.000	0.000	0.000
529	benzamide	1.80	0.832	1	1.492	1	3.464	-6.208	40	88	0.786	0.000	1.544	0.000	0.000	0.000
535	benzenepropanenitrile	2.14	2.200	1	2.513	3	2.921	3.835	42	133	2.143	0.000	1.245	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
536	benzenepropanol	2.31	2.003	1	2.966	4	1.611	-5.698	42	133	1.612	0.000	1.207	0.000	0.000	0.000
539	benzofuran	5.13	2.134	1	0.833	0	0.867	-3.792	46	79	2.433	0.000	1.273	1.000	0.000	0.000
540	benzoic acid	2.83	1.460	2	1.605	2	2.472	-3.883	40	88	1.385	0.500	1.429	0.000	0.000	0.000
541	benzonitrile	1.95	1.709	1	1.294	1	3.548	-0.528	34	64	1.558	0.000	1.296	0.000	0.000	0.000
544	benzothiophene	2.47	2.464	1	1.028	0	0.417	0.274	46	79	2.901	0.000	1.273	1.000	0.000	0.000
555	Bifenthrin	1.69	6.369	6	5.927	6	6.041	-9.008	156	2490	6.662	0.000	1.576	0.000	0.000	2.000
559	bisphenol a	1.99	3.779	2	3.007	4	2.468	-7.754	88	516	3.424	0.100	1.269	0.000	0.000	0.000
562	bromoacetic acid	1.97	0.473	3	2.405	2	0.627	2.070	16	18	0.466	0.500	1.906	0.000	0.000	0.000
567	bromofenoxim	2.25	4.503	9	5.986	4	8.057	39.043	120	1498	4.147	1.576	2.050	0.000	0.000	0.000
568	bromoform	0.33	2.229	3	3.625	0	1.159	0.071	12	9	2.455	0.000	1.371	0.000	0.000	0.000
569	bromotrifluoromethane	2.67	2.833	4	1.224	0	0.896	1.421	20	16	1.901	0.000	1.371	0.000	0.000	0.000
572	butachlor	2.23	4.754	3	8.396	10	5.975	-13.16	94	936	4.157	0.000	1.433	0.000	0.000	0.000
574	butane	1.26	2.196	0	3.000	1	0.000	-0.922	10	10	1.806	0.000	0.863	0.000	0.000	0.000
575	butralin	2.95	4.078	4	5.138	4	6.481	-0.702	104	860	4.011	1.442	1.623	0.000	0.000	0.000
578	butyl benzoate	2.66	3.014	2	4.194	5	2.099	-8.704	56	284	2.644	0.000	1.297	0.000	0.000	0.000
586	butyranilde	1.86	2.485	1	4.174	5	3.868	-16.67	62	316	2.840	0.000	1.325	0.000	0.000	0.000
587	butyric acid	1.71	0.919	2	2.670	3	1.922	2.117	20	32	0.871	0.500	1.379	0.000	0.000	0.000
591	carbaryl	2.30	2.502	2	2.649	3	3.831	6.820	74	362	2.558	0.000	1.505	0.000	0.000	0.000
597	carbon tetrachloride	3.24	3.585	4	2.146	0	0.002	0.001	20	16	2.553	0.000	0.722	0.000	0.000	0.000
599	carbophenothion methyl	2.02	4.503	6	6.588	6	3.601	-0.160	74	510	4.640	0.000	2.011	0.000	0.000	0.000
600	carbophenothion	4.66	5.200	6	8.118	8	4.035	-0.410	82	708	5.420	0.000	1.887	0.000	0.000	0.000
604	chloramben	1.25	2.042	4	2.569	2	4.427	-7.466	58	184	2.274	0.500	2.013	0.000	0.000	0.000
611	chlorimuron ethyl	2.04	2.441	9	6.797	9	7.896	-11.25	134	1958	1.826	1.424	2.042	1.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
612	chlornidine	3.94	2.354	3	2.794	2	3.416	-14.49	70	301	2.364	0.000	1.749	1.000	0.000	0.000
613	chloroacetic acid	1.50	0.328	3	2.140	2	0.539	2.265	16	18	0.310	0.500	1.906	0.000	0.000	0.000
615	chlorobenzilate	3.30	4.292	5	5.012	6	1.149	5.088	106	876	3.792	0.333	1.585	0.000	0.000	1.000
617	chlorofluoromethane	1.65	0.775	2	2.383	0	1.798	0.422	6	4	1.152	0.000	1.922	0.000	0.000	0.000
622	chlorotoluron	2.43	2.303	2	3.359	3	3.866	-14.39	66	321	2.742	0.000	1.669	0.000	0.000	0.000
629	chlor-thiamide	2.26	3.060	3	2.708	1	4.973	-8.159	52	144	2.628	0.000	1.921	0.000	0.000	0.000
630	chrysene	4.49	4.555	0	1.920	0	0.001	-19.76	102	545	5.146	0.000	0.971	0.000	0.000	0.000
635	cis-1,2-dichloroethylene	2.39	1.057	2	3.586	0	4.809	1.557	10	10	1.935	0.000	1.585	0.000	0.000	0.000
642	citric acid	0.44	-1.319	7	3.820	9	2.562	-0.229	58	246	-1.248	5.065	1.575	0.000	0.000	1.000
650	cycloheptane	3.55	3.193	0	2.249	0	0.013	0.053	28	42	2.731	0.000	0.918	0.000	0.000	0.000
658	cyclopentane	3.01	2.281	0	0.922	0	0.023	-0.384	20	15	1.951	0.000	0.918	0.000	0.000	0.000
661	cyhalothrin	5.26	5.791	8	6.557	8	7.101	-23.28	164	2982	6.544	0.000	1.759	0.000	0.000	2.000
666	DCPA	3.70	4.198	8	5.399	4	2.041	-7.402	88	555	3.873	0.143	1.888	0.000	0.000	0.000
667	decachlorobiphenyl	5.87	9.992	10	6.521	1	1.003	-12.53	118	907	9.888	0.000	0.994	0.000	0.000	0.000
668	decane	4.78	4.934	0	9.000	7	0.000	-2.698	34	165	4.147	0.000	0.896	0.000	0.000	0.000
669	decanoic acid	3.60	3.656	2	8.455	9	2.009	6.722	44	277	3.212	0.500	1.198	0.000	0.000	0.000
670	decylbenzene	5.38	6.422	0	7.844	9	0.631	-5.747	66	612	5.370	0.000	0.959	0.000	0.000	0.000
673	di-2-ethaylhexyl phthalate	4.94	7.574	4	12.674	16	2.388	-16.30	124	2388	6.433	0.200	1.234	0.000	0.000	2.000
680	dibenzyl ether	3.18	3.218	1	3.526	4	1.372	-11.73	70	436	3.403	0.000	1.182	0.000	0.000	0.000
690	dichloromethane	2.06	1.496	2	3.079	0	1.478	-1.962	6	4	1.734	0.000	1.522	0.000	0.000	0.000
693	dichlorvos	1.67	1.033	6	3.732	4	7.905	9.881	38	168	2.680	0.000	2.078	0.000	0.000	0.000
697	Dicrotofos (trans)	1.66	0.136	5	4.290	6	7.835	19.526	58	400	1.396	0.167	1.741	0.000	0.000	0.000
699	dicumyl peroxide	4.37	5.370	2	4.264	5	0.469	-3.035	102	848	4.805	0.000	1.222	0.000	0.000	2.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
705	diethyl ketone	1.82	1.230	1	2.726	2	2.781	1.424	20	31	1.376	0.000	1.198	0.000	0.000	0.000
707	diethyl oxalate	1.68	0.720	4	4.702	5	0.000	-2.304	38	135	0.113	0.333	1.485	0.000	0.000	0.000
713	diethylamine	1.69	0.482	1	3.928	2	1.113	-1.906	14	20	0.616	0.000	1.122	0.000	0.000	0.000
716	diethylene glycol dimethyl ether	1.18	-0.211	3	7.775	6	1.515	-4.727	30	120	0.296	0.000	1.325	0.000	0.000	0.000
718	diflubenzoron	4.06	3.665	5	4.493	5	5.645	-5.126	104	1020	3.580	0.250	1.979	0.000	0.000	0.000
719	difluoromethane	1.49	0.477	2	1.773	0	1.939	1.630	6	4	0.883	0.000	1.522	0.000	0.000	0.000
720	diiodomethane	2.74	2.300	2	5.144	0	0.204	-4.460	6	4	1.814	0.000	1.522	0.000	0.000	0.000
723	diisopropyl ether	2.20	1.503	1	3.010	2	2.558	2.075	26	48	1.820	0.000	1.116	0.000	0.000	0.000
724	diisopropylamine	2.14	1.237	1	3.010	2	2.013	1.612	26	48	1.393	0.000	1.091	0.000	0.000	0.000
732	dimethyl sulfoxide	0.64	-0.317	1	1.522	0	3.777	3.558	12	9	-0.005	0.000	1.571	0.000	0.000	0.000
733	dimethyl terephthalate	2.60	1.541	4	3.502	4	2.282	-1.051	64	327	1.260	0.143	1.483	0.000	0.000	0.000
736	di-n-butyl phthalate	3.14	4.198	4	7.766	10	2.314	-15.44	88	912	3.600	0.200	1.342	0.000	0.000	0.000
742	diphenyl ether	3.67	3.390	1	2.390	2	1.635	-2.011	62	264	3.479	0.000	1.209	0.000	0.000	0.000
743	diphenyl sulfide	3.80	3.948	1	2.579	2	1.714	-3.289	62	264	3.838	0.000	1.209	0.000	0.000	0.000
746	diphenylmethane	3.63	3.805	0	2.419	2	0.383	-6.954	62	264	3.277	0.000	0.999	0.000	0.000	0.000
748	dipropetryn	3.07	3.469	4	5.343	6	3.006	-10.12	78	546	2.624	0.000	1.514	1.000	0.000	0.000
749	dipropyl ether	2.48	1.796	1	5.926	4	1.343	-3.167	22	56	1.823	0.000	1.116	0.000	0.000	0.000
755	DNOC	1.81	1.863	5	2.654	1	5.204	15.407	68	286	1.517	2.252	1.883	0.000	0.000	0.000
759	Dowco275	2.41	3.357	6	5.445	6	7.049	-11.25	74	456	2.897	0.000	2.051	1.000	0.000	0.000
764	Endrin	4.20	3.407	7	2.179	0	1.131	5.357	134	520	4.481	0.000	1.698	1.000	1.000	6.000
766	EPN	3.12	4.164	5	5.334	5	3.796	-26.19	104	966	3.645	0.500	1.855	0.000	0.000	0.000
771	ethane	2.36	1.284	0	0.000	0	0.000	-0.344	2	1	1.026	0.000	0.811	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
775	ethyl acetate	1.77	0.370	2	2.670	2	1.666	-0.397	20	32	0.569	0.000	1.379	0.000	0.000	0.000
776	ethyl acetoacetate	1.51	0.281	3	3.879	4	2.616	7.651	34	102	0.529	0.250	1.433	0.000	0.000	0.000
784	ethyl hexanoate	2.06	2.405	2	6.496	6	1.936	0.536	36	150	2.130	0.000	1.239	0.000	0.000	0.000
786	ethyl methacrylate	2.43	1.514	2	3.116	3	1.687	-3.574	30	70	1.126	0.000	1.352	0.000	0.000	0.000
792	ethyl vinyl ether	1.94	0.670	1	3.478	2	1.762	-3.084	14	20	1.166	0.000	1.239	0.000	0.000	0.000
798	ethylbenzene	2.73	2.772	0	1.680	1	0.558	-5.773	34	64	2.249	0.000	0.991	0.000	0.000	0.000
802	ethylenediamine	0.27	-1.477	2	2.862	1	2.352	-0.994	10	10	-1.096	0.000	1.252	0.000	0.000	0.000
804	ethynylbenzene	2.68	2.957	0	1.344	1	0.380	-7.105	34	64	1.668	0.000	0.985	0.000	0.000	0.000
805	etridiazole	3.00	3.042	7	3.548	2	2.652	-0.772	58	204	2.764	0.000	2.324	1.000	0.000	0.000
810	fenarimol	2.78	3.828	5	3.996	4	3.327	16.026	116	942	4.068	0.000	1.661	1.000	0.000	1.000
814	fenoxaprop-P	3.65	4.071	7	4.402	6	1.663	-0.722	120	1391	4.125	0.500	1.740	1.000	0.000	0.000
817	fensulfothion	2.52	2.812	5	5.238	7	5.396	24.238	76	661	3.100	0.000	1.771	0.000	0.000	0.000
818	fensulfothion sulfide	3.18	3.923	5	5.122	7	2.916	-1.648	70	562	4.085	0.000	1.726	0.000	0.000	0.000
822	fenvalerate	3.72	6.565	5	7.372	9	2.325	26.994	150	2659	6.680	0.000	1.490	0.000	0.000	2.000
823	fipronil	3.08	5.579	11	5.195	3	7.145	-4.994	140	1575	4.279	0.000	2.356	1.000	0.000	0.000
825	fluchloralin	3.55	4.261	8	6.420	5	1.996	1.725	112	1082	3.977	1.442	2.152	0.000	0.000	0.000
826	flucythrinate	5.00	6.706	7	8.386	11	2.803	33.340	164	3560	6.628	0.000	1.589	0.000	0.000	2.000
827	flumetralin	4.00	5.526	9	6.320	4	1.527	-6.905	144	1865	5.341	1.442	2.128	0.000	0.000	0.000
828	fluometuron	1.96	2.095	4	3.413	3	4.764	-13.59	78	457	2.799	0.000	1.865	0.000	0.000	0.000
835	fluvalinate	6.00	7.289	8	8.410	10	4.178	8.630	186	4160	7.396	0.000	1.766	0.000	0.000	1.000
841	formic acid	1.08	-0.283	2	1.429	1	1.097	1.746	6	4	-0.299	0.500	1.522	0.000	0.000	0.000
842	fumaric acid	1.63	0.039	4	2.679	4	0.000	0.732	30	74	-0.288	1.629	1.585	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
843	furan	2.11	0.934	1	0.468	0	0.450	-0.994	20	15	1.280	0.000	1.392	1.000	0.000	0.000
844	furfural	1.60	0.985	2	0.941	1	3.594	1.496	30	43	1.092	0.000	1.495	1.000	0.000	0.000
852	glyphosate	3.46	-1.516	6	3.700	7	5.155	-5.756	42	139	-1.204	2.586	1.927	0.000	0.000	0.000
854	GS-39985	3.23	3.955	8	6.263	5	3.246	5.335	132	1522	3.917	1.442	1.942	1.000	0.000	0.000
855	halothane	2.63	2.509	5	2.396	0	1.364	2.316	30	42	2.508	0.000	2.156	0.000	0.000	0.000
861	hexachlorocyclopentadiene	4.12	3.498	6	2.971	0	0.501	-5.030	58	132	4.552	0.000	0.994	0.000	0.000	0.000
865	hexafluoroacetone	2.17	2.072	7	1.975	0	0.115	-2.224	48	111	1.680	0.000	1.295	0.000	0.000	0.000
867	hexafluoroethane	2.47	2.196	6	1.448	0	0.000	0.003	38	58	2.111	0.000	0.811	0.000	0.000	0.000
874	hexanoic acid	2.42	1.831	2	4.560	5	1.977	3.480	28	79	1.651	0.500	1.295	0.000	0.000	0.000
876	hexylamine	2.50	1.594	1	5.926	4	1.497	-1.360	22	56	1.525	0.000	1.091	0.000	0.000	0.000
878	hexythiazox	3.79	5.417	4	5.614	4	3.594	-17.96	124	1238	4.981	0.250	1.693	1.000	0.000	0.000
881	hydroxycaproic acid	1.82	0.605	3	5.461	7	1.758	5.058	32	114	0.624	0.651	1.379	0.000	0.000	0.000
882	imazalil	3.73	3.350	4	5.586	6	5.730	-22.40	96	721	4.134	0.000	1.693	1.000	0.000	0.000
889	indole	2.54	2.124	0	0.833	0	1.871	-10.01	46	79	2.168	0.000	1.272	1.000	0.000	0.000
894	iprodione	2.85	3.808	5	4.389	4	5.775	-5.905	108	915	2.880	0.696	1.919	1.000	0.000	0.000
895	isazofos	2.01	3.471	7	6.170	7	5.395	-5.022	86	630	3.189	0.000	2.057	1.000	0.000	0.000
898	isobutyl acetate	2.35	1.213	2	3.443	3	1.689	-0.257	30	74	1.206	0.000	1.295	0.000	0.000	1.000
899	isobutyl acrylate	2.59	1.911	2	3.970	4	2.466	-2.506	34	104	1.372	0.000	1.313	0.000	0.000	1.000
901	isobutylbenzene	3.56	3.480	0	2.494	2	0.514	-5.725	44	126	2.885	0.000	0.980	0.000	0.000	1.000
906	isophorone	2.30	2.196	1	1.672	0	3.890	2.894	50	109	2.322	0.000	1.175	0.000	0.000	0.000
910	isopropyl alcohol	1.40	0.368	1	1.285	1	1.611	-2.894	12	9	0.387	0.000	1.189	0.000	0.000	0.000
913	isopropylamine	1.52	0.079	1	1.285	0	1.441	0.671	12	9	0.354	0.000	1.140	0.000	0.000	0.000
914	isoproturon	2.35	2.346	1	3.718	4	3.130	-5.297	70	408	2.904	0.000	1.406	0.000	0.000	1.000

