Technical Appendix B

Physicochemical Properties for TRI Chemicals and Chemical Categories

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1 Introduction

To predict the fate and transport of the reportable TRI chemicals and chemical categories, the RSEI model relies on a database called "Chemical.db," which contains physicochemical properties and estimates of chemical removal efficiencies at incinerators and at publicly owned treatment works (POTWs). The physicochemical properties in the database include rates of chemical decay in air and water; organic carbon-water, octanol-water, and soil-water partition coefficients (K_{oc}, K_{ow}, and K_d, respectively); water solubilities; bioconcentration factors; Henry's Law constants (K_H); and molecular weights. To evaluate the effects of treatment and disposal, the model also requires incinerator destruction and removal efficiencies (DREs) as well as removal efficiencies for POTWs, including estimates of the percent of chemical removed due to volatilization, biodegradation, and sorption to sludge within a POTW. However, not all of the properties included in the model are currently used for modeling. Maximum Contaminant Levels (MCLs) for chemicals in drinking water also are included in the database.

The sources of values in this database were originally documented in November, 1992. Since that time, the data have been significantly updated, with several new sources being used. The most significant new data sources are the experimental and estimation databases from Syracuse Research Corporation (PHYSPROP, CHEMFATE, and the EPI Suite) and the RREL Treatability Database Version 5.0, maintained by the U.S. EPA Risk Reduction Engineering Laboratory (U.S. EPA, 1994). Table B-1 lists each parameter, its field name in Chemical.db, and the main data sources or estimation methods used to obtain chemical-specific values.

Table B-1. Physicochemical Properties and Data Sources

Property	Field Name in Chemical.db	Main Data Source(s)
Rate of Chemical Decay in Air	AirDecay	AOPWIN (SRC) PHYSPROP (SRC)
Organic Carbon-Water Partition Coefficient (K_{oc})	Koc	CHEMFATE (SRC) Lyman et al. (1990) PCKOC (SRC)
Rate of Chemical Decay in Water	H2ODecay	HYDROWIN (SRC)
Log of Octanol-Water Partition Coefficient (log K_{ow})	LogKow	PHYSPROP (SRC)
Soil-Water Partition Coefficient (K_d)	Kd	Gerritse et al. (1982)
Water Solubility	WaterSolubility	PHYSPROP (SRC)
Total Removal Efficiency for POTWs	POTWPartition(Removal)	RREL (U.S. EPA, 1994) STPWIN (SRC)
Within-POTW Sorption to Sludge	POTWPartition(Sludge)	EFDB (SRC) STPWIN (SRC)
Within-POTW Volatilization to Air	POTWPartition(Volatil)	EFDB (SRC) STPWIN (SRC)
Within-POTW Biodegradation	POTWPartition(Biod)	EFDB (SRC) STPWIN (SRC)

Property	Field Name in Chemical.db	Main Data Source(s)
Incinerator Destruction and Removal Efficiency	IncineratorDRE	Assumed
Bioconcentration Factor	BCF	CHEMFATE (SRC) Lyman et al. (1990)
Henry's Law Constant	Henrys	PHYSPROP (SRC)
Maximum Contaminant Level	MCL	U.S. EPA
Molecular Weight	Molecular Weight	PHYSPROP (SRC)

2 Physicochemical Properties of Chemicals Included in the RSEI Model

This Appendix describes the methods used to update Chemical.db and provides the sources for all of the data. Values for the physicochemical parameters for the TRI chemicals and chemical categories are divided between two tables (Tables B-6 and B-7) provided at the end of this Appendix. The chemicals in each table are listed in order by Chemical Abstract Service (CAS) number. Table B-6 shows values and reference codes for all chemicals for the parameters air decay, K_{oc}, water decay, log K_{ow}, K_d, and water solubility. Table B-7 shows values and reference codes for all chemicals for POTW removal rates and within-POTW partitioning percentages, incinerator DREs, BCFs, Henry's Law constants, MCLs (if applicable), and molecular weights. Explanations for the reference codes and full citations for the data sources can be found in Table B-8. All three tables can be found at the end of this Appendix; however, the following sections discuss the data sources and special issues for each physicochemical parameter presented. The methods for treating chemical categories are also presented, followed by a summary of the resolution of certain TRI reporting issues which affect the exposure modeling.

2.1 Rate of Chemical Decay in Air (hr^{-1})

This parameter describes how fast a chemical degrades in air, primarily due to photooxidation by hydroxyl radicals. The daughter products of photodegradation are not modeled further; that is, it is assumed that all chemicals are photodegraded into nontoxic compounds. The main source for decay rates is SRC's Atmospheric Oxidation Program (AOPWIN), which estimates the second-order rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. For the RSEI model, a concentration of hydroxyl radicals of 1.5 x 10^6 molecules/cm^3 is used to convert the second-order rate constant provided in AOPWIN to a first-order rate constant. Furthermore, the rate is divided by a factor of two to reflect an assumed average day length of 12 hours:

$$AirDecay\ (hr^{-1}) = AOPWIN\ estimate\ \left(\frac{cm^3}{molecule}\cdot sec\right) * 1.5 * 10^6 (\frac{molecules}{cm^3}) * 3600 \frac{sec}{hr} * 1/2$$

For details on the methodology used in AOPWIN, see Meylan and Howard (1993).

2.2 Organic Carbon-Water Partition Coefficient (K_{oc}, in units of L/kg)

K_{oc} is "the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium" (Lyman et al., 1990; p. 4-1). K_{oc} provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic systems. The K_{oc} values have units of L/kg.

Several sources were used for K_{oc} values. CHEMFATE, part of SRC's Environmental Fate Database, is an online database that presents experimental and estimated values for various parameters. CHEMFATE was the preferred data source. If an appropriate value from CHEMFATE was not available, regression equations from Lyman et al. (1990) were used to

estimate K_{oc}. If a solubility value was available, the following equation (Eq. 4-5 in Lyman et al., 1990) was used to estimate K_{oc}:

$$\log(K_{oc}) = -0.55 \log(S) + 3.64$$

Note that in this equation, solubility (S) must be entered in units of milligrams per liter (mg/L). In total, 261 chemicals were used to obtain this regression equation, which has an r^2 of 0.71. Solubility values ranged between approximately 5 x 10^{-4} mg/L to 1,000,000 mg/L.

If a solubility value was not available, or it did not fall within the range of solubility values used to develop the regression equation, then another equation, based on $\log(K_{ow})$, was used. If a $\log(K_{ow})$ value was available, Eq. 4-8 in Lyman et al. (1990) was used to estimate K_{oc}:

$$\log(K_{oc}) = 0.544 \log(K_{ow}) + 1.377$$

Fifty chemicals were used to obtain this regression equation, which has an r^2 of 0.74. Values of $\log(K_{ow})$ ranged between approximately -3 and 6.6.

If a $\log(K_{ow})$ value was not available, or it did not fall within the range of $\log(K_{ow})$ values used to develop the regression equation, then CHEMFATE or SRC's estimation program PCKOC was used. PCKOC uses an estimation method based on a first-order molecular conductivity index and a series of statistically derived fragment contribution factors for polar compounds to predict K_{oc} values. For details on the methodology used in this program, see Meylan et al. (1992).

2.3 Rate of Chemical Decay in Water (hr^{-1})

The primary source of water decay rates was SRC's estimation program HYDROWIN, which was developed for EPA. The program estimates abiotic hydrolysis rate constants and half-lives for esters, carbamates, epoxides, halomethanes, and selected alkyl halides. For the RSEI model, the half-life estimated for a pH of 7 was converted to a rate using the following equation:

$$k = -\ln(0{,}5)/t_{1/2}$$

For some chemicals, HYDROWIN stated that "Even at low pH, the hydrolysis rate is very fast: $t_{1/2}$ < 10 minutes." For these chemicals, a first-order decay rate of 4.2/hr was used.

For details on the methodology used in HYDROWIN, see Mill et al. (1987). A few decay rates were obtained from the Office of Pesticide Program's OneLiner database, as included in PIRANHA (U.S. EPA, 1991).

For a few chemicals which do not undergo hydrolysis, a water decay rate was estimated based on information in CHEMFATE on photodegradation. Twelve hours of sunlight per day were assumed, and thus the rates provided in CHEMFATE for photodegradation in water were halved to estimate an average rate over a 24 hour period.

2.4 Log of Octanol-Water Partition Coefficient (log(K_{ow}), unitless)

Log(K_{ow}) describes a chemical's lipophilic or hydrophobic properties. It is the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase system at equilibrium. It has been strongly correlated with environmental fate and transport parameters such as K_{oc} and BCF and therefore is often used to estimate values for those two parameters.

The primary source for values of log (K_{ow}) was SRC's PHYSPROP database, which contains experimental and estimated values. A few values were estimated using SRC's program KOWWIN. KOWWIN uses a fragment constant methodology, in which a compound's structure is divided into functional fragments, and the coefficients for all groups are summed to obtain the compound's coefficient. Coefficients for individual fragments are derived from multiple regression of more than 2400 reliably measured values. For details on the methodology used, see Meylan and Howard (1995). Note that the parameter log(K_{ow}) has no units because it is the ratio of two concentrations.

2.5 Soil-Water Partition Coefficient (K_d, in units of L/kg)

In the RSEI chemical database, explicit values for this parameter are provided only for inorganic compounds. Organic compounds are modeled by combining chemical-specific K_{oc} values, as listed in Chemical.db, with an estimate of the fraction of organic carbon, f_{oc}, to obtain a soil-water partition coefficient. For all the metals except aluminum, K_d values were estimated from column studies by Gerritse et al. (1982) using sand with an f_{oc} value of 0.0355 g/g, a cation exchange capacity of 0.22 meq/g, zero clay content, and a solution pH of 5.[1] The median of the range of K_d values for each metal was taken, assuming a log-normal distribution. For classes of inorganic compounds, the same values were used as for the elemental inorganic compound. For aluminum, the K_d value is based on Langmuir isotherm data presented in Bodek et al. (1988). The K_d values presented have units of L/kg.

2.6 Water Solubility (mg/L)

Water solubility values were primarily obtained from SRC's PHYSPROP database. The water solubility values have units of mg/L.