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916	isouron	2.47	1.837	3	3.021	4	3.180	-13.57	74	391	2.066	0.000	1.579	1.000	0.000	0.000
917	isoxaben	2.40	3.902	5	5.746	8	7.958	-19.20	120	1387	4.022	0.000	1.520	1.000	0.000	0.000
918	lactic acid	0.99	-0.392	3	1.764	3	3.203	0.972	22	29	-0.548	1.145	1.500	0.000	0.000	0.000
923	linoleic acid	5.21	6.416	2	15.446	15	1.489	8.351	76	1313	5.885	0.500	1.142	0.000	0.000	0.000
942	m-difluorobenzene	2.58	2.241	2	1.242	0	1.537	-1.600	36	61	1.965	0.000	1.459	0.000	0.000	0.000
948	metaldehyde	2.38	0.118	4	3.460	0	0.451	-8.831	56	188	1.450	0.000	1.379	1.000	0.000	0.000
949	metamitron	1.55	0.533	4	2.305	1	3.402	-6.994	76	352	0.328	0.000	1.666	1.000	0.000	0.000
951	methacrylic acid	1.88	0.940	2	1.540	2	1.945	-1.022	22	29	0.647	0.500	1.459	0.000	0.000	0.000
953	methamidophos	0.70	-0.087	4	2.916	2	5.471	-0.321	28	44	1.063	0.000	2.040	0.000	0.000	0.000
955	methazole	3.48	3.248	5	2.752	1	2.229	-7.772	84	422	1.436	0.250	2.060	1.000	0.000	0.000
957	methiocarb	2.25	3.108	3	4.054	4	4.219	-14.17	70	380	2.744	0.000	1.618	0.000	0.000	0.000
963	methyl alcohol	0.97	-0.358	1	0.000	0	1.624	-0.852	2	1	-0.392	0.000	1.252	0.000	0.000	0.000
966	methyl butanoate	2.08	1.144	2	3.606	3	1.765	0.715	24	50	0.960	0.000	1.333	0.000	0.000	0.000
969	methyl cyanoacetate	1.12	0.081	3	2.899	3	1.415	5.406	24	50	0.073	0.000	1.784	0.000	0.000	0.000
977	Methyl isothiocyanate	0.78	1.013	2	2.660	0	2.071	-0.418	10	10	0.719	0.000	1.842	0.000	0.000	0.000
978	methyl methacrylate	2.13	1.165	2	2.300	2	1.686	-2.434	26	46	0.736	0.000	1.400	0.000	0.000	0.000
979	methyl parathion	2.64	2.578	6	4.667	4	7.458	26.278	76	473	2.491	0.500	2.053	0.000	0.000	0.000
982	methyl propyl ketone	1.83	1.019	1	2.726	2	2.910	2.843	20	32	1.376	0.000	1.198	0.000	0.000	0.000
985	methylacetylene	1.89	1.925	0	1.331	0	0.407	-2.102	6	4	0.640	0.000	0.985	0.000	0.000	0.000
991	methyl-n-(3,4-dichlorophenyl)carbamate	2.74	2.922	4	3.539	3	3.161	-13.38	60	262	3.172	0.000	1.939	0.000	0.000	0.000
992	methyl-n-(3-chlorophenyl)carbamate	2.15	2.258	3	3.077	3	2.358	-13.58	54	211	2.518	0.000	1.822	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
995	m-ethyltoluene	3.54	3.259	0	1.884	1	0.634	-6.515	40	88	2.557	0.000	0.985	0.000	0.000	0.000
998	metoxuron	1.72	1.800	3	3.938	4	4.626	-15.93	70	394	2.442	0.000	1.760	0.000	0.000	0.000
999	metribuzin	1.71	1.606	5	2.944	2	1.579	-6.003	62	284	0.372	0.000	1.761	1.000	0.000	0.000
1002	mevinphos (trans)	2.30	0.578	6	5.831	6	6.234	3.791	60	332	1.481	0.167	1.671	0.000	0.000	0.000
1005	m-nitrotoluene	2.71	2.211	2	1.777	0	6.805	1.132	46	117	1.903	0.500	1.658	0.000	0.000	0.000
1009	monolinuron	2.10	1.663	3	3.734	4	5.094	-6.970	64	333	2.365	0.000	1.821	0.000	0.000	0.000
1016	m-toluidine	1.74	1.570	0	1.203	0	2.037	-9.893	36	61	1.577	0.000	1.253	0.000	0.000	0.000
1022	N,N-dimethylbenzamide	1.80	1.244	1	2.261	2	3.529	-4.296	50	156	1.388	0.000	1.433	0.000	0.000	0.000
1029	napropamide	2.54	3.170	2	4.745	6	3.387	5.355	98	832	3.476	0.000	1.364	0.000	0.000	0.000
1036	nitrapyrin	2.24	3.514	5	2.870	0	3.499	-6.266	54	148	3.562	0.000	1.788	1.000	0.000	0.000
1038	nitroethane	1.48	0.640	2	1.679	0	5.043	3.699	16	18	0.283	0.500	1.761	0.000	0.000	0.000
1039	nitroglycerine	2.26	0.078	9	6.267	5	4.506	-10.30	62	424	-1.020	2.657	1.839	0.000	0.000	0.000
1040	nitromethane	1.20	0.291	2	0.846	0	4.900	2.286	12	9	-0.107	0.500	1.842	0.000	0.000	0.000
1043	N-methylaniline	2.28	1.639	0	1.522	1	2.337	-8.342	34	64	1.728	0.000	1.253	0.000	0.000	0.000
1046	N-methylpyrrole	2.04	1.130	0	0.675	0	2.598	-1.973	26	26	1.025	0.000	1.296	1.000	0.000	0.000
1047	N-methylpyrrolidine	1.88	0.781	1	1.105	0	1.657	-2.143	26	26	0.712	0.000	1.166	1.000	0.000	0.000
1049	nonane	4.45	4.477	0	8.000	6	0.090	-2.395	30	120	3.757	0.000	0.894	0.000	0.000	0.000
1053	N-phenylbenzamide	2.80	2.615	1	2.789	3	3.640	-9.816	72	394	2.939	0.000	1.387	0.000	0.000	0.000
1062	o-chloroaniline	3.13	1.748	1	1.398	0	1.972	-8.723	36	60	1.922	0.000	1.592	0.000	0.000	0.000
1064	o-chloronitrobenzene	2.60	2.389	3	1.988	0	6.721	-1.664	46	114	2.248	0.500	1.985	0.000	0.000	0.000
1066	o-chlorotoluene	3.24	2.981	1	1.542	0	1.129	-6.157	36	60	2.648	0.000	1.287	0.000	0.000	0.000
1071	octanenitrile	2.87	2.992	1	7.066	6	3.417	9.724	30	120	2.870	0.000	1.143	0.000	0.000	0.000
1076	o-dichlorobenzene	2.78	3.159	2	1.765	0	1.986	-7.218	36	60	2.993	0.000	1.459	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1077	o-diethylbenzene	3.78	3.715	0	2.494	2	0.847	-5.523	44	117	2.811	0.000	0.980	0.000	0.000	0.000
1080	o-ethylaniline	2.32	2.026	0	1.730	1	3.105	-8.672	40	86	1.831	0.000	1.219	0.000	0.000	0.000
1081	o-ethylphenol	2.72	2.530	1	1.853	2	0.843	-6.016	40	86	1.955	0.000	1.236	0.000	0.000	0.000
1083	oleic acid	5.53	6.861	2	15.907	16	1.927	9.976	76	1313	6.109	0.500	1.125	0.000	0.000	0.000
1084	o-nitroaniline	2.38	0.978	2	1.639	0	6.355	-1.255	46	114	1.177	0.500	1.811	0.000	0.000	0.000
1085	o-nitroanisole	2.32	1.708	3	2.300	1	7.818	-0.494	50	150	1.603	0.500	1.722	0.000	0.000	0.000
1090	o-toluic acid	2.64	1.946	2	1.826	2	2.357	-4.126	46	114	1.693	0.500	1.392	0.000	0.000	0.000
1093	oxadiazon	3.51	5.225	6	4.822	4	5.093	-5.167	116	1031	4.217	0.000	1.762	1.000	0.000	0.000
1096	oxycarboxin	1.98	0.585	4	3.490	3	8.906	6.605	92	599	1.302	0.945	1.757	1.000	0.000	0.000
1097	oxydemeton-methyl	1.00	0.617	5	7.360	7	6.219	8.204	54	286	1.889	0.167	1.803	0.000	0.000	0.000
1099	o-xylene	2.70	2.802	0	1.335	0	0.756	-6.120	36	60	2.303	0.000	0.991	0.000	0.000	0.000
1100	oxythioquinox	3.36	4.133	5	1.835	0	4.581	-7.655	84	341	2.575	0.000	1.881	2.000	0.000	0.000
1101	pp-dde	4.82	5.930	4	4.579	2	0.529	-0.871	90	603	6.188	0.000	1.420	0.000	0.000	0.000
1107	p-benzidine	5.36	1.855	0	2.108	1	0.001	-25.92	70	315	2.518	0.000	1.314	0.000	0.000	0.000
1108	p-bromoaniline	1.96	1.832	1	1.534	0	3.846	-13.90	36	62	2.031	0.000	1.592	0.000	0.000	0.000
1109	p-bromophenol	2.41	2.336	2	1.655	1	1.274	-5.168	36	62	2.155	0.000	1.614	0.000	0.000	0.000
1114	p-chlorotoluene	3.19	2.981	1	1.542	0	1.824	-6.178	36	62	2.648	0.000	1.287	0.000	0.000	0.000
1125	pentachloroaniline	4.62	4.405	5	3.240	0	3.138	-12.40	60	174	4.536	0.000	1.727	0.000	0.000	0.000
1126	pentachlorobenzene	4.10	5.152	5	3.184	0	0.759	-7.611	54	140	4.954	0.000	1.325	0.000	0.000	0.000
1128	pentachloronitrobenzene	3.70	5.046	7	3.857	0	5.560	-0.153	70	268	4.862	0.500	1.727	0.000	0.000	0.000
1132	pentane	3.25	2.653	0	4.000	2	0.090	-1.206	14	20	2.197	0.000	0.874	0.000	0.000	0.000
1134	pentylamine	2.19	1.137	1	4.927	3	1.557	-1.175	18	35	1.135	0.000	1.105	0.000	0.000	0.000
1145	phenmedipham	3.40	3.420	4	5.239	7	3.152	-43.08	106	1221	3.784	0.125	1.616	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1146	phenol	1.74	1.588	1	1.089	1	1.262	-4.697	30	42	1.392	0.000	1.314	0.000	0.000	0.000
1149	phenyl formate	2.06	1.519	2	1.988	2	4.079	0.566	38	94	1.222	0.000	1.429	0.000	0.000	0.000
1151	phenylacetic acid	1.45	1.495	2	2.179	3	1.579	-10.14	44	126	1.314	0.500	1.392	0.000	0.000	0.000
1162	p-hydroxybenzaldehyde	2.11	1.347	2	1.605	2	2.008	-1.428	40	90	1.205	0.167	1.429	0.000	0.000	0.000
1163	picloram	1.20	2.194	6	2.975	2	8.436	0.372	64	226	2.322	0.500	2.186	1.000	0.000	0.000
1167	piperophos	3.44	3.971	5	9.458	10	3.651	-30.67	96	1022	4.198	0.000	1.642	1.000	0.000	0.000
1168	pirimicarb	1.90	2.012	4	4.007	4	3.851	-8.436	82	518	1.220	0.000	1.612	1.000	0.000	0.000
1169	pirimiphos methyl	3.00	3.108	6	6.292	7	5.840	-4.536	90	714	2.527	0.000	1.849	1.000	0.000	0.000
1172	p-nitrophenol	2.72	1.482	3	1.749	1	6.548	4.186	46	120	1.300	0.721	1.782	0.000	0.000	0.000
1173	p-nitrotoluene	2.69	2.211	2	1.777	0	7.300	1.889	46	120	1.903	0.500	1.658	0.000	0.000	0.000
1177	profluralin	4.01	4.416	7	5.187	5	7.598	-10.44	124	1212	4.148	1.442	1.952	0.000	0.000	1.000
1179	pronamide	2.31	4.142	3	3.851	4	2.721	-2.993	78	448	3.135	0.000	1.678	0.000	0.000	1.000
1186	propazine	2.19	2.913	4	4.082	4	3.162	-6.827	70	386	2.166	0.000	1.595	1.000	0.000	0.000
1188	propiconazole	3.39	3.801	6	4.682	5	4.137	-12.84	116	1000	3.653	0.000	1.777	2.000	0.000	0.000
1192	propyl acetate	2.05	0.894	2	3.606	3	1.578	-0.839	24	52	0.960	0.000	1.333	0.000	0.000	0.000
1194	propyl formate	1.83	0.815	2	4.344	3	4.304	4.097	18	35	0.569	0.000	1.379	0.000	0.000	0.000
1199	propylene	2.34	1.350	0	1.589	0	0.276	-1.801	6	4	1.192	0.000	0.918	0.000	0.000	0.000
1202	p-toluic acid	2.65	1.946	2	1.826	2	3.015	-4.346	46	120	1.693	0.500	1.392	0.000	0.000	0.000
1204	p-xylene	2.77	2.802	0	1.335	0	0.044	-6.583	36	62	2.303	0.000	0.991	0.000	0.000	0.000
1207	pyrimidine	1.16	0.051	2	0.707	0	2.084	-0.087	24	27	0.477	0.000	1.522	1.000	0.000	0.000
1209	pyrrole	1.79	0.924	0	0.468	0	2.186	-1.934	20	15	1.015	0.000	1.361	1.000	0.000	0.000
1212	quinoxaline	1.87	1.294	2	1.104	0	0.650	-5.576	50	109	1.630	0.000	1.406	1.000	0.000	0.000
1216	salicylaldehyde	2.36	1.347	2	1.605	2	4.191	-2.480	40	86	1.205	0.250	1.429	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1226	sec-butylbenzene	3.86	3.480	0	2.494	2	0.475	-5.022	44	121	3.200	0.000	0.980	0.000	0.000	1.000
1227	sethoxydim	2.00	3.436	5	8.981	10	4.201	-9.296	100	1139	4.502	0.250	1.454	0.000	0.000	1.000
1234	succinic acid	1.06	-0.359	4	2.982	5	0.000	7.577	30	74	-0.064	1.629	1.557	0.000	0.000	0.000
1237	sulfometuron methyl	1.62	1.261	7	5.445	7	10.423	-18.66	126	1564	1.390	1.424	1.889	1.000	0.000	0.000
1238	sulfometuron	1.89	1.035	7	4.904	7	10.925	-15.10	122	1398	1.302	2.348	1.926	1.000	0.000	0.000
1245	terbufos sulfone	2.18	2.875	6	7.221	8	3.263	-2.682	80	538	3.188	0.500	1.734	0.000	0.000	1.000
1252	tert-butyl acetate	2.33	0.952	2	2.161	2	1.243	-0.730	34	66	1.348	0.000	1.295	0.000	0.000	1.000
1259	tetrachlorophthalate	3.30	0.799	8	4.174	0	5.866	0.391	80	382	1.027	1.629	1.500	0.000	0.000	0.000
1263	tetrahydropyran	1.83	0.968	1	0.892	0	1.593	-2.842	20	27	1.187	0.000	1.198	1.000	0.000	0.000
1269	thiobencarb	3.27	3.727	3	5.565	6	2.124	-9.488	72	505	4.035	0.000	1.656	0.000	0.000	0.000
1274	toluene	1.97	2.316	0	1.116	0	0.464	-5.611	30	42	1.995	0.000	0.997	0.000	0.000	0.000
1278	trans-2,trans-4-hexadiene	3.01	2.220	0	4.092	1	0.057	-4.688	18	35	2.139	0.000	0.954	0.000	0.000	0.000
1280	trans-2-methylcyclohexanol	2.37	1.820	1	1.896	1	1.599	-0.040	36	60	1.557	0.000	1.143	0.000	0.000	1.000
1283	trans-stilbene	3.99	3.816	0	2.770	2	0.341	-12.60	66	343	3.857	0.000	0.996	0.000	0.000	0.000
1300	triethyl phosphate	1.81	1.255	4	5.779	6	8.780	8.281	44	166	2.204	0.000	1.542	0.000	0.000	0.000
1301	triethylamine	2.17	1.367	1	4.104	3	1.264	-3.128	24	48	1.348	0.000	1.091	0.000	0.000	0.000
1307	trimethylamine	1.46	0.320	1	1.285	0	1.428	-2.045	12	9	0.178	0.000	1.140	0.000	0.000	0.000
1308	trimethylolpropane	0.57	-0.618	3	3.770	7	2.250	-0.816	36	88	-0.640	0.750	1.325	0.000	0.000	0.000
1310	triphenyl phosphate	3.87	4.938	4	5.008	6	9.294	0.080	116	1204	5.332	0.000	1.520	0.000	0.000	0.000
1311	triphenylamine	4.50	5.163	0	3.283	3	1.053	-7.215	96	666	5.156	0.000	1.156	0.000	0.000	0.000
1320	vernolate	2.33	3.399	2	8.098	8	1.491	-9.632	50	282	3.372	0.000	1.398	0.000	0.000	0.000
1322	vinyl acetate	1.77	0.105	2	2.326	2	1.584	-1.407	20	32	0.693	0.000	1.459	0.000	0.000	0.000
1325	vinylacetonitrile	1.60	0.777	1	2.733	2	3.089	2.321	14	20	1.086	0.000	1.361	0.000	0.000	0.000