2.7 POTW Removal Efficiencies and Within-POTW Partitioning Percentages

The POTW removal efficiency and the three within-POTW partitioning percentages describe the fate of chemicals during treatment at POTWs. The 'POTW Partition Removal' is the total POTW removal efficiency, or the total percentage of the chemical removed by the POTW (influent concentration minus effluent concentration divided by influent concentration). The

[1]The assumption that the waste in landfills is similar to the above conditions results in a conservative estimate of the leachate concentration of metals, because low clay content and relatively low pH tend to increase the mobility of metals.

three within-POTW partitioning percentages describe the fate of the total amount of chemical removed by the POTW; the chemical may be removed by sorbing to sludge (POTW Partition Sludge), by volatilizing into the air (POTW Partition Volatil) or by being biodegraded by microorganisms (POTW Partition Biodeg). Note that the within-POTW partitioning percentages sum to 100 percent.

POTW removal efficiencies were available from the RREL Treatability Database maintained by the U.S. EPA Risk Reduction Engineering Laboratory (U.S. EPA, 1994). For any given chemical, the RREL Treatability Database provides a list of removal efficiencies published in the scientific literature. Each value is characterized by the technology used, the type of influent, and the scale of the experiment. For all values associated with activated sediment and full scale experiments, a geometric mean was derived and used as the POTW removal efficiency. Within-POTW partitioning values for most organic chemicals were supplied by David Lynch of the Exposure Assessment Branch of Office of Pollution Prevention and Toxics. Inorganic chemicals, except for ammonia, were assumed to partition 100 percent to sludge.

For those chemicals without data provided by David Lynch, SRC's STPWIN program was used to estimate total removal efficiency and within-POTW partitioning values. Details on the methodology used in STPWIN can be found in Clark et al. (1995). One value was obtained from Howard et al. (1991).

2.8 Bioconcentration Factor (BCF, in units of L/kg)

Bioconcentration factors (BCFs) are used to describe the equilibrium concentrations of chemicals in aquatic organisms living in contaminated water. The BCF is defined as the ratio of the chemical concentration in the organism (mg/kg) to that in the surrounding water (mg/L). Many experimental and estimated BCF values were obtained from SRC's CHEMFATE database. If an appropriate BCF value from CHEMFATE was not available, regression equations from Lyman et al. (1990) were used to estimate BCF values, as described below.

If a log(K_{ow}) value was available for a chemical and was within the range used to develop the regression equation (0.90 to 6.9), Eq. 5-2 in Lyman et al. (1990) was used to estimate a BCF:

$$logBCF = 0.76\ \log(K_{ow}) - 0.23$$

Two hundred and fifty-five chemicals used this regression equation, which has an r^2 of 0.823.

If a log (K_{ow}) value was not available, or it did not fall within the range of values used to develop the regression equation, then another equation, based on water solubility, was used. If a water solubility value was available and within the range of 0.001 to 50,000 mg/L, Eq. 5-3 in Lyman et al. (1990) was used to estimate a BCF:

$$logBCF = 2.791 - 0.564\ log(S)$$

Thirty-nine chemicals were used to obtain this regression equation, which has an r^2 of 0.49.

If the above two equations could not be applied to estimate BCF values, then Chemfate or SRC's BCFWIN program was used.

2.9 Incinerator Destruction/Removal Efficiencies

This parameter describes the percentage of a chemical removed or destroyed during combustion in an incinerator. We assume that the typical municipal waste combustor destruction/removal efficiency for organics is 99 percent. This assumption ignores the fact that chemicals of concern, such as dioxins, may be formed during the incineration process. The exceptions to the 99 percent removal assumption are PCBs and dioxin and dioxin-like compounds, both of which are assumed to have a DRE of 99.9999 percent, as required by TSCA regulation.

For incinerator destruction/removal efficiencies for inorganic chemicals, values were taken from multiple hearth sludge incinerator studies, as reported in U.S. EPA, 1992.

2.10 Henry's Law Constant (atm·m^3/mol)

The Henry's Law constant is defined as the ratio of a chemical concentration in air (often expressed as a partial pressure with units of atmospheres) to the chemical concentration in water (often expressed as moles per cubic meter) under equilibrium conditions. This constant is used to model volatilization from off-site landfills. The primary source for this parameter is SRC's PHYSPROP database. The units of the Henry's Law constants are atm≅m^3/mol.

2.11 Maximum Contaminant Level (mg/L)

Maximum Contaminant Levels (MCLs) are enforceable standards for chemicals in drinking water and are to be set as close to the Maximum Contaminant Level Goals (MCLGs), which are based on health effects, as is feasible. MCLs are based upon the availability of analytical methods, treatment technologies, and costs for achieving various levels of removal. MCLs have not been set for most TRI chemicals. For those chemicals that do have MCLs, the RSEI model limits the concentrations in drinking water so that they cannot exceed the appropriate MCLs.

2.12 Molecular Weight (g/mol)

The molecular weight is not specifically used in the RSEI model, but values are provided as part of the physicochemical database. The primary source for molecular weights is SRC's PHYSPROP database.

3 Chemical Categories

EPA's annual 'Reporting Form R and Instructions' describes the reporting requirements for several categories that combine similar chemicals into one release report. For these categories, facilities are not required to report the pounds released of each individual chemical in the category, but only the total pounds released for the entire category. Because it is not known in what proportion individual chemicals within each category are released, professional judgment was used to assign surrogate values for the various physicochemical properties to each category. In most cases, the most toxic chemical of each category, based on the calculated toxicity weight, was selected, and the toxicity and physicochemical data for that chemical were assigned to the entire chemical category. In these cases, the actual risk for the chemical category would be less than or equal to the modeled risk.

The rest of this section describes the decisions made for each chemical category. Note that a chemical category does not have a CAS number in Chemical.db; instead, it has a three digit number preceded by an 'N.'[2]

3.1 Metal/Metalloid Compounds

Metal/metalloid compounds are reported separately in TRI, but in RSEI each compound category is combined with the metal/metalloid elemental form. The physicochemical properties from the elemental form are used to represent the combined category. Table B-2 shows the metal compound categories included in TRI. Most categories include any unique chemical substance that contains the metal as part of that chemical's infrastructure. Any additional restrictions are noted in the table.

[2] The only exception is the category polychlorinated biphenyls (PCBs), which has been assigned a CAS number. Physicochemical data are readily available for this category, and therefore this category is not discussed further here.

Table B-2. Metal Categories

CAS Number	Name	Exclusions
N010	Antimony compounds	None.
N020	Arsenic compounds	None.
N040	Barium compounds	Does not include Barium sulfate (CAS# 7727-43-7).
N050	Beryllium compounds	None.
N078	Cadmium compounds	None.
N090	Chromium compounds	None.
N096	Cobalt compounds	None.
N100	Copper compounds	Does not include copper phthalocyanine compounds that are substituted with only hydrogen, and/or chlorine, and/or bromine.
N420	Lead compounds	None.
N450	Manganese compounds	None.
N458	Mercury compounds	None.
N495	Nickel compounds	None.
N725	Selenium compounds	None.
N740	Silver compounds	None.
N760	Thallium compounds	None.
N770	Vanadium compounds	None.
N982	Zinc compounds	None.

3.2 Chlorophenols

Of the 19 chlorophenols which have the formula $C_6OHCl_xH_{(5-x)}$, where x = 1 to 5, toxicity data were available for six. Pentachlorophenol (CAS# 87-86-5) had the highest toxicity value, so that chemical was used as a surrogate for the category for both toxicity and physicochemical data.

3.3 Cyanide Compounds

This category includes only chemicals that can be represented by the formula $X^{y+}(CN^-)_y$, where $X = H^+$ or any other ion where a formal dissociation may occur, for example, KCN or $Ca(CN)_2$. Because cyanide compounds in a gaseous state exhibit markedly different properties than compounds in solution, two surrogate compounds were used for toxicity scores and physicochemical data for the chemical category. For the inhalation toxicity score, the air decay rate, and the Henry's Law constant, the properties of hydrogen cyanide, the most toxic gaseous compound, were used. For the oral exposure pathway, toxicity data were collected for metal cyanide compounds, the most toxic group of nongaseous cyanide compounds. Copper cyanide ($Cu(CN)_2$)was found to be the most toxic metal cyanide compound. Thus, for the oral toxicity

score and for all physicochemical properties other than the air decay rate and the Henry's Law constant, the properties of ($Cu(CN)_2$) were used for this chemical category.

3.4 Diisocyanates

This category only includes those chemicals listed in Table B-3. At this time, toxicity and physicochemical data have not been obtained or estimated for this category.

Table B-3. Members of Diisocyanates Category

CAS Number	Chemical
822-06-0	1,6-Hexamethylene diisocyanate
101-68-8	Methylene bis(phenylisocyanate) (MDI) and polymeric MDI
38661-72-2	1,3-Bis(methylisocyanate)-cyclohexane
10347-54-3	1,4-Bis(methylisocyanate)-cyclohexane
2556-36-7	1,4-Cyclohexane diisocyanate
134190-37-7	Diethyldiisocyanatobenzene
4128-73-8	4,4'-Diisocyanatodiphenyl ether
75790-87-3	2,4'-Diisocyanatodiphenyl sulfide
91-93-0	3,3'-Dimethoxybenzidene-4,4'-diisocyanate
91-97-4	3,3'-Dimethyl-4,4'-diphenylene diisocyanate
139-25-3	3,3'-Dimethyldiphenylmethane-4,4'-diisocyanate
4098-71-9	Isophorone diisocyanate
75790-84-0	4-Methyldiphenylmethane-3,4-diisocyanate
5124-30-1	1,1-Methylene bis(4-isocyanatocyclohexane)
3173-72-6	1,5-Naphthalene diisocyanate
123-61-5	1,3-Phenylene diisocyanate
104-49-4	1,4-Phenylene diisocyanate
9016-87-9	Polymeric diphenylmethane diisocyanate
16938-22-0	2,2,4-Trimethylhexamethylene diisocyanate
15646-96-5	2,4,4-Trimethylhexamethylene diisocyanate

3.5 Dioxin and Dioxin-like Compounds

This category includes manufacturing and the processing or otherwise use of dioxin and dioxin-like compounds if the dioxin and dioxin-like compounds are present as contaminants in a chemical and if they were created during the manufacture of that chemical. Of the 17 congeners reportable under this category and shown below in Table B-4, physicochemical data were available only for TCDD (2,3,7,8-Tetrachlorodibenzo-p-dioxin), which was used as a surrogate for the entire category. However, POTW removal rates were not available, so dioxin transfers to POTWs are not currently modeled in RSEI. Fugitive and stack air releases, direct releases to water and transfers off-site to incineration are modeled. The incineration destruction removal efficiency is assumed to be 99.9999, as required by TSCA.