Code	name	log Koc	AlogP98	HBA	MF	nRB	TD	QM-zz	ZI	WI	SlogP	MDEO-11	IC0	nHRing	nG12FAHRing	C3SP3
1327	α-epichlorohydrin	1.54	0.563	2	0.791	1	1.122	1.842	22	17	0.624	0.000	1.685	1.000	0.000	0.000
1331	γ-terpinene	3.08	3.449	0	2.530	1	0.203	-2.881	46	120	3.309	0.000	0.961	0.000	0.000	1.000

Table B-1 values of calculated log K_{OC} in a training set

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0001	2.36	2.37	2.47	2.37	2.35	2.38
0002	3.86	2.65	2.60	2.63	2.50	2.40
0003	2.97	2.73	2.81	2.82	2.80	2.86
0004	1.60	2.21	2.22	2.05	2.55	1.96
0005	2.01	2.41	2.26	2.40	2.67	2.48
0006	2.68	2.63	2.40	2.58	2.81	2.67
0007	3.10	2.85	2.46	2.70	3.01	2.82
0008	1.80	2.37	2.24	2.40	2.45	2.26
0010	1.49	1.96	1.93	2.03	2.31	2.18
0012	2.05	1.88	1.83	1.91	2.04	1.84
0014	1.43	2.02	2.21	1.96	2.38	2.03
0015	1.72	1.89	2.13	1.79	2.29	2.09
0017	3.28	3.18	3.37	3.40	2.79	3.13
0019	3.55	3.43	3.59	3.61	3.02	3.36
0020	3.52	3.84	3.59	3.75	3.90	3.79
0021	3.61	3.43	3.59	3.62	3.02	3.36
0022	3.23	3.45	3.30	3.36	3.48	3.34
0025	3.72	3.84	3.59	3.79	3.90	3.79
0027	3.11	3.45	3.30	3.43	3.48	3.34
0029	2.44	2.28	2.25	2.40	2.29	2.16
0031	2.53	3.01	2.86	2.86	3.00	2.50
0032	1.65	2.11	2.09	2.25	2.09	1.96
0036	2.51	2.28	2.36	2.27	2.24	2.24
0037	1.26	1.19	1.31	1.28	1.33	1.40
0038	3.72	3.39	3.61	3.67	3.36	3.68
0039	3.94	3.71	3.94	3.92	3.37	3.69
0041	1.39	1.38	1.50	1.52	1.41	1.63

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0044	2.85	3.45	3.30	3.48	3.48	3.34
0045	2.02	2.11	1.97	2.34	2.05	2.61
0046	2.51	2.16	2.24	2.26	2.05	2.14
0047	1.51	2.12	2.12	2.18	2.41	2.25
0048	3.78	3.39	3.61	3.70	3.36	3.68
0050	1.30	1.20	1.32	1.34	1.41	1.63
0052	2.72	2.31	2.46	2.57	2.36	2.71
0053	3.75	3.39	3.61	3.72	3.36	3.68
0054	1.15	1.08	1.18	1.26	1.17	1.32
0055	2.73	2.32	2.46	2.53	2.27	2.64
0058	2.90	2.59	2.74	2.77	2.52	2.89
0059	3.79	3.39	3.61	3.67	3.36	3.68
0060	4.32	3.79	4.14	4.02	3.97	4.30
0061	4.51	3.79	4.14	4.03	3.97	4.30
0062	6.10	4.22	4.65	4.48	4.74	5.08
0064	2.60	3.12	3.07	3.10	3.13	2.87
0066	2.60	3.12	3.07	3.15	3.13	2.87
0067	2.42	2.67	2.62	2.53	2.66	2.24
0069	2.42	2.67	2.62	2.59	2.66	2.24
0070	2.87	2.58	2.63	2.64	2.54	2.69
0072	3.44	3.11	3.18	3.13	3.04	3.24
0073	4.04	3.64	3.72	3.63	3.54	3.76
0076	1.83	1.80	1.92	1.88	1.65	1.84
0078	2.56	2.56	2.41	2.42	2.53	2.33
0079	2.81	2.50	2.55	2.58	2.44	2.59
0080	3.64	3.29	3.37	3.32	3.19	3.40
0082	2.86	2.76	2.82	2.82	2.69	2.87
0086	3.77	3.37	3.59	3.65	3.32	3.65

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0088	2.65	2.61	2.67	2.69	2.52	2.70
0089	2.11	2.02	2.20	2.05	2.15	2.23
0091	3.55	3.08	3.22	3.23	2.91	3.31
0092	2.48	2.33	2.46	2.37	2.15	2.38
0097	3.01	2.89	2.92	2.95	2.57	2.72
0098	2.74	2.63	2.64	2.71	2.32	2.43
0099	4.08	3.54	3.82	3.86	3.43	3.76
0100	3.48	3.11	3.33	3.41	3.16	3.49
0101	4.17	3.63	3.93	3.84	3.90	4.22
0102	2.00	2.27	2.56	2.34	2.34	2.31
0105	3.58	2.39	2.69	2.65	2.70	2.81
0106	2.18	2.18	2.20	2.11	1.83	1.79
0107	2.47	2.44	2.47	2.37	2.08	2.10
0109	3.56	3.12	3.28	3.11	2.89	3.15
0110	4.18	3.61	3.76	3.72	3.41	3.81
0111	3.05	2.86	3.00	2.86	2.64	2.90
0112	3.86	3.34	3.49	3.47	3.16	3.56
0113	2.20	2.06	2.19	2.12	1.90	2.11
0114	2.45	2.88	2.97	3.06	2.06	2.43
0119	4.66	4.44	4.64	4.42	4.14	4.42
0122	3.12	3.65	3.31	3.55	3.48	3.25
0125	1.08	1.08	1.22	0.98	1.17	1.22
0126	2.55	2.78	2.94	2.82	2.95	3.07
0127	2.36	3.09	2.96	2.92	2.53	1.98
0128	2.36	2.41	2.42	2.37	2.61	2.25
0129	1.94	1.73	1.61	1.61	1.69	0.92
0131	1.60	1.61	1.46	1.46	1.50	1.01
0132	5.02	5.88	5.40	5.62	6.21	6.14

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0134	5.24	6.65	5.97	6.26	7.04	7.13
0135	5.00	6.26	5.69	5.96	6.63	6.61
0136	4.11	5.49	5.12	5.27	5.79	5.68
0137	6.00	4.72	4.55	4.66	4.96	4.86
0138	4.50	3.57	3.73	3.78	3.61	4.03
0139	3.83	5.88	5.40	5.56	6.21	6.14
0140	5.60	5.10	4.83	4.91	5.38	5.26
0141	3.83	5.49	5.12	5.36	5.79	5.68
0144	5.37	4.72	4.55	4.66	4.96	4.86
0145	5.21	4.33	4.26	4.28	4.54	4.49
0146	5.37	4.72	4.55	4.67	4.96	4.86
0147	5.21	4.33	4.26	4.28	4.54	4.49
0150	4.70	3.95	3.98	3.99	4.13	4.14
0152	3.46	2.78	2.89	3.01	2.71	3.15
0154	4.80	5.10	4.83	4.93	5.38	5.26
0156	5.64	4.72	4.55	4.57	4.96	4.86
0157	4.85	4.72	4.55	4.61	4.96	4.86
0158	4.23	3.78	3.43	3.47	3.84	3.41
0159	2.88	3.70	3.40	3.48	3.71	3.34
0160	3.94	3.41	3.23	3.21	3.63	3.22
0161	2.88	3.70	3.40	3.50	3.71	3.34
0162	2.60	3.02	2.94	2.83	3.21	2.80
0165	3.76	3.00	3.11	3.10	2.63	2.77
0168	5.21	4.33	4.26	4.29	4.54	4.49
0169	1.96	3.31	3.11	3.18	3.29	2.89
0170	3.76	3.00	3.11	3.09	2.63	2.77
0171	1.96	3.31	3.11	3.16	3.29	2.89
0173	0.67	2.64	2.66	2.56	2.80	2.45

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0175	4.06	2.27	2.47	2.37	2.22	2.33
0176	4.06	2.77	2.91	2.88	2.35	2.47
0177	2.54	2.33	2.49	2.45	2.19	2.42
0178	3.47	2.80	2.92	3.04	2.62	2.78
0180	2.66	2.72	2.83	2.83	2.43	2.55
0181	5.21	4.33	4.26	4.34	4.54	4.49
0182	3.85	3.07	3.21	3.27	3.07	3.47
0184	5.21	4.33	4.26	4.33	4.54	4.49
0187	3.76	3.00	3.11	3.08	2.63	2.77
0188	5.21	4.33	4.26	4.33	4.54	4.49
0189	1.96	3.31	3.11	3.22	3.29	2.89
0190	3.76	3.00	3.11	3.09	2.63	2.77
0191	2.40	2.24	2.40	2.34	2.43	2.71
0192	2.25	2.40	2.25	2.57	2.25	2.78
0193	4.55	3.95	3.98	3.93	4.13	4.14
0194	2.70	3.58	3.46	3.46	3.53	3.29
0196	2.55	2.93	2.83	2.86	2.87	2.52
0197	2.11	2.76	2.60	2.63	2.72	2.47
0198	3.68	3.35	3.30	3.37	3.26	3.18
0199	2.39	2.49	2.59	2.57	2.34	2.26
0202	0.67	2.64	2.66	2.63	2.80	2.45
0204	2.55	2.93	2.83	2.90	2.87	2.52
0205	1.63	1.43	1.56	1.57	1.52	1.71
0206	3.28	3.04	3.18	3.24	3.01	3.39
0207	2.66	2.72	2.83	2.81	2.43	2.55
0209	0.67	2.64	2.66	2.69	2.80	2.45
0211	2.60	3.00	2.91	2.84	2.98	2.68
0212	4.70	3.95	3.98	3.94	4.13	4.14

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0214	3.05	2.88	3.01	2.94	2.71	2.68
0215	3.72	3.39	3.61	3.69	3.36	3.68
0216	2.29	1.96	2.11	2.09	2.24	2.48
0218	2.52	2.46	2.41	2.41	2.31	2.33
0219	2.56	2.29	2.10	2.33	2.49	2.17
0220	4.15	4.06	4.25	4.17	3.89	4.11
0221	2.66	2.72	2.83	2.82	2.43	2.55
0224	1.96	2.58	2.71	2.64	2.64	2.49
0226	2.57	2.52	2.48	2.41	2.52	2.39
0227	2.41	2.23	2.26	2.37	2.29	2.41
0228	1.83	1.72	1.86	1.73	1.66	1.78
0229	2.47	2.12	2.15	2.24	2.27	2.28
0232	3.84	3.56	3.70	3.64	3.71	3.84
0233	2.65	2.45	2.49	2.55	2.44	2.59
0234	1.39	1.41	1.45	1.47	1.29	1.02
0235	3.54	3.21	3.33	3.40	3.38	3.49
0236	2.60	2.54	2.54	2.51	2.46	2.22
0238	2.41	2.15	2.18	2.28	2.19	2.31
0239	1.71	1.98	2.11	2.08	1.98	2.06
0240	3.43	3.15	3.31	3.19	3.27	3.51
0241	1.20	1.15	1.28	1.21	1.16	1.23
0243	2.68	2.25	2.34	2.41	2.33	2.56
0246	3.79	3.41	3.57	3.56	2.98	3.33
0250	2.45	2.36	2.49	2.41	2.53	2.73
0251	2.33	2.28	2.40	2.32	2.15	2.38
0252	2.13	2.09	2.22	2.15	2.28	2.46
0253	2.17	1.94	2.06	2.02	2.11	2.31
0255	1.99	2.19	2.29	2.23	1.96	1.82

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0256	1.26	1.34	1.38	1.16	0.97	0.94
0257	2.95	2.54	2.54	2.68	2.32	2.43
0258	2.11	2.07	2.20	2.17	2.17	2.18
0262	2.08	1.98	2.10	2.06	1.81	1.88
0263	2.61	2.38	2.38	2.18	2.18	2.12
0264	2.87	2.57	2.69	2.68	2.43	2.54
0266	2.61	2.44	2.57	2.49	2.31	2.40
0267	3.13	2.56	2.72	2.72	2.90	3.14
0268	2.38	1.86	1.97	2.06	2.17	2.35
0269	3.55	3.11	3.33	3.39	3.16	3.49
0270	1.98	1.79	1.94	1.92	2.04	2.25
0271	2.79	2.57	2.75	2.68	2.77	3.03
0272	2.38	1.75	1.88	1.86	1.91	2.21
0274	2.22	2.47	2.69	2.62	2.64	2.77
0275	2.85	2.68	2.86	2.91	2.78	2.89
0276	3.58	2.39	2.69	2.57	2.70	2.81
0277	1.45	1.66	1.76	1.52	1.59	1.43
0278	1.88	1.83	1.84	1.76	1.58	1.47
0279	3.10	2.89	3.03	2.92	3.03	3.25
0280	2.96	2.81	2.94	2.81	2.64	2.90
0281	2.67	2.62	2.76	2.66	2.78	2.99
0282	2.06	2.02	2.13	2.08	1.90	2.11
0285	2.12	2.13	2.30	2.22	1.93	2.05
0286	2.40	2.55	2.69	2.59	2.46	2.56
0287	2.97	2.97	3.07	3.04	2.65	2.79
0288	0.92	1.02	1.22	1.10	1.09	1.05
0289	3.60	3.41	3.58	3.46	3.52	3.77
0290	2.46	2.56	2.60	2.33	2.90	2.38

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0291	2.53	2.90	3.07	2.79	3.17	2.92
0292	1.73	2.47	2.74	2.45	2.68	2.60
0293	1.84	2.16	2.27	1.93	2.49	2.06
0294	2.10	2.45	2.60	2.32	2.68	2.34
0295	1.79	2.29	2.46	2.17	2.70	2.36
0297	1.73	2.02	2.21	1.93	2.38	2.03
0298	1.72	1.89	2.13	1.78	2.29	2.09
0300	1.43	2.02	2.21	1.96	2.38	2.03
0301	1.40	1.89	2.13	1.79	2.29	2.09
0302	1.51	2.19	2.46	2.17	2.48	2.37
0303	2.36	3.09	2.96	2.88	2.53	1.98
0305	3.83	3.42	3.25	3.21	2.99	2.43
0306	3.83	5.49	5.12	5.38	5.79	5.68
0308	4.70	3.95	3.98	4.04	4.13	4.14
0309	2.18	2.10	2.22	2.20	2.05	2.29
0310	1.96	3.31	3.11	3.18	3.29	2.89
0311	3.76	3.00	3.11	3.07	2.63	2.77
0312	4.70	3.95	3.98	3.92	4.13	4.14
0313	2.34	2.56	2.58	2.36	3.04	2.57
0315	2.33	3.04	2.98	2.94	2.88	2.63
0316	2.53	3.01	2.86	2.85	3.00	2.50
0317	2.55	2.93	2.83	2.84	2.87	2.52
0318	2.49	2.44	2.47	2.30	2.74	2.14
0319	1.53	1.96	1.83	1.64	1.92	2.53
0322	0.67	2.64	2.66	2.55	2.80	2.45
0323	2.55	2.93	2.83	2.90	2.87	2.52
0324	2.83	2.72	2.83	2.80	2.43	2.55
0326	2.31	1.60	1.60	1.56	1.54	1.72

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0327	2.66	2.72	2.83	2.80	2.43	2.55
0328	0.99	2.84	2.68	2.61	2.87	2.62
0329	2.30	2.71	2.53	2.47	2.68	2.55
0330	0.77	0.58	0.73	0.58	0.72	0.68
0332	2.35	2.17	2.22	2.27	2.15	2.16
0333	1.96	2.58	2.71	2.57	2.64	2.49
0334	1.96	2.58	2.71	2.57	2.64	2.49
0335	2.69	2.98	2.87	2.94	2.94	2.44
0338	1.89	1.61	1.70	1.21	1.92	1.57
0339	2.12	2.10	2.23	2.05	2.39	1.91
0340	2.60	3.06	2.90	2.92	3.07	2.44
0342	2.00	2.04	2.14	1.89	2.33	1.83
0344	1.93	2.24	2.33	2.11	2.38	2.02
0345	3.87	3.56	3.70	3.64	3.71	3.84
0347	2.01	2.05	2.18	2.00	2.32	1.84
0348	3.74	3.41	3.57	3.57	2.98	3.33
0349	1.66	1.72	1.91	1.38	1.79	1.78
0350	1.57	1.91	2.05	1.83	2.29	1.95
0351	1.77	1.78	1.94	1.74	1.99	1.51
0352	2.60	2.59	2.70	2.63	2.39	2.64
0354	0.98	2.02	2.07	1.98	1.85	1.86
0355	1.61	1.43	1.41	1.36	1.40	1.24
0356	1.55	2.15	2.21	2.11	2.05	2.01
0358	2.07	1.95	2.06	2.03	1.81	1.88
0362	2.26	2.58	2.71	2.53	2.64	2.49
0363	2.37	2.38	2.51	2.35	2.59	2.18
0365	2.61	2.38	2.38	2.23	2.18	2.09
0366	1.45	2.07	2.29	2.09	2.40	2.33