Table B-4. Members of the Dioxin and Dioxin-like Compounds Category

CAS	Dioxin and Dioxin-like Compounds Name
01746–01–6	2,3,7,8-Tetrachlorodibenzo- p-dioxin
40321–76–4	1,2,3,7,8-Pentachlorodibenzo- p-dioxin
39227–28–6	1,2,3,4,7,8-Hexachlorodibenzo- p-dioxin
57653–85–7	1,2,3,6,7,8-Hexachlorodibenzo- p-dioxin
19408–74–3	1,2,3,7,8,9-Hexachlorodibenzo- p-dioxin
35822–46–9	1,2,3,4,6,7,8-Heptachlorodibenzo- p-dioxin
03268–87–9	1,2,3,4,6,7,8,9-Octachlorodibenzo- p-dioxin
51207–31–9	2,3,7,8-Tetrachlorodibenzofuran
57117–41–6	1,2,3,7,8-Pentachlorodibenzofuran
57117–31–4	2,3,4,7,8-Pentachlorodibenzofuran
70648–26–9	1,2,3,4,7,8-Hexachlorodibenzofuran
57117–44–9	1,2,3,6,7,8-Hexachlorodibenzofuran
72918–21–9	1,2,3,7,8,9-Hexachlorodibenzofuran
60851–34–5	2,3,4,6,7,8-Hexachlorodibenzofuran
67562–39–4	1,2,3,4,6,7,8-Heptachlorodibenzofuran
55673–89–7	1,2,3,4,7,8,9-Heptachlorodibenzofuran
39001–02–0	1,2,3,4,6,7,8,9-Octachlorodibenzofuran

3.6 Ethylenebisdithiocarbamic (EBDC) Acids, Salts, and Esters

This category contains any unique chemical substance that contains an EBDC or an EBDC salt as a part of that chemical's infrastructure. According to EPA's 1998 Status of Pesticides in Registration, Reregistration, and Special Review (The Rainbow Report), chemicals regulated in the category EBDCs include maneb, mancozeb, metiram, nabam, zineb, and amobam. Maneb, metiram, nabam, and zineb are separately reported in TRI. Toxicity data were available for four compounds (mancozeb, maneb, metiram, and zineb); of these, metiram had the highest toxicity weight. Therefore, metiram was selected as the surrogate for both toxicity and physicochemical data.

3.7 Glycol Ethers

This category includes chemicals that can be represented by the formula R-$(OCH_2CH_2)_n$ -OR' where n = 1, 2, or 3; R = alkyl C7 or less, or, R = phenyl or alkyl substituted phenyl; R' = H, or alkyl C7 or less; or, OR' consists of carboxylic acid ester, sulfate, phosphate, nitrate, or sulfonate. Eight common glycol ethers were identified: ethylene glycol monobutyl ether (CAS#111-76-2), dipropylene glycol monomethyl ether (CAS#34590-94-8), ethylene glycol diethyl ether (CAS#629-14-1), ethylene glycol monoethyl ether acetate (CAS#11-15-9), ethylene glycol monoethyl ether (CAS#110-80-5), monomethyl ether acetate (CAS#110-49-6), ethylene glycol monomethyl ether (CAS#109-86-4), and propylene glycol monomethyl ether (CAS#107-98-2). Of these, four chemicals had available toxicity data. Ethylene glycol monomethyl ether had the highest toxicity weight of the four and therefore was used as a surrogate for the category for both the toxicity data and the physicochemical data.

3.8 Nicotine and Salts

This category includes any unique chemical substance that contains nicotine or a nicotine salt as part of that chemical's infrastructure. Nicotine was selected as a surrogate for both toxicity and physicochemical values. However, no toxicity values were available for nicotine.

3.9 Nitrate Compounds

This category only includes compounds that are water dissociable and are reportable only when in an aqueous solution. Toxicity data for nitrate were available from IRIS; however, at this time, physicochemical data have not been determined for this category.

3.10 Polybrominated Biphenyls (PBBs)

This category includes chemicals that can be represented by the formula $C_{12}Br_xH_{(10-x)}$, where x = 1 to 10. Toxicity data for a PBB mixture were available from HEAST. However, no physicochemical data was available for PBB mixtures. According to the Consumer Product Safety Commission, hexabromobiphenyl (CAS#36355-01-8) was the major component in the most widely used mixture of PBBs. Therefore, this chemical was selected as a surrogate for the entire class for physicochemical data.

3.11 Polychlorinated Alkanes

This category includes chemicals that can be represented by the formula $C_xH_{2x+2-y}Cl_y$, where x = 10 to 13 and y = 3 to 12, and the average chlorine content ranges from 40 to 70 percent, with the limiting molecular formulas $C_{10}H_{19}Cl_3$ and $C_{13}H_{16}Cl_{12}$. At this time, toxicity and physicochemical data have not been determined for this category.

3.12 Polycyclic Aromatic Compounds (PACs)

There are 21 members of this class listed in the Form R instructions as reportable under TRI, as shown in Table B-5. Of these 21 chemicals, only benzo(a)pyrene (CAS# 50-32-8) and benzo(j,k)fluorene (CAS#206-44-0) had available toxicity data. The toxicity weight for benzo(j,k)fluorene (tox weight = 13) is approximately 1,000-fold lower than that for benzo(a)pyrene (tox weight = 15,000). However, absent information on the composition of the total PAC emissions, the model uses a conservative approach and uses the benzo(a)pyrene value to represent the group. This chemical was selected as a surrogate for the entire class for physicochemical data. For toxicity data, the toxicity of this group is assumed to be 18% of the toxicity for benzo(a)pyrene. This approach follows that used in EPA's National-Scale Air Toxics Assessment (NATA) evaluation for polycyclic organic matter (POM).

Table B-5. Members of Polycyclic Aromatic Compounds Category

CAS Number	Chemical
56-55-3	Benz(a)anthracene
205-99-2	Benzo(b)fluoranthene
205-82-3	Benzo(j)fluoranthene
207-08-9	Benzo(k)fluoranthene
189-55-9	Benzo(rst)pentaphene
218-01-9	Benzo(a)phenanthrene
50-32-8	Benzo(a)pyrene
226-36-8	Dibenzo(a,h)acridine
224-42-0	Dibenzo(a,j)acridine
53-70-3	Dibenz(a,h)anthracene
194-59-2	7H-Dibenzo(c,g)carbazole
5385-75-1	Dibenzo(a,e)fluoranthene
192-65-4	Dibenzo(a,e)pyrene
189-64-0	Dibenzo(a,h)pyrene
191-30-0	Dibenzo(a,l)pyrene
57-97-6	7,12-Dimethylbenz(a)anthracene
193-39-5	Indenol[1,2,3-cd]pyrene

CAS Number	Chemical
3697-24-3	5-Methylchrysene
5522-43-0	l-Nitropyrene
206-44-0	Benzo(j,k)fluorene
56-49-5	3-Methylcholanthrene

3.13 Strychnine and salts

This category includes any unique chemical substance that contains strychnine or a strychnine salt as part of that chemical's infrastructure. Strychnine (CAS#57-24-9) was used as a surrogate for both toxicity and physicochemical data for this category.

3.14 Warfarin and salts

This category includes any unique chemical substance that contains warfarin or a warfarin salt as part of that chemical's infrastructure. Warfarin (CAS# 81-81-2) was used as a surrogate for both toxicity and physicochemical data for this category.

4 Summary of Resolution of Certain TRI Reporting Issues

In March 1996, several reporting issues pertaining to the TRI chemicals ammonia, ammonium sulfate, and mineral acids were resolved. These issues and the corresponding modifications or recommendations which were agreed upon are summarized below.

4.1 Ammonia and Ammonium Sulfate

Effective for the 1994 reporting year, only the ammonia or a fraction of the water-dissociable portion of ammonia in a compound will be reportable to TRI. This includes anhydrous ammonia, aqueous ammonia, and ammonia from water-dissociable ammonium salts and other sources (the latter includes ammonium sulfate). The total quantity of ammonia is calculated, but only 10% of this quantity counts towards threshold levels for reporting and it is this 10% which is actually reported. To re-calculate the original quantity of ammonia, one must multiply the reported quantity of releases and transfers (e.g., POTW) to water and land by 10 (air emissions are reported at 100%).

Because of these reporting changes, comparisons should not be made between ammonia reporting before 1995 and after 1995.

4.2 Mineral Acids

Mineral acids include sulfuric and hydrochloric acid. The Agency has made the decision to modify reporting to include only the more highly toxic exposures to aerosol releases of certain of these acids. The acid aerosols include mists, vapors, gas, fog and other airborne forms of any particle size. For sulfuric acid, this change in reporting takes place in 1994, while for hydrochloric acid the change takes place for reporting year 1995. The very high decay rate in water of these acids will greatly reduce any risk-based impacts associated with releases or transfers to water.

5 Physicochemical Property Data Tables for TRI Chemicals

The following two tables present the physicochemical properties used for the chemicals currently included in the RSEI Model and the references for those properties. Table B-6 provides the following seven physicochemical parameters and references:

- Chemical Name;
- CAS Number;
- Air Decay (hr^{-1}): decay rate in air due to photooxidation (and in rare instances hydrolysis in air);
- Koc (milliliters/gram): organic carbon-water partition coefficient;
- H2O Decay (hr^{-1}): decay rate in water due to hydrolysis or aerobic biodegradation;
- LOG Kow: base 10 log of the octanol-water partition coefficient;
- Kd (liter/kilogram): soil-water partition coefficient;
- Water Solubility (milligrams/liter): water solubility
- Inciner. DRE (percent): incinerator destruction/removal efficiency.