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0368	2.82	2.57	2.69	2.68	2.43	2.54
0369	2.25	2.23	2.38	2.31	2.10	2.22
0370	2.01	1.91	1.96	1.95	1.86	1.92
0371	3.34	2.92	3.03	3.13	2.71	3.01
0372	1.48	1.46	1.65	1.12	1.63	1.57
0373	1.56	1.95	2.18	1.99	2.10	1.90
0374	2.03	1.91	2.04	2.01	2.04	2.25
0375	2.65	2.17	2.25	2.36	2.46	2.64
0377	1.95	1.66	1.76	1.69	1.59	1.40
0378	2.80	2.78	2.61	2.59	2.82	2.33
0380	2.37	3.13	3.42	3.24	3.40	3.38
0381	2.07	2.86	3.15	2.85	3.16	3.10
0382	1.93	2.60	2.88	2.57	2.91	2.83
0383	1.72	2.07	2.36	2.04	2.41	2.26
0385	1.75	2.33	2.33	2.10	2.85	2.38
0386	2.36	2.41	2.42	2.25	2.61	2.25
0387	1.98	2.21	2.22	2.05	2.55	1.96
0388	2.36	3.09	2.96	2.82	2.53	1.98
0390	2.36	3.42	3.25	3.12	2.99	2.43
0391	5.27	3.95	3.98	4.07	4.13	4.14
0393	2.99	3.30	3.07	3.11	3.30	2.83
0394	1.88	1.80	1.93	1.51	1.90	1.66
0395	2.69	2.83	3.06	2.87	2.97	3.11
0397	1.96	2.58	2.71	2.52	2.64	2.49
0398	1.96	2.58	2.71	2.53	2.64	2.49
0399	1.95	2.22	2.34	2.12	2.69	2.35
0403	2.01	3.30	3.42	3.30	2.80	2.46
0404	2.41	2.59	2.59	2.62	2.53	2.29

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0405	2.12	2.10	2.23	2.06	2.39	1.91
0406	3.36	3.23	3.34	3.28	2.90	3.06
0407	1.96	2.25	2.38	2.22	2.38	2.16
0408	2.19	2.59	2.56	2.36	2.45	1.97
0409	1.98	2.66	2.69	2.61	2.46	2.32
0410	3.89	3.56	3.70	3.65	3.71	3.84
0411	1.90	3.25	3.38	3.26	2.74	2.39
0412	3.81	3.41	3.57	3.59	2.98	3.33
0414	1.48	1.91	2.05	1.86	2.29	1.95
0415	1.87	2.39	2.45	2.37	2.13	2.00
0416	1.68	2.99	3.13	3.02	2.41	2.07
0417	1.52	1.78	1.94	1.77	1.99	1.51
0418	2.59	2.59	2.70	2.63	2.39	2.64
0420	2.17	3.56	3.80	3.58	3.04	2.80
0421	1.94	1.87	2.08	1.54	2.15	2.04
0423	1.80	2.26	2.36	2.19	2.05	1.97
0424	1.83	2.86	3.05	2.86	2.32	2.10
0425	1.40	1.17	1.32	0.72	1.44	1.32
0426	2.74	2.69	2.82	2.89	2.57	2.83
0427	0.63	1.97	2.10	2.06	2.19	2.22
0428	2.61	2.38	2.38	2.19	2.18	2.12
0429	2.57	2.43	2.59	2.47	2.55	2.67
0430	1.60	2.15	2.38	2.27	2.16	2.26
0431	2.91	2.57	2.69	2.66	2.43	2.54
0432	1.78	2.00	2.20	2.01	1.85	1.74
0434	1.77	2.36	2.44	2.33	2.23	2.38
0437	2.70	2.44	2.54	2.53	2.24	2.32
0438	2.53	2.44	2.54	2.37	2.38	2.38

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0440	2.16	3.27	3.42	3.30	2.90	3.06
0441	1.93	1.66	1.76	1.60	1.59	1.38
0446	2.71	2.74	2.96	2.86	3.01	3.02
0449	2.07	1.99	2.22	1.68	2.26	2.33
0451	1.96	2.58	2.71	2.55	2.64	2.49
0452	3.85	3.41	3.57	3.59	2.98	3.33
0453	1.93	1.87	2.01	1.94	2.14	2.27
0454	1.69	2.20	2.30	2.27	1.78	1.87
0458	1.37	2.17	2.07	1.94	2.07	1.81
0459	5.58	3.44	3.88	3.56	4.17	4.34
0460	1.82	4.44	4.81	4.70	4.83	5.15
0462	2.48	3.92	4.21	4.11	4.09	4.41
0463	4.47	3.14	3.34	3.10	3.51	3.74
0464	2.54	3.00	3.29	3.18	3.38	3.53
0469	0.30	1.69	1.80	1.68	2.05	2.16
0471	1.62	0.75	0.92	0.83	0.83	0.57
0472	0.69	1.79	2.01	1.81	2.20	2.09
0474	1.29	3.16	3.29	2.93	3.14	2.99
0475	2.32	1.18	1.30	1.30	1.53	1.60
0476	1.25	1.26	1.35	1.37	1.49	1.41
0477	1.19	2.15	2.31	2.21	2.36	2.45
0478	2.26	1.12	1.24	1.23	1.51	1.56
0479	1.60	2.38	2.41	2.65	1.31	1.66
0481	2.05	3.18	3.39	3.30	3.31	3.61
0482	3.23	1.53	1.63	1.71	1.39	1.36
0484	0.95	1.52	1.54	1.62	1.32	1.34
0486	1.51	1.56	1.54	1.58	1.61	1.95
0488	1.20	3.22	3.35	3.15	3.06	2.90

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0489	2.48	1.91	1.91	1.60	2.09	1.59
0491	0.42	0.90	0.96	0.77	0.94	0.48
0492	0.56	3.71	3.61	3.59	4.51	3.48
0494	2.17	1.61	1.68	1.64	1.62	1.59
0496	1.47	1.22	1.35	1.35	1.24	1.36
0497	1.39	4.01	3.68	3.86	4.78	4.00
0498	5.15	3.65	3.31	3.45	3.48	3.25
0499	3.30	2.83	2.81	2.60	2.33	2.28
0500	2.13	4.34	4.54	4.39	4.26	4.31
0501	3.00	0.88	0.99	0.85	0.76	0.77
0503	2.33	2.23	2.40	2.17	2.51	2.23
0504	2.08	3.78	3.51	3.60	3.43	3.09
0505	3.00	1.86	2.09	1.99	1.96	2.03
0506	1.87	2.29	2.41	2.39	2.23	2.32
0507	2.25	3.35	3.64	3.64	3.70	4.04
0510	3.22	0.25	0.22	-0.08	0.25	1.04
0511	0.49	1.48	1.60	1.00	1.35	1.13
0513	2.24	2.35	2.35	2.36	2.36	2.68
0514	2.23	3.15	2.94	2.58	2.43	1.86
0517	3.13	2.82	3.05	2.99	2.93	3.27
0518	3.13	2.54	2.47	2.26	2.30	2.07
0521	3.99	2.96	3.08	2.84	2.79	2.71
0523	2.60	3.37	3.27	3.08	3.56	3.30
0526	4.59	2.41	2.60	2.46	2.61	2.73
0530	1.46	2.30	2.45	2.54	2.23	2.57
0531	1.87	2.12	2.28	2.22	2.06	2.16
0532	2.35	2.10	2.20	2.07	1.99	2.14
0533	2.14	2.25	2.39	2.31	2.27	2.35

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0534	2.23	1.97	2.15	2.09	1.91	2.05
0537	2.40	4.05	4.48	4.31	4.81	5.16
0538	4.75	4.22	4.71	4.50	5.19	5.55
0542	2.23	3.11	3.31	3.17	3.01	3.16
0543	2.64	2.55	2.59	2.60	2.62	2.56
0545	1.97	2.07	2.15	2.07	1.76	1.76
0546	3.07	2.84	2.78	2.78	2.88	2.74
0547	3.04	2.17	2.29	2.19	2.27	2.27
0548	2.44	1.95	2.10	2.02	1.90	1.99
0549	1.95	3.13	3.29	3.13	3.09	3.15
0550	3.54	2.65	2.73	2.74	2.70	2.76
0551	2.63	2.39	2.55	2.44	2.57	2.71
0552	2.55	2.18	2.34	2.25	2.32	2.44
0553	2.11	3.21	3.40	3.30	3.24	3.38
0554	3.44	1.78	1.95	1.87	1.88	1.99
0556	5.38	3.83	3.62	3.76	4.01	3.79
0557	3.04	3.18	3.41	3.36	3.29	3.62
0558	3.30	2.04	2.03	2.08	2.10	1.84
0560	3.18	3.12	3.25	3.03	3.01	2.81
0561	1.71	2.36	2.46	2.26	2.16	2.01
0563	1.60	2.73	2.78	2.83	2.71	2.74
0564	3.00	1.98	1.94	2.05	2.16	1.64
0565	2.14	2.89	2.93	3.01	2.88	3.03
0566	3.12	2.01	2.05	2.13	2.05	2.11
0570	2.39	4.67	4.52	4.53	4.56	4.28
0571	4.00	2.95	2.82	2.86	2.93	2.40
0573	2.86	1.40	1.57	1.44	1.33	1.23
0576	3.98	2.02	2.09	2.02	2.01	2.08

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0577	2.37	2.42	2.48	2.35	2.12	2.17
0579	3.47	2.36	2.43	2.39	2.25	2.44
0580	2.62	2.68	2.74	2.64	2.37	2.44
0581	2.94	1.63	1.77	1.74	1.63	1.86
0582	1.85	3.27	3.39	3.20	3.37	3.06
0583	2.11	3.37	3.53	3.52	3.08	3.43
0584	3.69	2.93	3.06	2.84	3.09	2.99
0585	2.26	1.78	1.89	1.88	1.78	1.90
0588	1.81	1.91	2.00	1.98	1.99	2.07
0589	1.70	3.57	3.31	3.34	3.40	2.65
0590	3.32	3.87	3.61	3.65	3.01	2.25
0592	2.02	2.19	2.30	2.15	2.26	2.05
0593	2.35	2.10	2.30	1.96	2.27	2.12
0594	1.95	2.53	2.68	2.54	2.50	2.35
0595	1.79	2.19	2.11	2.36	1.80	2.22
0596	2.54	3.57	3.23	3.54	3.18	3.77
0598	2.27	2.65	2.36	2.65	2.09	2.69
0601	4.67	2.16	2.34	2.19	2.82	2.70
0602	2.41	3.63	3.46	3.38	2.79	2.60
0603	3.36	2.55	2.51	2.32	2.66	2.12
0605	2.74	1.83	1.78	1.52	1.73	1.72
0606	2.00	2.63	2.64	2.33	3.15	2.53
0607	2.58	3.46	3.46	3.27	3.01	2.67
0608	2.47	3.63	3.41	3.34	4.81	4.30
0609	2.47	3.63	3.41	3.24	4.81	4.30
0610	2.04	1.61	1.82	1.40	2.09	1.80
0614	2.22	2.68	2.74	2.79	2.64	2.67
0616	1.97	1.95	1.81	1.99	2.08	1.55

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0618	1.65	2.17	2.03	2.21	2.42	2.41
0619	3.22	3.05	2.93	3.00	3.07	2.73
0620	1.79	3.14	2.78	2.97	2.17	1.89
0621	2.98	3.70	3.38	3.49	3.73	3.70
0623	2.28	2.82	2.52	2.79	2.27	2.26
0624	3.55	3.19	3.37	3.24	3.85	3.55
0625	2.53	2.97	3.00	2.81	3.26	2.94
0626	3.79	4.12	3.70	3.49	4.16	3.47
0627	3.52	3.72	3.28	3.21	3.66	2.83
0628	1.60	2.31	2.19	2.11	2.01	1.79
0631	2.14	1.99	2.22	1.98	1.91	1.81
0632	2.54	2.35	2.45	2.30	2.29	2.45
0633	2.44	2.50	2.64	2.52	2.57	2.67
0634	4.79	2.07	2.32	2.04	2.16	2.44
0636	2.48	2.15	2.12	2.18	2.64	2.47
0637	2.68	2.29	2.44	2.50	2.27	2.64
0638	2.90	2.52	2.68	2.73	2.52	2.89
0639	2.65	2.25	2.38	2.50	2.16	2.58
0640	2.38	2.29	2.42	2.43	2.15	2.21
0641	3.19	4.39	4.44	4.44	5.05	4.61
0643	4.67	4.40	4.95	4.70	5.57	5.94
0644	2.00	2.71	2.69	2.68	3.46	3.29
0645	3.37	2.99	3.16	3.18	2.94	3.14
0646	2.26	2.59	2.52	2.38	2.22	1.92
0647	1.42	1.28	1.29	1.46	1.17	1.52
0648	2.54	3.17	3.29	3.18	3.39	3.34
0649	3.61	3.59	3.73	3.69	3.61	3.85
0651	3.25	2.82	2.93	3.09	2.65	3.05

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0652	2.05	2.11	2.23	2.19	1.99	2.17
0653	1.82	2.00	2.12	2.09	2.12	2.25
0654	1.83	2.05	2.10	2.13	2.29	2.22
0655	2.93	2.57	2.70	2.81	2.50	2.88
0656	2.19	1.94	2.08	2.08	1.97	2.18
0657	3.80	3.35	3.47	3.61	3.14	3.55
0659	2.31	2.03	2.14	2.31	1.90	2.32
0660	5.00	4.43	4.37	4.50	5.18	4.52
0662	5.00	4.31	4.33	4.31	5.09	4.55
0663	2.30	1.42	1.56	1.42	0.90	0.90
0664	0.40	1.77	1.65	1.65	1.96	1.60
0665	1.85	2.68	2.57	2.66	2.67	2.27
0671	1.49	2.24	2.15	1.82	2.99	2.61
0672	3.18	3.14	3.27	2.88	3.62	3.41
0674	3.28	3.13	3.11	3.02	3.88	3.52
0675	3.28	3.13	3.11	2.97	3.88	3.52
0676	2.36	3.45	3.31	2.98	3.44	3.05
0677	6.07	4.40	4.84	4.75	5.17	5.51
0678	3.62	3.17	3.36	3.32	3.44	3.72
0679	3.40	3.16	3.45	3.37	3.27	3.55
0681	2.63	2.10	2.06	2.16	2.26	2.11
0682	3.12	2.81	2.68	2.85	2.81	3.06
0683	3.95	3.67	3.46	3.69	3.45	3.52
0684	2.92	2.65	2.55	2.70	2.54	2.81
0686	2.33	3.00	2.86	3.03	2.98	2.68
0687	1.88	1.81	1.79	1.88	1.71	1.29
0688	2.55	2.98	2.84	3.02	2.44	2.29
0689	2.22	2.06	2.02	2.12	2.25	1.72

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0691	3.00	3.86	3.74	3.58	3.78	3.56
0692	3.00	3.04	2.88	2.77	2.97	2.76
0694	4.20	3.94	3.79	3.85	4.11	3.98
0695	4.20	4.07	3.94	4.02	4.17	3.89
0696	3.70	4.50	4.29	4.39	4.72	4.30
0698	1.66	1.31	1.37	0.90	2.04	1.75
0700	4.11	3.21	3.13	3.06	4.01	4.34
0701	0.60	0.49	0.62	0.38	0.23	0.18
0702	3.15	3.34	3.44	3.20	3.03	2.92
0703	2.04	2.03	2.00	1.89	1.90	1.86
0704	1.86	1.67	1.80	1.79	1.82	2.01
0706	1.90	1.67	1.67	1.56	1.47	1.48
0708	2.72	2.53	2.57	2.34	2.45	2.46
0709	2.03	1.69	1.73	1.67	1.72	1.74
0710	2.00	1.33	1.31	1.10	1.35	1.25
0711	2.44	2.10	2.20	2.16	2.27	2.46
0712	1.84	1.40	1.62	1.44	1.71	1.71
0714	2.42	2.65	2.84	2.52	2.83	2.97
0715	1.59	1.52	1.68	1.41	1.84	1.92
0717	1.68	1.65	1.80	1.51	1.67	1.75
0721	3.14	3.51	3.56	3.39	3.27	3.05
0722	0.93	0.92	1.04	0.83	0.73	0.75
0725	0.48	1.02	1.13	1.00	1.20	1.52
0726	2.56	1.66	1.61	1.52	1.78	1.16
0727	2.34	2.04	2.02	2.10	2.19	2.18
0728	1.43	1.27	1.37	1.42	1.32	1.46
0729	1.63	2.13	2.15	1.95	1.96	1.91
0730	2.01	0.93	0.88	0.69	0.85	0.68