Table B-7 provides the remaining eight physicochemical parameters with references:

- Chemical Name;
- CAS number;
- 4 POTW Partition Rates:
    - Total Removal: percent of the chemical that is removed by a POTW;
    - Part. to Sludge: percent of the chemical removed by a POTW that partitions to sludge;
    - Part. to Volat.: percent of the chemical removed by a POTW that volatilizes to the air;
    - Part. to Biodeg.: percent of the chemical removed by a POTW that biodegrades;
- BCF (liter/kilogram): bioconcentration factor;
- Henry's Law ($atm\text{-}m^3/mol$): Henry's Law Constant;
- MCL (milligram/liter): Maximum Contaminant Level for drinking water;
- Mol. Weight (gram/mole): molecular weight.

Table B-8 provides explanations for the reference codes found in tables B-6 and B-7.

6 References

Bodek, I., W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt (eds.). 1988. Environmental Inorganic Chemistry: Properties, Processes and Estimation Methods. Pergamon Press, New York.

Budavari, S. (ed.). 1989. The Merck Index. Merck & Co., Inc., Rahway, NJ.

Clark, B., Henry, J.G., and D. Mackay. 1995. Fugacity analysis and model of organic chemical fate in a sewage treatment plant. Environ. Sci. Technol. 29: 1488-1494.

Gerritse, R. G., R. Vriesema, J. W. Dalenberg, and H. P. De Roos (1982). Effect of sewage sludge on trace element mobility in soils. J. Environ. Qual. 11(3):359-364.

Hine, J. and P. K. Mookerjee (1975). The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. J. Org. Chem. 40(3):292-298.

Howard, P. H., R. S. Boethling, W. F. Jarvis, W. M. Meylan, and E. M. Michalenko. 1991. Handbook of Environmental Degradation Rates. Chelsea, MI. Lewis Publishers, Inc.

Jørgensen, S. E. and I. Johnsen. 1981. Principles of Environmental Science and Technology. Elsevier, New York.

Lyman, W. J., W. F. Reehl, and D. H. Rosenblatt. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society. Washington, D.C.

Mabey, W. R., J. H. Smith, R. T. Podoll, H. L. Johnson, T. Mill, T.-W. Chou, J. Gates, I. W. Partridge, H. Jaber, and D. Vandenberg. 1982. Aquatic Fate Process Data for Organic Priority Pollutants, Chapter 4, EPA Report No. 440/4-81-014.

Mackay, D. and W. Y. Shiu. 1981. A critical review of Henry's Law constants for chemicals of environmental interest. J. Phys. Chem. Ref. Data 10:1175-1199.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic chemicals with hydroxyl radicals and ozone. Chemosphere 26: 2293-99.

Meylan, W.M. and P.H. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84: 83-92.

Meylan, W., P.H. Howard, and R.S. Boethling. 1992. Molecular topology/ fragment contribution method for predicting soil sorption coefficients. Environ. Sci. Technol. 26:1560-1567.

Mill, T., W. Haag, P. Penwell, T. Pettit, and H. Johnson. 1987. Environmental fate and exposure studies development of a PC-SAR for hydrolysis: Esters, alkyl halides and epoxides. EPA Contract Number 68-02-4254. Menlo Park, CA. SRI International.

Morel, F.M.M. 1983. Principles of Aquatic Chemistry. John Wiley & Sons. New York.

O'Connor, G. 1992. Professor and Chairman, Soil and Water Science Dept., University of Florida. Personal Communication.

Syracuse Research Corporation. 1995. Environmental Fate Data Base. Syracuse, New York.

Tetra Tech. 1985. Bioaccumulation Monitoring Guidance: 1. Estimating the Potential for Bioaccumulation of Priority Pollutants and 301(h) Pesticides Discharged into Marine and Estuarine Waters. Final Report. Office of Marine and Estuary Protection, U.S. EPA.

U.S. EPA. 1986. Report to Congress on the Discharge of Hazardous Wastes to Publicly Owned Treatment Works. Office of Water Regulations and Standards. EPA/530-SW-86-004. February.

U.S. EPA. 1987. Ambient Aquatic Life Water Quality Criteria for Silver. Draft. Environmental Research Laboratories, Duluth, MN and Narragansett, RI. September.

U.S. EPA. 1988a. Ambient Water Quality Criteria for Aluminum--1988. EPA 440/5-86-008. August.

U.S. EPA. 1988b. Ambient Aquatic Life Water Quality Criteria for Antimony (III). Draft. Environmental Research Laboratories, Duluth, MN and Narragansett, RI. August.

U.S. EPA. 1991. PIRANHA, Pesticide and Industrial Chemical Risk Analysis and Hazard Assessment, Version 2.0. Environmental Research Laboratory, Office of Research and Development.

U.S. EPA. 1992. Human Health Risk Assessment for the Use and Disposal of Sewage Sludge: Benefits of Regulation. Prepared by Abt Associates Inc., Cambridge, MA, for the U.S. EPA Office of Water.