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0731	0.61	1.11	1.18	1.11	0.94	0.82
0734	2.17	2.32	2.43	2.58	1.81	2.18
0735	2.72	1.11	1.23	1.28	1.05	1.25
0737	4.72	4.73	4.78	4.68	4.44	4.57
0738	3.63	2.79	2.68	2.80	3.03	2.86
0739	1.59	2.99	2.91	2.93	2.89	3.14
0740	5.51	5.79	5.86	5.97	5.44	5.59
0741	2.08	2.84	3.19	3.02	3.01	2.90
0744	3.98	3.52	3.77	3.69	3.12	3.47
0745	2.78	3.20	3.45	3.38	3.34	3.47
0747	2.83	2.88	3.11	3.04	2.92	3.07
0750	1.59	2.12	2.21	2.08	1.93	2.03
0751	2.29	2.12	2.28	2.19	2.04	2.30
0752	6.00	2.35	2.75	2.46	1.75	3.62
0753	3.22	3.16	3.06	2.73	3.56	3.26
0754	2.82	2.67	2.74	2.47	3.12	2.66
0756	4.97	4.63	4.79	4.71	4.30	4.70
0757	3.88	3.89	3.97	3.87	3.70	4.04
0758	6.08	5.49	5.69	5.66	5.08	5.42
0760	3.44	3.32	3.34	3.07	3.80	3.54
0761	6.43	6.00	6.15	6.26	5.69	6.07
0762	4.13	2.48	2.22	2.29	3.51	3.78
0763	2.14	1.04	1.08	0.84	1.12	1.54
0765	4.85	2.58	2.83	2.65	2.63	2.97
0767	1.27	1.55	1.75	1.64	1.58	1.67
0768	2.38	2.90	3.01	2.81	3.05	2.98
0769	3.72	5.04	5.12	5.35	5.41	4.97
0770	3.60	3.63	3.47	3.56	3.66	3.55

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0772	3.94	3.86	3.55	3.59	4.35	3.89
0773	2.17	2.66	2.70	2.49	2.46	2.59
0774	1.80	3.22	3.16	2.79	3.97	3.73
0777	2.10	1.86	1.90	1.83	1.62	1.59
0778	1.21	1.23	1.34	1.37	1.15	1.29
0779	2.81	2.42	2.51	2.39	2.34	2.34
0780	2.48	2.24	2.38	2.30	2.32	2.54
0781	2.16	1.93	1.97	2.06	1.95	2.01
0782	1.50	1.40	1.46	1.37	1.27	1.21
0783	2.61	2.90	2.98	2.85	2.76	2.89
0785	2.47	2.32	2.34	2.44	2.07	2.13
0787	3.02	3.16	3.25	3.12	3.01	3.15
0788	1.97	2.37	2.44	2.35	2.26	2.35
0789	1.89	2.44	2.56	2.39	2.30	2.33
0790	2.31	1.84	1.89	1.86	1.76	1.80
0791	2.24	2.21	2.26	2.12	2.17	2.16
0793	2.74	2.29	2.18	2.18	2.22	2.49
0794	2.21	2.28	2.32	2.23	2.15	2.14
0795	2.59	2.70	2.79	2.65	2.54	2.57
0796	2.48	2.35	2.35	2.24	2.28	2.19
0797	1.31	1.06	1.19	1.23	1.13	1.33
0799	1.99	1.79	1.88	2.07	1.66	2.08
0800	0.64	0.72	0.81	0.83	0.50	0.62
0801	1.21	1.16	1.27	1.31	1.16	1.31
0803	1.82	2.36	2.49	2.29	2.59	2.42
0806	1.80	3.26	3.05	2.98	3.24	2.98
0807	2.52	3.12	3.10	2.97	3.86	3.55
0808	1.64	2.53	2.54	2.60	3.01	2.84

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0809	1.57	2.47	2.55	2.56	3.23	2.92
0811	3.51	3.01	2.85	2.57	2.94	2.52
0812	1.71	4.36	4.56	4.53	4.16	4.35
0813	3.98	3.93	3.80	3.99	4.09	3.92
0815	3.00	3.30	3.42	3.63	3.45	3.31
0816	3.40	4.05	4.31	4.38	3.88	4.03
0819	2.17	2.92	2.84	2.34	2.92	2.67
0820	3.18	3.39	3.26	3.15	3.46	3.06
0821	1.40	1.90	2.17	1.89	2.29	2.14
0824	3.76	4.27	4.05	4.29	4.34	4.13
0829	4.14	3.52	3.88	3.73	4.01	4.37
0830	3.66	3.26	3.54	3.59	3.23	3.57
0831	2.61	2.42	2.49	2.53	2.32	2.35
0832	1.73	1.83	1.70	1.86	1.90	1.90
0833	1.53	2.31	2.06	1.90	2.16	1.58
0834	3.01	3.43	3.61	3.30	4.17	4.08
0836	3.27	4.11	3.82	3.75	3.23	2.71
0837	1.78	3.37	3.10	3.41	3.54	3.46
0838	1.57	0.72	0.83	0.95	1.03	0.92
0839	0.56	0.71	0.86	0.93	0.58	0.19
0840	2.00	1.74	1.94	1.83	1.95	1.79
0845	1.53	1.47	1.55	1.55	1.64	1.71
0847	2.00	0.62	0.63	0.40	0.95	1.06
0848	1.22	1.29	1.27	1.27	1.36	1.72
0849	0.99	1.58	1.67	1.55	1.92	1.83
0850	0.42	0.42	0.50	0.25	0.09	0.38
0851	1.51	1.08	1.06	0.97	1.18	1.20
0853	3.17	3.23	3.08	3.22	3.40	3.46

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0856	3.83	3.30	3.43	3.46	3.05	3.49
0857	2.69	2.56	2.61	2.55	2.45	2.71
0858	2.78	2.42	2.58	2.47	2.37	2.64
0859	4.00	3.34	2.98	3.15	4.19	4.53
0860	4.49	4.61	4.16	4.40	4.73	5.04
0862	3.55	3.19	2.79	3.07	3.53	4.03
0863	3.52	5.47	5.00	5.20	5.37	5.03
0864	5.28	4.94	5.06	5.01	4.69	5.06
0866	2.76	3.01	2.70	2.98	2.76	3.09
0868	1.53	0.59	0.71	0.48	1.65	1.46
0869	3.93	3.99	4.15	4.20	3.41	3.76
0870	3.66	3.26	3.33	3.40	2.86	2.88
0871	2.35	2.31	2.44	2.38	2.28	2.46
0872	3.55	3.04	3.16	3.22	2.80	3.24
0873	2.25	2.44	2.55	2.48	2.49	2.64
0875	1.73	2.74	2.92	2.78	1.48	1.52
0877	4.38	3.90	4.07	4.03	3.58	3.93
0879	5.86	4.98	4.93	5.81	5.22	5.07
0880	2.98	3.21	3.49	3.42	3.15	3.18
0883	2.04	2.70	2.85	2.64	2.42	2.32
0884	2.35	2.00	2.09	1.77	1.84	1.78
0885	2.64	1.84	1.89	1.64	1.59	1.50
0886	1.33	1.07	1.23	1.11	1.41	1.41
0887	3.19	2.91	3.10	3.16	2.54	2.88
0888	2.97	2.65	2.87	2.86	2.59	2.93
0890	3.16	2.63	2.70	2.72	2.61	2.64
0891	2.30	2.76	2.65	2.68	2.73	2.20
0892	3.39	3.11	3.09	2.93	2.55	2.51

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0893	2.40	3.44	3.46	3.17	4.26	4.05
0896	1.79	1.72	1.82	1.83	1.56	1.61
0897	2.66	2.28	2.38	2.51	2.16	2.58
0900	1.77	1.55	1.67	1.68	1.54	1.62
0902	1.89	1.77	1.80	1.83	1.62	1.64
0903	1.63	1.92	1.99	2.00	1.90	1.83
0904	2.78	3.38	3.33	2.94	3.63	3.32
0905	2.63	2.66	2.76	2.89	2.46	2.77
0907	2.28	1.87	1.86	1.86	1.84	2.19
0908	2.69	2.32	2.44	2.53	2.27	2.64
0909	4.00	3.97	4.03	3.97	3.87	3.98
0911	3.11	2.63	2.74	2.63	2.59	2.62
0912	1.95	2.58	2.71	2.51	2.84	2.71
0915	2.51	2.16	2.35	2.26	2.58	2.82
0919	0.87	1.15	1.21	1.11	1.08	0.79
0920	4.50	4.71	4.48	4.63	4.61	3.93
0921	1.11	1.09	1.14	1.15	1.43	1.61
0924	4.89	4.70	4.89	4.92	4.76	5.10
0925	2.43	2.59	2.59	2.30	3.08	2.53
0927	3.07	2.49	2.28	1.68	2.51	2.17
0928	1.12	1.26	1.20	1.09	0.97	1.34
0929	0.45	-0.04	0.09	-0.24	-0.43	-0.77
0930	1.05	1.30	1.34	1.33	1.42	1.25
0931	1.96	2.30	2.42	2.29	2.45	2.23
0932	2.41	2.59	2.59	2.57	2.53	2.29
0933	3.13	2.25	2.38	2.25	2.38	2.16
0934	2.72	2.62	2.57	2.48	2.59	2.17
0935	1.82	2.54	2.54	2.53	2.46	2.22

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0936	1.73	2.65	2.60	2.63	2.50	2.40
0937	1.54	2.44	2.54	2.54	2.24	2.32
0938	3.83	3.27	3.44	3.45	3.14	3.34
0939	3.42	3.17	3.11	3.19	3.20	3.10
0940	2.78	3.07	3.02	3.10	3.06	2.96
0941	3.86	3.39	3.55	3.54	2.95	3.29
0943	2.19	2.17	2.13	2.08	2.11	2.10
0944	2.10	2.94	2.88	2.73	2.75	2.69
0945	1.71	2.72	2.84	2.60	2.44	2.31
0946	3.24	3.14	3.30	3.36	2.82	3.16
0947	1.66	2.43	2.59	2.44	2.33	2.28
0950	2.72	2.46	2.57	2.32	2.47	2.23
0952	1.75	1.93	1.99	2.02	1.84	1.85
0954	1.97	2.03	2.09	2.31	1.56	2.16
0956	1.53	2.82	2.47	2.18	2.12	1.47
0958	1.86	1.61	1.59	1.40	1.81	1.33
0959	4.90	4.12	4.06	4.20	4.47	4.10
0960	2.43	2.72	2.74	2.57	2.12	2.10
0961	1.48	1.25	1.30	1.33	1.27	1.21
0962	1.81	1.65	1.69	1.66	1.37	1.29
0964	2.57	2.21	2.30	2.21	2.09	2.06
0965	0.79	1.81	1.80	1.93	1.80	1.79
0967	1.87	1.73	1.73	1.86	1.70	1.69
0968	2.80	2.48	2.60	2.44	2.35	2.36
0970	3.78	3.49	3.58	3.47	3.26	3.41
0971	1.54	1.56	1.68	1.66	1.78	1.90
0972	2.22	1.90	1.98	1.98	2.03	2.19
0973	1.65	1.57	1.59	1.73	1.53	1.52

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
0974	1.39	1.20	1.24	1.18	1.02	0.90
0975	1.04	2.12	2.08	2.25	1.82	1.82
0976	1.68	1.83	1.95	1.93	1.94	1.95
0980	1.83	1.64	1.68	1.69	1.52	1.51
0981	2.04	1.77	1.89	1.88	1.82	2.01
0983	2.76	2.07	2.11	1.94	1.90	1.89
0984	1.89	1.81	1.93	1.94	2.07	2.14
0986	1.07	0.86	0.95	1.03	0.88	1.09
0987	3.49	2.97	3.09	3.24	2.80	3.07
0988	3.21	2.71	2.83	2.96	2.55	2.82
0989	0.87	0.80	0.92	0.85	0.64	0.59
0990	1.46	1.31	1.45	1.46	1.30	1.51
0993	1.73	2.16	2.28	2.12	2.34	2.12
0994	2.74	2.70	2.81	2.79	2.40	2.51
0996	2.02	2.25	2.36	2.04	2.73	2.30
0997	2.20	3.19	3.35	3.09	3.17	3.04
1000	1.54	1.85	1.76	1.37	1.46	1.54
1001	2.30	1.57	1.48	1.22	2.10	1.87
1003	2.12	1.80	1.93	1.61	1.90	1.66
1004	1.72	2.10	2.10	1.88	1.98	1.87
1006	1.92	2.69	2.80	2.72	2.90	2.93
1007	0.00	1.20	1.23	0.92	1.82	1.49
1008	0.66	0.55	0.66	0.63	0.47	0.37
1010	1.70	2.29	2.46	2.19	2.70	2.36
1011	1.83	2.06	2.37	2.14	1.92	3.43
1012	0.40	0.93	1.05	1.02	0.90	0.96
1013	1.20	1.43	1.73	1.54	1.69	1.66
1014	1.45	1.71	2.02	1.90	1.89	1.90

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1015	2.67	2.36	2.44	2.34	2.23	2.38
1017	2.46	2.86	3.02	3.07	2.62	2.96
1018	1.54	2.87	3.09	2.88	2.32	2.16
1019	3.18	2.80	3.04	2.85	2.77	2.94
1020	0.96	0.99	1.19	1.07	1.21	1.12
1021	2.63	2.39	2.62	2.49	2.27	2.40
1023	2.45	2.34	2.51	2.43	2.27	2.43
1024	0.83	0.95	1.12	1.03	0.96	0.80
1025	2.48	2.96	3.14	3.06	3.03	3.09
1026	2.26	2.90	2.49	2.34	3.48	2.56
1027	4.51	3.88	4.24	4.14	4.44	4.78
1028	3.00	2.82	3.05	3.14	2.96	3.30
1030	3.21	3.82	3.91	3.77	3.70	3.76
1031	3.40	3.45	3.52	3.28	3.87	3.55
1032	3.07	2.51	2.63	2.78	2.46	2.91
1033	1.70	2.77	2.83	2.67	2.64	2.58
1034	2.26	1.63	1.63	1.18	1.22	1.47
1035	2.92	1.63	1.63	1.30	1.22	1.47
1037	2.01	2.24	2.29	2.12	2.17	2.00
1041	1.17	1.14	1.36	1.22	1.30	1.34
1042	0.81	0.87	1.06	0.94	0.99	0.83
1044	1.42	1.84	2.06	1.85	1.82	1.71
1045	0.85	0.83	1.00	0.90	0.75	0.48
1048	2.50	2.90	3.07	2.79	3.17	2.92
1050	3.24	3.09	3.16	3.06	2.95	3.25
1051	5.25	4.70	4.88	4.82	4.33	4.68
1052	2.66	2.41	2.39	2.02	3.03	2.52
1054	2.37	3.13	3.42	3.26	3.40	3.38

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1055	2.07	2.86	3.15	3.04	3.16	3.10
1056	1.93	2.60	2.88	2.60	2.91	2.83
1057	1.74	2.07	2.36	2.07	2.41	2.26
1058	1.29	1.78	2.03	1.80	2.07	1.87
1059	1.29	1.78	2.04	1.93	1.92	1.73
1060	1.96	2.30	2.42	2.36	2.45	2.23
1061	2.41	2.59	2.59	2.54	2.53	2.29
1063	2.49	2.47	2.44	2.37	2.45	2.32
1065	1.71	2.54	2.54	2.51	2.46	2.22
1067	1.34	2.96	3.02	3.07	2.84	2.90
1068	5.85	5.47	5.61	5.62	5.19	5.57
1069	4.15	4.88	4.71	4.88	2.99	2.93
1070	4.18	3.57	3.70	3.71	3.30	3.73
1072	3.04	2.83	2.89	2.80	2.70	2.98
1073	2.96	2.69	2.85	2.72	2.62	2.89
1074	4.80	4.43	4.61	4.55	4.08	4.43
1075	3.76	3.27	3.44	3.42	3.14	3.34
1078	2.67	2.54	2.53	2.55	2.41	2.31
1079	2.30	2.17	2.13	1.80	2.11	2.17
1082	3.30	3.13	3.28	3.27	2.78	3.13
1086	2.06	2.10	2.10	1.84	1.98	1.92
1087	2.63	2.52	2.57	2.43	2.37	2.26
1088	1.46	1.43	1.73	1.50	1.69	1.66
1089	3.40	2.53	2.48	2.71	2.29	2.85
1091	1.74	2.15	2.38	2.27	2.16	2.26
1092	3.51	1.13	1.09	1.17	1.20	0.81
1094	0.90	1.36	1.37	0.97	1.22	0.79
1095	1.44	1.08	1.14	1.19	1.58	1.32

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1098	5.00	4.27	3.98	4.44	4.63	4.18
1102	5.31	4.91	4.72	4.88	5.30	5.02
1103	3.23	3.24	3.35	3.06	3.50	3.45
1104	2.93	2.75	3.05	2.78	3.03	3.16
1105	1.74	1.29	1.36	1.31	1.85	1.98
1106	3.02	3.14	2.99	2.80	3.24	2.87
1110	3.23	3.01	3.06	3.08	2.91	2.97
1111	3.13	2.25	2.38	2.22	2.38	2.16
1112	2.68	2.62	2.57	2.52	2.59	2.17
1113	1.85	2.54	2.54	2.58	2.46	2.22
1115	1.69	2.44	2.54	2.53	2.24	2.32
1116	3.61	3.27	3.44	3.47	3.14	3.34
1117	2.78	3.07	3.02	3.17	3.06	2.96
1118	3.87	3.39	3.55	3.56	2.95	3.29
1119	2.54	2.54	2.53	2.68	2.41	2.31
1120	2.36	2.25	2.46	2.16	2.15	2.08
1121	2.17	2.17	2.13	2.39	2.11	2.05
1122	2.80	3.17	3.28	3.07	3.30	3.26
1123	3.33	4.02	4.30	4.11	4.54	4.40
1124	3.70	3.66	3.69	3.50	3.53	3.73
1127	2.95	2.91	2.59	2.81	3.17	3.22
1129	3.73	4.08	3.68	3.84	4.12	3.87
1130	0.46	-0.02	0.10	-0.16	-0.16	0.34
1131	3.86	3.71	3.87	3.90	3.21	3.56
1133	2.13	2.03	2.07	2.05	1.96	2.16
1135	4.04	3.64	3.80	3.77	3.33	3.68
1136	2.61	3.20	3.33	3.10	3.34	3.27
1137	5.00	4.39	4.44	4.44	5.05	4.61

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1138	4.78	4.05	4.48	4.31	4.81	5.16
1139	2.74	2.70	2.81	2.78	2.40	2.51
1140	3.35	3.13	3.28	3.32	2.78	3.13
1141	2.78	2.70	2.78	2.79	2.51	2.58
1142	3.77	3.35	3.64	3.56	3.70	4.04
1143	2.92	3.01	3.15	3.12	2.93	3.10
1144	2.74	2.49	2.62	2.57	2.48	2.60
1147	2.19	2.16	2.25	2.10	2.18	2.15
1148	3.33	3.13	3.26	3.14	3.01	3.04
1150	2.75	2.51	2.58	2.58	2.41	2.45
1152	2.06	1.88	2.04	1.88	1.77	1.74
1153	2.25	2.10	2.28	2.15	2.27	2.51
1154	1.35	1.67	1.90	1.70	1.90	1.65
1155	2.82	3.15	3.01	2.59	3.53	3.19
1156	2.93	3.77	3.57	3.54	3.85	3.32
1157	2.91	2.89	2.81	2.51	2.74	2.36
1158	0.85	1.93	1.93	1.52	2.90	2.53
1159	1.77	1.87	1.86	1.65	1.84	2.25
1160	2.25	1.99	2.05	1.89	1.79	1.94
1161	1.70	2.02	2.07	2.01	1.85	1.84
1164	3.70	3.85	3.82	3.89	3.97	3.90
1165	0.74	0.78	0.91	1.00	0.63	0.85
1166	1.83	1.64	1.78	1.84	1.64	1.97
1170	1.75	2.15	2.21	2.13	2.05	2.01
1171	2.13	1.80	1.93	1.51	1.90	1.66
1174	1.21	1.43	1.73	1.64	1.69	1.66
1175	4.13	3.79	3.72	3.68	4.09	3.76
1176	3.30	4.12	3.89	3.72	4.83	4.24

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1178	2.80	3.05	3.03	2.88	2.58	2.55
1180	2.42	2.64	2.80	2.48	2.85	2.68
1181	2.66	2.25	2.34	2.51	2.06	2.54
1182	2.48	2.94	2.95	2.74	3.28	2.89
1183	1.56	1.50	1.53	1.56	1.46	1.57
1184	3.60	4.30	4.40	4.44	3.48	3.58
1185	1.17	1.72	1.80	1.80	0.90	0.88
1187	1.83	2.58	2.71	2.51	2.84	2.71
1189	1.70	1.52	1.62	1.63	1.53	1.60
1190	1.46	1.65	1.73	1.73	1.74	1.75
1191	1.67	2.57	2.67	2.37	2.55	2.39
1193	1.51	1.53	1.64	1.64	1.40	1.57
1195	2.36	2.10	2.16	2.15	2.00	2.16
1196	1.64	1.37	1.49	1.50	1.38	1.59
1197	3.38	3.11	3.27	3.27	2.84	3.18
1198	0.36	0.93	1.02	0.93	0.74	0.90
1200	2.06	2.67	2.79	2.58	2.84	2.71
1201	4.66	4.06	4.37	4.33	4.36	4.68
1203	1.90	2.15	2.38	2.27	2.16	2.26
1205	4.38	3.52	3.88	3.74	4.08	4.43
1206	1.73	1.63	1.76	1.75	1.84	2.01
1208	2.07	2.02	2.07	2.00	1.85	1.89
1210	1.63	1.38	1.51	1.53	1.39	1.70
1211	2.48	2.41	2.58	2.51	2.58	2.82
1213	2.71	3.89	3.79	4.02	3.96	3.77
1214	2.55	3.15	3.04	3.03	3.39	2.79
1215	1.02	2.02	2.07	1.98	1.85	1.86
1217	2.57	1.94	1.96	1.80	1.85	2.04

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1218	2.37	1.99	1.99	1.90	1.77	2.24
1219	3.10	3.21	3.22	3.13	3.02	3.67
1220	3.30	2.50	2.50	2.41	2.27	2.82
1221	2.56	2.40	2.41	2.29	2.27	2.82
1222	2.71	2.60	2.62	2.50	2.52	3.11
1223	2.78	2.81	2.81	2.61	2.12	2.10
1224	1.73	1.75	1.85	1.84	1.65	1.84
1225	2.31	1.97	2.04	1.92	2.01	2.08
1228	2.31	3.05	3.35	3.05	3.31	3.14
1229	3.28	3.42	3.16	3.10	3.38	3.10
1230	2.08	2.49	2.44	2.21	2.04	1.90
1231	0.18	-0.47	-0.40	-0.84	-1.14	0.05
1232	4.14	1.90	2.47	2.31	2.49	4.26
1233	3.04	2.62	2.79	2.82	2.64	2.97
1235	0.84	1.32	1.40	1.52	1.67	1.53
1236	0.96	1.38	1.48	1.27	1.28	1.35
1239	4.08	4.14	4.00	3.69	4.46	4.14
1240	2.67	3.34	3.45	3.16	3.28	3.10
1241	1.83	2.34	2.37	2.02	2.18	2.00
1242	5.00	4.52	4.22	4.28	4.74	4.23
1243	1.63	2.12	2.26	2.08	1.95	1.67
1244	2.50	3.49	3.36	2.98	4.03	3.62
1246	2.18	2.85	2.81	2.27	3.40	2.94
1247	2.85	2.95	2.94	2.70	2.58	2.41
1248	2.32	2.83	2.81	2.63	2.53	2.32
1249	2.47	1.87	1.86	1.79	1.84	2.14
1250	3.81	3.35	3.52	3.58	3.36	3.72
1251	1.57	1.57	1.69	1.67	1.65	1.70

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1253	1.60	1.40	1.54	1.57	1.63	1.71
1254	3.61	3.11	3.30	3.30	3.06	3.40
1255	1.86	1.87	1.99	1.95	1.90	1.97
1256	2.31	2.64	2.41	2.62	3.11	3.51
1257	2.85	3.69	3.35	3.39	3.71	3.22
1258	1.80	3.32	2.98	3.29	2.78	3.37
1260	5.29	5.16	5.34	5.23	4.79	5.19
1261	4.70	4.41	4.52	4.43	4.20	4.55
1262	1.63	1.53	1.65	1.64	1.66	1.93
1264	3.24	2.61	2.69	2.50	2.87	2.89
1265	1.62	1.53	1.55	1.59	1.88	1.61
1266	2.04	2.06	2.11	1.89	2.54	2.19
1267	1.65	1.56	1.35	1.12	1.44	1.85
1268	1.60	1.69	1.50	1.29	1.50	1.62
1270	2.54	2.46	2.19	2.03	3.12	2.59
1271	3.26	2.81	2.80	2.38	2.30	1.74
1272	2.36	1.89	1.97	2.09	2.27	2.39
1273	3.01	3.07	2.96	2.57	2.47	2.12
1275	5.00	5.25	5.07	5.31	5.91	5.27
1276	2.43	1.85	1.84	2.00	2.39	2.18
1277	2.70	2.29	2.44	2.50	2.27	2.64
1279	2.63	2.25	2.38	2.51	2.16	2.58
1281	5.15	4.01	3.68	3.77	4.78	4.00
1282	3.19	4.39	4.44	4.52	5.05	4.61
1284	2.71	3.35	3.33	3.26	3.15	2.94
1285	1.95	3.12	3.13	3.01	3.01	2.84
1286	3.35	3.53	3.41	3.32	4.24	3.80
1287	3.70	4.64	4.58	4.13	5.42	5.30

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1288	1.90	1.89	1.63	1.62	2.53	1.97
1289	1.92	2.10	1.92	2.07	2.14	1.70
1290	0.99	1.73	1.61	1.62	1.69	0.92
1291	2.15	2.25	2.12	2.20	2.75	2.65
1292	2.75	3.15	2.83	3.11	2.61	2.60
1293	1.43	2.91	2.58	2.60	2.75	2.37
1294	3.09	2.57	2.64	2.40	2.59	2.59
1295	6.47	5.75	5.96	5.95	5.32	5.67
1296	3.31	4.83	5.01	5.00	4.60	4.94
1297	3.75	3.54	3.33	3.36	4.33	3.98
1298	2.74	2.90	2.87	2.63	2.30	2.23
1299	0.83	0.48	0.60	0.22	0.05	0.12
1302	1.44	1.38	1.29	1.26	1.17	0.41
1303	4.49	3.83	3.64	3.71	3.80	3.72
1304	2.30	2.45	2.14	2.37	2.10	1.63
1305	2.60	3.01	3.13	2.88	2.64	2.55
1306	1.02	1.36	1.30	0.98	1.81	1.54
1309	1.14	0.98	0.99	0.98	1.10	1.13
1312	4.36	3.88	4.24	4.13	4.44	4.78
1313	3.38	3.72	4.03	3.99	3.69	3.72
1314	4.47	4.55	4.84	4.86	3.35	3.53
1315	2.90	2.94	3.09	2.95	2.76	3.04
1316	5.81	5.23	5.42	5.38	4.83	5.18
1317	1.86	2.18	2.28	2.23	2.24	2.36
1318	2.04	2.01	2.05	1.94	1.93	1.88
1319	2.51	2.30	2.30	1.75	2.38	2.18
1321	2.43	3.72	3.61	3.58	3.33	2.95
1323	2.23	1.87	1.91	2.04	2.12	2.03

Code	Exp log Koc	Cal log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1324	2.13	1.82	1.86	1.95	2.03	1.94
1326	3.52	2.75	2.92	2.98	2.77	2.98
1328	3.27	2.88	3.06	3.07	2.89	3.22
1329	4.01	2.90	3.15	3.18	3.07	3.14
1330	1.03	1.40	1.46	1.38	1.36	1.42

Table 3.2 values of predicted log K_{OC} in a test set

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
9	2.37	2.51	2.70	2.49	2.93	3.25
11	2.54	2.22	2.15	2.21	2.39	2.18
13	1.73	2.02	2.21	1.93	2.38	2.03
16	3.52	3.84	3.59	3.70	3.90	3.79
18	2.62	2.49	2.75	2.73	2.46	2.73
23	2.61	2.52	2.40	2.51	2.47	2.30
24	3.34	3.14	3.30	3.33	2.82	3.16
26	3.61	3.43	3.59	3.64	3.02	3.36
28	3.35	3.14	3.30	3.34	2.82	3.16
30	2.91	2.74	2.35	2.59	2.84	2.71
33	2.47	2.33	2.29	2.45	2.33	2.26
34	6.10	4.51	4.92	4.75	4.69	5.02
35	2.85	2.90	2.82	2.99	2.34	2.21
40	0.88	0.93	1.02	1.03	0.74	0.90
42	2.46	2.06	2.19	2.32	2.02	2.39
43	3.05	2.32	2.53	2.59	2.57	2.90
49	0.81	0.75	0.88	0.71	0.74	0.87
51	0.93	1.09	1.22	1.16	0.99	1.13
56	3.10	2.84	3.00	3.10	2.86	3.21
57	3.76	3.39	3.61	3.72	3.36	3.68
63	0.86	0.77	0.87	0.83	0.72	0.67
65	2.42	2.67	2.62	2.44	2.66	2.24
68	2.60	3.12	3.07	3.21	3.13	2.87
71	3.75	3.38	3.45	3.38	3.29	3.50
74	3.21	2.85	2.91	2.88	2.79	2.97
75	2.52	2.32	2.36	2.40	2.29	2.41

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
77	2.68	2.28	2.40	2.51	2.16	2.58
81	3.50	3.21	3.33	3.39	3.38	3.49
83	2.49	2.23	2.28	2.33	2.20	2.31
84	3.86	3.39	3.55	3.36	3.14	3.41
85	4.17	3.92	4.09	3.88	3.64	3.92
87	2.78	2.34	2.40	2.44	2.27	2.42
90	2.80	2.59	2.73	2.61	2.40	2.64
93	3.23	2.81	2.95	2.98	2.66	3.07
94	2.86	3.15	3.24	3.30	2.31	2.69
95	1.71	2.00	2.16	2.00	2.08	2.15
96	1.45	1.39	1.52	1.53	1.41	1.41
103	2.22	2.47	2.69	2.71	2.64	2.77
104	2.92	2.68	2.86	2.87	2.78	2.89
108	1.85	1.91	1.92	1.86	1.58	1.47
115	2.57	2.53	2.68	2.58	2.61	2.72
116	2.16	2.16	2.35	2.19	2.31	2.43
117	1.57	2.17	2.33	2.26	2.26	2.38
118	0.48	1.53	1.64	1.64	1.40	1.57
120	4.54	4.18	4.37	4.15	3.89	4.17
121	3.95	3.65	3.82	3.62	3.39	3.66
123	3.41	3.65	3.31	3.41	3.48	3.25
124	3.30	3.65	3.31	3.48	3.48	3.25
130	2.11	1.95	1.79	1.82	2.01	1.52
133	5.82	5.49	5.12	5.34	5.79	5.68
142	5.64	5.49	5.12	5.30	5.79	5.68
143	4.80	5.10	4.83	4.96	5.38	5.26
148	4.89	4.72	4.55	4.60	4.96	4.86
149	4.26	3.89	4.11	4.06	3.99	4.37

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
151	2.09	1.88	1.99	1.99	1.81	2.02
153	3.83	5.49	5.12	5.36	5.79	5.68
155	3.03	3.41	3.23	3.19	3.63	3.22
163	5.21	4.33	4.26	4.22	4.54	4.49
164	1.96	3.31	3.11	3.12	3.29	2.89
166	4.05	3.78	3.43	3.41	3.84	3.41
167	2.88	3.70	3.40	3.52	3.71	3.34
172	3.76	3.00	3.11	3.10	2.63	2.77
174	2.55	2.93	2.83	2.79	2.87	2.52
179	3.77	3.39	3.61	3.66	3.36	3.68
183	5.21	4.33	4.26	4.29	4.54	4.49
185	1.96	3.31	3.11	3.22	3.29	2.89
186	1.72	3.14	2.88	2.98	3.14	2.82
195	0.67	2.64	2.66	2.57	2.80	2.45
200	2.45	2.46	2.50	2.39	2.31	2.33
201	2.66	2.72	2.83	2.82	2.43	2.55
203	4.70	3.95	3.98	4.01	4.13	4.14
208	3.00	2.57	2.50	2.25	2.74	2.16
210	0.53	2.49	2.49	2.32	2.49	1.96
213	2.55	2.93	2.83	2.85	2.87	2.52
217	3.61	3.12	2.92	3.05	3.29	3.07
222	4.48	2.92	3.29	3.04	3.43	3.58
223	2.60	2.98	2.87	2.88	2.94	2.44
225	1.96	2.58	2.71	2.62	2.64	2.49
230	2.75	2.57	2.62	2.67	2.69	2.73
231	1.51	2.10	2.21	2.05	2.07	1.66
237	1.61	2.05	2.18	1.99	2.32	1.84
242	2.29	2.30	2.33	2.32	2.11	2.21

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
244	3.71	3.41	3.57	3.54	2.98	3.33
245	3.76	3.37	3.59	3.63	3.32	3.65
247	1.31	1.78	1.94	1.74	1.99	1.51
248	2.13	2.34	2.45	2.33	2.30	2.43
249	2.63	2.55	2.67	2.56	2.39	2.64
254	2.03	2.20	2.32	2.27	2.36	2.57
259	0.96	0.95	1.06	1.05	0.91	0.95
260	1.60	2.15	2.21	2.13	2.05	2.01
261	2.57	2.51	2.67	2.68	2.44	2.52
265	4.18	3.63	3.93	3.90	3.90	4.22
273	2.65	2.05	2.15	2.24	2.46	2.64
283	2.96	2.87	3.11	2.87	2.97	2.98
284	3.11	3.13	3.36	3.18	3.14	3.29
296	1.93	2.17	2.32	2.04	2.49	2.08
299	1.84	2.20	2.31	2.02	2.66	2.23
304	2.36	2.41	2.42	2.25	2.61	2.25
307	5.00	4.72	4.55	4.71	4.96	4.86
314	0.67	2.64	2.66	2.49	2.80	2.45
320	2.51	2.46	2.41	2.08	2.31	2.39
321	2.66	2.72	2.83	2.81	2.43	2.55
325	2.55	1.74	1.77	1.54	1.84	1.79
331	1.73	1.80	1.93	1.62	1.90	1.66
336	2.01	2.22	2.34	2.10	2.69	2.35
337	2.94	2.52	2.48	2.49	2.52	2.39
341	1.95	2.45	2.61	2.36	2.82	2.54
343	1.86	2.17	2.29	2.07	2.62	2.28
346	2.54	2.54	2.54	2.53	2.46	2.22
353	2.28	2.32	2.43	2.38	2.15	2.38

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
357	1.44	1.17	1.32	0.71	1.44	1.32
359	2.07	1.94	2.05	2.02	1.80	1.88
360	2.61	2.38	2.38	2.15	2.18	2.17
361	0.63	2.10	2.21	2.18	2.19	2.22
364	1.75	2.07	2.22	2.06	2.19	1.78
367	1.65	2.15	2.38	2.27	2.16	2.26
376	1.94	1.73	1.85	1.47	2.14	1.97
379	2.04	2.06	2.16	2.13	1.90	2.11
384	1.29	1.78	2.03	1.76	2.07	1.87
389	2.36	2.41	2.42	2.20	2.61	2.25
392	4.15	3.74	3.98	3.91	3.69	4.01
396	2.60	2.98	2.87	2.90	2.94	2.44
400	2.42	2.57	2.66	2.63	2.69	2.47
401	1.96	2.30	2.42	2.24	2.45	2.23
402	2.93	2.52	2.48	2.50	2.52	2.39
413	3.83	3.41	3.57	3.58	2.98	3.33
419	1.43	1.94	1.96	1.89	1.85	1.97
422	1.40	1.78	1.97	1.69	2.21	2.04
433	2.24	2.23	2.38	2.30	2.10	2.22
435	3.90	3.46	3.70	3.63	3.49	3.81
436	1.76	3.15	3.38	3.15	2.52	2.38
439	2.04	1.91	2.04	2.00	2.04	2.25
442	1.54	2.02	1.99	1.93	1.98	2.04
443	2.37	2.10	2.10	1.93	1.98	1.84
444	2.84	2.85	2.98	2.87	2.64	2.90
445	2.56	2.57	2.81	2.64	3.05	2.84
447	2.79	2.51	2.72	2.60	2.91	3.18
448	3.12	2.97	3.07	3.02	2.65	2.79

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
450	5.17	4.97	5.20	5.28	5.12	5.45
455	2.40	2.24	2.37	2.31	2.44	2.49
456	2.61	2.38	2.38	2.11	2.18	2.17
457	2.97	2.77	2.91	2.80	2.93	3.02
461	5.29	2.27	2.38	2.26	2.39	2.41
465	3.43	2.93	3.18	3.02	3.00	3.16
466	3.33	3.63	3.93	3.92	3.90	4.22
467	4.14	3.17	3.44	3.34	3.03	3.36
468	3.53	1.18	1.20	0.72	1.94	1.42
470	1.83	1.13	1.24	1.26	1.28	1.28
473	2.01	1.12	1.15	1.21	1.21	1.26
480	1.58	3.86	3.51	3.84	4.19	4.06
483	1.37	1.16	1.31	1.35	0.93	0.65
485	1.57	1.67	1.74	1.76	1.60	1.52
487	1.42	1.85	1.94	2.06	2.17	2.13
490	1.30	1.32	1.34	1.22	1.25	0.89
493	4.69	1.96	2.07	2.28	1.76	2.12
495	1.91	1.39	1.50	1.49	1.26	1.33
502	2.00	2.18	2.37	2.27	2.16	2.32
508	3.86	3.14	3.34	3.10	3.51	3.74
509	2.74	2.86	3.08	2.98	2.72	2.86
512	2.48	2.71	2.67	2.49	2.29	2.18
515	3.17	3.55	3.35	2.76	2.93	2.46
516	2.69	3.67	3.71	3.72	3.77	3.79
519	1.34	2.09	2.19	1.95	2.37	2.28
520	2.76	3.79	3.61	3.68	3.80	3.72
522	3.28	2.25	2.18	2.12	1.75	1.85
524	3.00	1.63	1.87	1.45	1.92	1.95

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
525	1.53	3.88	4.24	4.12	4.44	4.78
527	2.50	2.16	2.29	2.22	2.11	2.17
528	2.18	2.20	2.27	2.05	2.03	1.75
529	1.80	1.72	1.92	1.74	1.65	1.49
535	2.14	2.51	2.66	2.59	2.52	2.62
536	2.31	2.40	2.56	2.44	2.18	2.32
539	5.13	2.47	2.61	2.63	2.70	2.93
540	2.83	2.08	2.15	2.07	2.04	2.15
541	1.95	2.23	2.35	2.27	2.15	2.21
544	2.47	2.67	2.79	2.87	3.00	3.22
555	1.69	4.93	4.92	5.10	5.40	4.88
559	1.99	3.43	3.60	3.45	3.34	3.45
562	1.97	1.51	1.45	1.56	1.45	1.12
567	2.25	3.85	3.50	3.85	3.80	3.68
568	0.33	2.53	2.36	2.54	2.72	2.70
569	2.67	2.88	2.58	2.84	2.36	2.35
572	2.23	3.99	4.13	3.75	3.80	3.72
574	1.26	2.51	2.61	2.75	2.30	2.77
575	2.95	3.60	3.67	3.48	3.71	3.95
578	2.66	2.98	3.08	2.93	2.84	2.89
586	1.86	2.68	2.93	2.57	2.96	2.99
587	1.71	1.77	1.80	1.80	1.71	1.87
591	2.30	2.69	2.87	2.76	2.78	2.64
597	3.24	3.32	2.98	3.29	2.78	3.37
599	2.02	3.85	3.59	3.55	4.11	3.49
600	4.66	4.25	4.02	3.95	4.61	4.09
604	1.25	2.42	2.36	2.18	2.60	2.16
611	2.04	2.65	2.51	2.34	2.32	2.32

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
612	3.94	2.60	2.68	2.45	2.66	2.44
613	1.50	1.43	1.37	1.48	1.35	1.02
615	3.30	3.73	3.70	3.78	3.57	3.32
617	1.65	1.69	1.66	1.77	1.89	1.37
622	2.43	2.57	2.74	2.46	2.90	2.61
629	2.26	3.01	2.96	2.80	2.83	2.30
630	4.49	3.88	4.24	4.13	4.44	4.78
635	2.39	1.85	1.84	1.80	2.39	2.18
642	0.44	0.47	0.35	0.10	0.36	1.78
650	3.55	3.09	3.20	3.35	2.89	3.30
658	3.01	2.56	2.67	2.82	2.40	2.81
661	5.26	4.59	4.48	4.60	5.33	4.64
666	3.70	3.67	3.29	3.32	3.62	3.17
667	5.87	7.03	6.26	6.64	7.46	7.75
668	4.78	4.10	4.25	4.20	3.80	4.21
669	3.60	3.36	3.43	3.33	3.20	3.52
670	5.38	4.96	5.15	5.10	4.58	4.93
673	4.94	5.63	5.71	5.77	5.26	5.12
680	3.18	3.10	3.33	3.19	3.32	3.48
690	2.06	2.10	2.04	2.17	2.26	2.11
693	1.67	1.84	1.58	1.41	2.86	2.19
697	1.66	1.31	1.31	1.09	2.04	1.75
699	4.37	4.35	4.51	4.56	4.22	4.04
705	1.82	1.95	2.06	2.02	2.03	2.18
707	1.68	1.65	1.62	1.60	1.22	1.23
713	1.69	1.52	1.66	1.64	1.54	1.78
716	1.18	1.11	1.25	1.03	1.34	1.38
718	4.06	3.36	3.35	3.21	3.44	2.93

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
719	1.49	1.51	1.49	1.60	1.72	1.57
720	2.74	2.57	2.49	2.66	2.31	2.16
723	2.20	2.11	2.23	2.19	2.31	2.54
724	2.14	1.95	2.09	2.06	2.04	2.30
732	0.64	1.05	1.20	1.16	1.15	0.96
733	2.60	2.13	2.15	2.05	1.96	1.89
736	3.14	3.67	3.71	3.50	3.45	3.52
742	3.67	3.20	3.36	3.34	3.37	3.50
743	3.80	3.53	3.66	3.64	3.60	3.73
746	3.63	3.44	3.68	3.66	3.24	3.57
748	3.07	3.25	3.24	3.07	2.83	2.82
749	2.48	2.28	2.41	2.33	2.32	2.54
755	1.81	2.32	2.22	2.22	2.12	2.41
759	2.41	3.18	2.98	2.65	3.00	2.50
764	4.20	3.21	3.13	3.16	4.01	4.34
766	3.12	3.65	3.63	3.39	3.48	3.18
771	2.36	1.98	2.05	2.26	1.81	2.32
775	1.77	1.45	1.51	1.50	1.52	1.51
776	1.51	1.40	1.46	1.39	1.49	1.52
784	2.06	2.63	2.71	2.60	2.51	2.62
786	2.43	2.11	2.16	2.11	1.87	1.88
792	1.94	1.62	1.75	1.71	1.90	2.01
798	2.73	2.84	3.00	3.03	2.59	2.93
802	0.27	0.38	0.51	0.44	0.45	0.57
804	2.68	2.95	3.09	3.13	2.22	2.57
805	3.00	3.00	2.61	2.68	2.92	2.16
810	2.78	3.46	3.48	3.57	3.75	3.46
814	3.65	3.60	3.44	3.63	3.78	3.73

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
817	2.52	2.87	2.79	2.81	3.13	2.74
818	3.18	3.51	3.34	3.31	3.76	3.40
822	3.72	5.04	5.12	5.73	5.41	4.97
823	3.08	4.47	3.95	4.06	3.88	3.08
825	3.55	3.71	3.45	3.59	3.69	3.43
826	5.00	5.13	5.08	5.96	5.38	4.85
827	4.00	4.44	4.15	4.47	4.56	4.32
828	1.96	2.45	2.50	2.22	2.94	2.46
835	6.00	5.46	5.39	6.19	5.87	5.31
841	1.08	1.07	1.09	1.19	0.96	1.00
842	1.63	1.26	1.20	1.24	0.97	1.34
843	2.11	1.78	1.86	1.97	1.97	2.09
844	1.60	1.81	1.85	1.80	1.85	1.88
852	3.46	0.36	0.27	-0.10	0.38	0.77
854	3.23	3.53	3.38	3.54	3.65	3.74
855	2.63	2.69	2.38	2.59	2.75	2.01
861	4.12	3.26	2.93	3.09	4.06	4.38
867	2.47	2.51	2.14	2.39	2.50	3.01
874	2.42	2.30	2.34	2.29	2.21	2.44
876	2.50	2.16	2.31	2.22	2.13	2.38
878	3.79	4.38	4.47	4.35	4.33	4.23
881	1.82	1.59	1.64	1.53	1.55	1.77
882	3.73	3.18	3.27	2.84	3.79	3.61
889	2.54	2.47	2.70	2.60	2.54	2.76
894	2.85	3.44	3.44	3.27	2.99	2.85
895	2.01	3.25	3.01	2.81	3.19	2.67
898	2.35	1.94	2.01	1.97	1.92	1.84
899	2.59	2.34	2.40	2.30	2.03	1.93

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
901	3.56	3.25	3.43	3.43	2.99	3.20
906	2.30	2.51	2.68	2.59	2.63	2.80
910	1.40	1.45	1.55	1.57	1.40	1.57
913	1.52	1.28	1.40	1.46	1.38	1.59
914	2.35	2.60	2.88	2.66	3.00	2.81
916	2.47	2.30	2.43	2.17	2.47	2.41
917	2.40	3.50	3.57	3.19	3.72	3.70
918	0.99	1.01	1.02	0.93	0.80	1.08
923	5.21	4.96	5.13	5.14	4.91	5.25
942	2.58	2.54	2.53	2.61	2.41	2.31
948	2.38	1.30	1.37	1.31	2.08	2.21
949	1.55	1.54	1.66	1.46	1.36	1.23
951	1.88	1.78	1.80	1.81	1.56	1.65
953	0.70	1.19	1.13	0.95	1.83	1.20
955	3.48	3.12	3.02	2.99	2.07	1.65
957	2.25	3.04	3.09	2.83	2.90	2.66
963	0.97	1.03	1.10	1.19	0.90	1.02
966	2.08	1.90	1.95	1.93	1.76	1.80
969	1.12	1.28	1.29	1.32	1.20	0.82
977	0.78	1.82	1.80	1.88	1.61	1.17
978	2.13	1.91	1.95	1.94	1.62	1.59
979	2.64	2.73	2.57	2.54	2.74	2.26
982	1.83	1.83	1.95	1.91	2.03	2.18
985	1.89	2.35	2.43	2.59	1.56	1.92
991	2.74	2.93	2.85	2.69	3.18	2.63
992	2.15	2.55	2.56	2.40	2.76	2.32
995	3.54	3.13	3.28	3.30	2.78	3.13
998	1.72	2.28	2.41	2.07	2.71	2.33

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
999	1.71	2.17	2.07	2.04	1.39	1.17
1002	2.30	1.57	1.48	1.20	2.10	1.87
1005	2.71	2.52	2.57	2.39	2.37	2.26
1009	2.10	2.20	2.31	2.02	2.66	2.23
1016	1.74	2.15	2.38	2.27	2.16	2.26
1022	1.80	1.96	2.19	1.99	2.04	1.97
1029	2.54	3.07	3.36	3.24	3.37	3.35
1036	2.24	3.27	3.02	3.03	3.42	3.16
1038	1.48	1.61	1.62	1.57	1.33	1.14
1039	2.26	1.28	0.95	0.73	0.50	0.99
1040	1.20	1.40	1.41	1.37	1.08	0.82
1043	2.28	2.19	2.41	2.29	2.25	2.36
1046	2.04	1.89	2.09	2.05	1.81	2.02
1047	1.88	1.69	1.82	1.83	1.61	1.94
1049	4.45	3.83	3.97	3.95	3.55	3.97
1053	2.80	2.75	3.02	2.77	3.03	2.99
1062	3.13	2.25	2.38	2.32	2.38	2.16
1064	2.60	2.62	2.57	2.41	2.59	2.17
1066	3.24	2.96	3.02	3.07	2.84	2.90
1071	2.87	2.97	3.09	2.99	2.98	3.18
1076	2.78	3.07	3.02	3.06	3.06	2.96
1077	3.78	3.39	3.55	3.55	2.95	3.29
1080	2.32	2.41	2.64	2.48	2.32	2.45
1081	2.72	2.70	2.81	2.80	2.40	2.51
1083	5.53	5.22	5.37	5.37	5.05	5.41
1084	2.38	1.80	1.93	1.70	1.90	1.66
1085	2.32	2.23	2.24	1.97	2.17	2.01
1090	2.64	2.36	2.44	2.36	2.23	2.38

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1093	3.51	4.27	4.13	4.07	3.84	3.60
1096	1.98	1.58	1.78	1.39	1.98	2.09
1097	1.00	1.59	1.59	1.29	2.36	2.00
1099	2.70	2.86	3.02	3.05	2.62	2.96
1100	3.36	3.63	3.46	3.38	2.79	2.60
1101	4.82	4.68	4.56	4.74	5.10	5.01
1107	5.36	2.31	2.70	2.46	2.76	2.80
1108	1.96	2.30	2.42	2.24	2.45	2.23
1109	2.41	2.59	2.59	2.62	2.53	2.29
1114	3.19	2.96	3.02	3.04	2.84	2.90
1125	4.62	3.79	3.51	3.50	4.05	3.68
1126	4.10	4.22	3.87	4.06	4.31	4.32
1128	3.70	4.16	3.71	3.75	4.25	4.06
1132	3.25	2.77	2.89	2.98	2.55	3.00
1134	2.19	1.90	2.04	1.98	1.88	2.12
1145	3.40	3.22	3.34	2.98	3.57	3.36
1146	1.74	2.16	2.26	2.26	2.04	2.09
1149	2.06	2.12	2.18	2.07	1.93	1.87
1151	1.45	2.10	2.20	2.07	1.99	2.14
1162	2.11	2.02	2.09	2.05	1.92	1.92
1163	1.20	2.51	2.28	2.03	2.63	2.18
1167	3.44	3.54	3.56	3.17	3.83	3.70
1168	1.90	2.40	2.48	2.25	1.93	1.85
1169	3.00	3.04	2.94	2.68	2.76	2.45
1172	2.72	2.10	2.10	1.93	1.98	1.84
1173	2.69	2.52	2.57	2.38	2.37	2.26
1177	4.01	3.80	3.66	3.44	3.80	3.59
1179	2.31	3.64	3.66	3.59	3.15	2.70

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1186	2.19	2.93	2.90	2.76	2.53	2.46
1188	3.39	3.44	3.39	3.22	3.48	3.38
1192	2.05	1.75	1.82	1.78	1.76	1.80
1194	1.83	1.71	1.76	1.65	1.52	1.51
1199	2.34	2.02	2.13	2.27	1.91	2.33
1202	2.65	2.36	2.44	2.33	2.23	2.38
1204	2.77	2.86	3.02	3.08	2.62	2.96
1207	1.16	1.27	1.33	1.35	1.46	1.46
1209	1.79	1.77	1.96	1.95	1.80	1.95
1212	1.87	1.99	2.10	2.10	2.19	2.30
1216	2.36	2.02	2.09	1.94	1.92	1.95
1226	3.86	3.25	3.43	3.44	3.19	3.40
1227	2.00	3.23	3.29	3.05	4.02	3.86
1234	1.06	1.03	1.00	1.05	1.11	1.50
1237	1.62	1.97	2.03	1.55	2.04	2.19
1238	1.89	1.84	1.89	1.37	1.98	2.42
1245	2.18	2.90	2.78	2.60	3.19	2.86
1252	2.33	1.79	1.87	1.86	2.01	1.93
1259	3.30	1.70	1.46	1.32	1.81	2.24
1263	1.83	1.80	1.89	1.93	1.91	2.21
1269	3.27	3.40	3.45	3.31	3.73	3.44
1274	1.97	2.58	2.73	2.79	2.42	2.76
1278	3.01	2.52	2.68	2.74	2.52	2.89
1280	2.37	2.29	2.42	2.42	2.15	2.21
1283	3.99	3.45	3.71	3.65	3.61	3.94
1300	1.81	1.96	1.95	1.58	2.56	2.39
1301	2.17	2.03	2.17	2.11	2.01	2.27
1307	1.46	1.42	1.52	1.57	1.27	1.48

Code	Exp log Koc	Pred log Koc				
		Model 1	Model 2	Model 3	Model 4	Model 5
1308	0.57	0.88	1.00	0.76	0.74	1.05
1310	3.87	4.10	4.17	3.92	4.55	4.38
1311	4.50	4.23	4.55	4.50	4.44	4.61
1320	2.33	3.21	3.32	3.10	3.30	3.26
1322	1.77	1.30	1.37	1.35	1.59	1.51
1325	1.60	1.69	1.79	1.75	1.84	1.85
1327	1.54	1.56	1.59	1.67	1.55	1.40
1331	3.83	3.24	3.42	3.47	3.26	3.48

Table C-1 Adjustment of the correlation of model 1

Eq. no.	Outlier	n	r^2	q^2
1	-	928	0.598	0.596
2	492 488	926	0.607	0.606
3	497 812	924	0.617	0.616
4	460 500	922	0.625	0.623
5	570 501	920	0.633	0.629
6	510 1092	918	0.644	0.642
7	1232 601	916	0.652	0.651
8	634 765	914	0.660	0.659
9	752 589	912	0.672	0.671
10	504 537	910	0.676	0.675
11	735 482	908	0.681	0.680
12	863 139	906	0.682	0.681
13	576 175	904	0.688	0.688
14	526 2	902	0.692	0.691
15	173 202	900	0.697	0.696
16	209 322	898	0.702	0.701
17	806 1258	896	0.706	0.705
18	169 171	894	0.709	0.706
19	609 462	892	0.711	0.710
20	1285 289	890	0.712	0.711
21	1257 753	888	0.713	0.712
22	1220 1296	886	0.715	0.714
23	240 554	884	0.717	0.717
24	105 276	882	0.720	0.719
25	136 762	880	0.722	0.721
26	328 1290	878	0.725	0.724
27	474 1058	876	0.728	0.726

Eq. no.	Outlier	n	r^2	q^2
28	837 295	874	0.730	0.729
29	582 665	872	0.732	0.731
30	644 847	870	0.734	0.733
31	494 420	868	0.736	0.736
32	390 676	866	0.738	0.738
33	641 1282	864	0.739	0.737
34	1191 416	862	0.741	0.739
35	938 141	860	0.743	0.739
36	305 306	858	0.745	0.743
37	602 608	856	0.747	0.747
38	1281 1213	854	0.750	0.749
39	839 1287	852	0.754	0.753
40	1321 596	850	0.757	0.756

Table C-2 Adjustment of the correlation of model 2

Eq. no.	Outlier	n	r^2	q^2
1	-	928	0.614	0.610
2	1296 470	926	0.610	0.605
3	1012 701	924	0.607	0.604
4	173 556	922	0.610	0.607
5	202 209	920	0.614	0.611
6	322 472	918	0.616	0.613
7	1158 354	916	0.616	0.613
8	328 1215	914	0.618	0.615
9	477 488	912	0.621	0.618
10	1067 474	910	0.623	0.621
11	497 821	908	0.627	0.625
12	14 300	906	0.627	0.625
13	1293 366	904	0.628	0.626
14	530 302	902	0.628	0.624
15	937 1018	900	0.630	0.626
16	809 739	898	0.630	0.621
17	479 498	896	0.631	0.625
18	1281 1242	894	0.631	0.625
19	430 565	892	0.632	0.628
20	1243 808	890	0.632	0.629
21	947 416	888	0.634	0.628
22	1033 589	886	0.636	0.632
23	875 993	884	0.637	0.633
24	765 1057	882	0.640	0.635
25	1091 434	880	0.640	0.633
26	837 295	878	0.642	0.633
27	774 806	876	0.644	0.638

Eq. no.	Outlier	n	r^2	q^2
28	803 935	874	0.644	0.639
29	1011 424	872	0.646	0.641
30	1187 582	870	0.648	0.642
31	415 411	868	0.650	0.644
32	382 1006	866	0.651	0.647
33	1056 592	864	0.651	0.645
34	549 912	862	0.653	0.648
35	1285 169	860	0.655	0.651
36	171 189	858	0.657	0.651
37	333 501	856	0.661	0.652
38	334 397	854	0.662	0.654
39	398 883	852	0.663	0.655
40	481 1200	850	0.665	0.655
41	1055 294	848	0.666	0.659
42	944 563	846	0.667	0.661
43	420 773	844	0.670	0.661
44	1246 507	842	0.672	0.667
45	663 478	840	0.673	0.666
46	1228 390	838	0.675	0.667
47	570 1180	836	0.679	0.676
48	714 1017	834	0.679	0.674
49	1249 1025	832	0.680	0.673
50	1182 463	830	0.680	0.675
51	158 176	828	0.681	0.676
52	175 1329	826	0.683	0.677
53	571 859	824	0.685	0.677
54	2 306	822	0.687	0.682
55	141 139	820	0.689	0.683
56	276 1287	818	0.690	0.682

Eq. no.	Outlier	n	r^2	q^2
57	550 105	816	0.691	0.687
58	1089 1326	814	0.692	0.686
59	603 892	812	0.693	0.683
60	558 1123	810	0.695	0.693
61	206 482	808	0.697	0.691
62	510 927	806	0.707	0.700
63	834 691	804	0.707	0.705
64	505 880	802	0.708	0.702
65	257 638	800	0.708	0.701
66	573 726	798	0.711	0.709
67	1217 607	796	0.712	0.706
68	523 783	794	0.713	0.706
69	1136 1279	792	0.713	0.711
70	885 375	790	0.714	0.708
71	1015 1240	788	0.714	0.718
72	395 194	786	0.715	0.713
73	735 52	784	0.717	0.712
74	605 793	782	0.719	0.713
75	983 745	780	0.720	0.717
76	904 1122	778	0.720	0.715
77	779 44	776	0.720	0.715
78	752 1257	774	0.729	0.723
79	492 427	772	0.738	0.733
80	3 965	770	0.739	0.734
81	4 7	768	0.739	0.734
82	526 584	766	0.743	0.741
83	451 459	764	0.744	0.740
84	403 160	762	0.746	0.739
85	769 665	760	0.748	0.748

Eq. no.	Outlier	n	r^2	q^2
86	664 561	758	0.749	0.746
87	812 945	756	0.758	0.757
88	1065 383	754	0.759	0.756
89	292 936	752	0.761	0.757
90	385 423	750	0.761	0.759
91	1241 293	748	0.761	0.758
92	1113 506	746	0.762	0.759
93	789 399	744	0.762	0.760
94	310 606	742	0.764	0.761
95	102 644	740	0.764	0.762
96	847 730	738	0.767	0.766
97	197 553	736	0.769	0.767
98	1244 46	734	0.770	0.766
99	807 31	732	0.771	0.767
100	291 431	730	0.771	0.768
101	655 1044	728	0.771	0.766
102	811 1092	726	0.778	0.773
103	1184 863	724	0.781	0.773
104	1007 1059	722	0.781	0.771
105	373 1258	720	0.782	0.773
106	1048 6	718	0.783	0.775
107	968 911	716	0.783	0.780
108	566 1321	714	0.786	0.774
109	763 609	712	0.788	0.785
110	521 356	710	0.789	0.787
111	988 576	708	0.793	0.790
112	344 710	706	0.793	0.791
113	499 301	704	0.794	0.789
114	15 1078	702	0.793	0.790

Eq. no.	Outlier	n	r^2	q^2
115	281 204	700	0.794	0.790
116	64 554	698	0.796	0.795
117	1313 997	696	0.798	0.792
118	741 583	694	0.802	0.793

Table C-3 Adjustment of the correlation of model 3

Eq. no.	Outlier	n	r^2	q^2
1	-	928	0.622	0.616
2	427 752	926	0.631	0.625
3	173 202	924	0.634	0.628
4	209 322	922	0.639	0.632
5	601 488	920	0.645	0.640
6	497 526	918	0.652	0.648
7	175 576	916	0.657	0.651
8	847 769	914	0.661	0.653
9	570 501	912	0.668	0.661
10	558 492	910	0.675	0.670
11	589 837	908	0.680	0.677
12	762 634	906	0.687	0.679
13	1092 1232	904	0.694	0.686
14	1067 821	902	0.696	0.686
15	460 482	900	0.705	0.699
16	683 459	898	0.706	0.701
17	474 500	896	0.713	0.702
18	504 1296	894	0.717	0.712
19	765 554	892	0.722	0.717
20	927 863	890	0.726	0.721
21	328 583	888	0.729	0.726
22	573 498	886	0.732	0.726
23	739 479	884	0.734	0.730
24	937 1018	882	0.736	0.732
25	1191 416	880	0.738	0.731
26	420 773	878	0.740	0.733
27	169 171	876	0.742	0.732

Eq. no.	Outlier	n	r^2	q^2
28	609 462	874	0.745	0.737
29	1035 1143	872	0.747	0.742
30	641 1282	870	0.750	0.741
31	753 510	868	0.760	0.752
32	139 141	866	0.764	0.761
33	806 1258	864	0.767	0.763
34	1171 763	862	0.769	0.762
35	1034 478	860	0.771	0.768
36	663 1001	858	0.772	0.769
37	286 537	856	0.776	0.770
38	934 735	854	0.778	0.775
39	933 1111	852	0.780	0.775
40	305 306	850	0.782	0.777
41	430 563	848	0.783	0.779
42	875 936	846	0.785	0.780
43	582 665	844	0.787	0.781
44	1285 189	842	0.789	0.786
45	224 310	840	0.791	0.788
46	463 812	838	0.800	0.795

Table C-4 Adjustment of the correlation of model 4

Eq. no.	Outlier	n	r^2	q^2
1	-	928	0.552	0.549
2	510 492	926	0.567	0.561
3	460 672	924	0.572	0.571
4	812 1092	922	0.580	0.578
5	501 537	920	0.587	0.583
6	497 608	918	0.598	0.596
7	609 774	916	0.604	0.601
8	570 893	914	0.610	0.608
9	173 202	912	0.615	0.612
10	209 322	910	0.620	0.617
11	175 500	908	0.626	0.625
12	474 809	906	0.630	0.628
13	634 752	904	0.647	0.646
14	176 837	902	0.651	0.648
15	576 641	900	0.656	0.655
16	481 482	898	0.660	0.658
17	462 1244	896	0.663	0.661
18	735 1035	894	0.668	0.667
19	554 1282	892	0.672	0.670
20	526 765	890	0.678	0.674
21	488 605	888	0.681	0.679
22	581 582	886	0.684	0.683
23	671 644	884	0.687	0.686
24	306 803	882	0.690	0.689
25	507 573	880	0.693	0.693
26	139 141	878	0.699	0.697
27	769 1287	876	0.703	0.700

Eq. no.	Outlier	n	r^2	q^2
28	589 1246	874	0.706	0.705
29	1213 807	872	0.709	0.706
30	1158 328	870	0.715	0.710
31	806 169	868	0.718	0.716
32	1067 808	866	0.721	0.718
33	171 189	864	0.724	0.721
34	136 1296	862	0.727	0.724
35	1176 310	860	0.730	0.728
36	601 1232	858	0.735	0.732
37	663 2	856	0.738	0.736
38	579 834	854	0.740	0.739
39	1123 558	852	0.743	0.741
40	730 549	850	0.745	0.743
41	134 135	848	0.747	0.746
42	1034 701	846	0.747	0.746
43	505 566	844	0.749	0.749
44	1089 504	842	0.752	0.751
45	1220 498	840	0.754	0.753
46	847 863	838	0.758	0.758
47	1257 1258	836	0.760	0.759
48	1191 1285	834	0.762	0.761

Table C-5 Adjustment of the correlation of model 5

Eq. no.	Outlier	n	r^2	q^2
1	-	928	0.637	0.623
2	492 812	926	0.644	0.622
3	460 1011	924	0.655	0.647
4	537 1092	922	0.666	0.654
5	501 497	920	0.673	0.660
6	608 609	918	0.677	0.667
7	252 500	916	0.680	0.668
8	173 202	914	0.683	0.669
9	209 322	912	0.687	0.675
10	837 774	910	0.692	0.681
11	806 1258	908	0.694	0.682
12	175 176	906	0.698	0.687
13	570 893	904	0.703	0.696
14	462 1244	902	0.706	0.698
15	1213 735	900	0.709	0.700
16	505 564	898	0.711	0.706
17	510 672	896	0.714	0.708
18	1296 590	894	0.717	0.710
19	139 141	892	0.722	0.717
20	305 306	890	0.726	0.719
21	474 809	888	0.729	0.723
22	553 583	886	0.732	0.721
23	481 507	884	0.737	0.729
24	573 482	882	0.742	0.736
25	641 1282	880	0.745	0.734
26	1271 558	878	0.749	0.740
27	576 634	876	0.755	0.749

Eq. no.	Outlier	n	r^2	q^2
28	554 1035	874	0.758	0.752
29	863 1287	872	0.762	0.758
30	2 571	870	0.765	0.759
31	663 730	868	0.768	0.761
32	134 135	866	0.771	0.763
33	549 1256	864	0.773	0.761
34	381 1055	862	0.775	0.764
35	997 596	860	0.777	0.768
36	169 171	858	0.779	0.769
37	189 310	856	0.780	0.772
38	644 498	854	0.784	0.777
39	582 464	852	0.786	0.780
40	834 671	850	0.788	0.781
41	605 752	848	0.790	0.786
42	1069 488	846	0.794	0.789
43	581 726	844	0.797	0.795
44	526 765	842	0.799	0.798
45	105 136	840	0.804	0.802

Table D-1 The statistical data of each group

Gr.	Nov.	used SlogP		Added properties											
		r_m^2	q_m^2	r_n^2	Δr^2	*%increase	%increase /nov.	r_n^2/ nov.	**%increase	q_n^2	Δq^2	*%increase	%increase /nov.	q_n^2 / nov.	**%increase
1	1	0.344	0.310	0.344	0.000	0.00	0.00	0.344	0.00	0.310	0.000	0.00	0.00	0.31	0.00
2	1	0.494	0.339	0.494	0.000	0.00	0.00	0.494	0.00	0.339	0.000	0.00	0.00	0.34	0.00
3	2	0.922	0.877	0.960	0.038	4.12	4.12	0.480	-47.94	0.895	0.018	2.05	2.05	0.45	-48.97
4	2	0.278	0.225	0.334	0.056	20.14	20.14	0.167	-39.93	0.188	-0.037	-16.44	-16.44	0.09	-58.22
5	2	0.517	0.403	0.723	0.206	39.85	39.85	0.362	-30.08	0.693	0.290	71.96	71.96	0.35	-14.02
6	2	0.738	0.723	0.796	0.058	7.86	7.86	0.398	-46.07	0.742	0.019	2.63	2.63	0.37	-48.69
7	2	0.370	-0.401	0.546	0.176	47.57	47.57	0.273	-26.22	-0.407	-0.006	-1.50	-1.50	-0.20	-49.25
8	3	0.555	0.550	0.647	0.092	16.58	8.29	0.216	-61.14	0.607	0.057	10.36	5.18	0.20	-63.21
9	4	0.594	0.582	0.665	0.071	12.00	4.00	0.166	-72.00	0.614	0.032	5.41	1.80	0.15	-73.65
10	4	0.566	0.562	0.639	0.073	12.90	4.30	0.160	-71.78	0.627	0.065	11.57	3.86	0.16	-72.11
11	4	0.326	0.316	0.417	0.091	27.91	9.30	0.104	-68.02	0.281	-0.035	-11.08	-3.69	0.07	-77.77

Where, nov = number of variable (number of properties showed in **table 3.2**)

$\Delta r^2 = r_n^2 - r_m^2$, $\Delta q^2 = q_n^2 - q_m^2$

* % increase of $r^2 = \frac{\Delta r^2}{r_m^2} \times 100$, * % increase of $q^2 = \frac{\Delta q^2}{q_m^2} \times 100$

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