U.S. EPA. 1994. RREL Treatability Database, Version 5.0. Risk Reduction Engineering Laboratory. U.S. EPA, Cincinnati, OH.

Weast, R.C. (ed.). 1990. CRC Handbook of Chemistry and Physics. CRC Press, Inc. Boca Raton, FL.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Abamectin	71751412	3.45	AOPWIN	1800	Lyman, 4-5			4.98	HL			5	HL	99	Assump.
Acephate	30560191	0.0302	AOPWIN	2.4	Lyman, 4-5			-0.85	PHYS			818000	PHYS	99	Assump.
Acetaldehyde	75070	0.0427	AOPWIN; exp	2	Lyman, 4-5			-0.34	PHYS			1000000	PHYS	99	Assump.
Acetamide	60355	0.00568	AOPWIN	4.9	Lyman, 4-8	2E-08	CHMF	-1.26	PHYS			2250000	PHYS	99	Assump.
2,4-D ((2,4-dichlorophenoxy)acetic acid)	94757	0.0179	AOPWIN	84	CHMF	0.0018	PRNA	2.81	PHYS			677	PHYS	99	Assump.
Acetonitrile	75058	0.000071	AOPWIN; exp	2	Lyman, 4-5	5.8E-10	CHMF	-0.34	PHYS			1000000	PHYS	99	Assump.
Acetophenone	98862	0.0074	AOPWIN; exp	57	CHMF			1.58	PHYS			6130	PHYS	99	Assump.
2-Acetylaminofluorene	53963	0.0729	AOPWIN	1700	Lyman, 4-5	0.0000023	CHMF	3.12	PHYS			5.534	PHYS	99	Assump.
Acifluorfen, sodium salt	62476599	0.00148	AOPWIN	38	Lyman, 4-8			0.37	PHYS			250000	PHYS	99	Assump.
Acrolein	107028	0.0537	AOPWIN; exp	5	CHMF	0.019	PRNA	-0.01	PHYS			212000	PHYS	99	Assump.
Acrylamide	79061	0.0303	AOPWIN	50	CHMF	0.0000021	CHMF	-0.67	PHYS			640000	PHYS	99	Assump.
Acrylic acid	79107	0.0263	AOPWIN		Ion			0.35	PHYS			1000000	PHYS	99	Assump.
Acrylonitrile	107131	0.0111	AOPWIN; exp	9	CHMF	6.1E-08	CHMF	0.25	PHYS			74500	PHYS	99	Assump.
Alachlor	15972608	0.122	AOPWIN	191	CHMF			3.52	PHYS			240	PHYS	99	Assump.
Aldicarb	116063	0.0249	AOPWIN	21	CHMF	6.31E-07	HYDRO	1.13	PHYS			6030	PHYS	99	Assump.
Aldrin	309002	0.174	AOPWIN	8220	CHMF	0.000038	CHMF	6.5	PHYS			0.017	PHYS	99	Assump.
Allyl alcohol	107186	0.07	AOPWIN; exp	2	Lyman, 4-5			0.17	PHYS			1000000	PHYS	99	Assump.
Allyl chloride	107051	0.0459	AOPWIN; exp	50	CHMF			1.93	PHYS			3370	PHYS	99	Assump.
Allylamine	107119	0.151	AOPWIN	2	Lyman, 4-5			0.03	PHYS			1000000	PHYS	99	Assump.
Aluminum (fume or dust)	7429905			14	PCKOC			0.33	KOWWIN	4	Bodek	59400	WSKOW		

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Aluminum oxide (fibrous forms)	1344281			81	PCKOC			-0.83	KOWWIN						
Aluminum phosphide	20859738			14	PCKOC			-0.17	PHYS			192000	PHYS		
Ametryn	834128	0.077	AOPWIN	389	CHMF			2.98	PHYS			209	PHYS	99	Assump.
1-Amino-2,4-dibromoanthraquinone	81492							5.68	Chem Spider			0.00442	EPI	99	Assump.
1-Amino-2-methyl-anthraquinone	82280	0.139	AOPWIN	8000	CHMF			4.07	PHYS			0.332	PHYS	99	Assump.
2-Aminoanthraquinone	117793	0.114	AOPWIN	11800	CHMF			3.31	PHYS			0.163	PHYS	99	Assump.
4-Aminoazobenzene	60093	0.117	AOPWIN	650	Lyman, 4-5			3.41	PHYS			32	PHYS	99	Assump.
4-Aminodiphenyl	92671	0.217	AOPWIN	223	Lyman, 4-5			2.86	PHYS			223.9	PHYS	99	Assump.
Amitraz	33089611	0.36	AOPWIN	4400	Lyman, 4-5			5.5	PHYS			1	PHYS	99	Assump.
Amitrole	61825	0.0149	AOPWIN	4.4	CHMF			-0.86	PHYS			280000	PHYS	99	Assump.
Ammonia	7664417			14	PCKOC			0.23	PHYS			482000	PHYS		
Ammonium Nitrate	6484522	0.000972	AOPWIN	14	PCKOC			-4.39	KOWWIN			2000000	Merck	99	Assump.
Ammonium sulfate	7783202			24	PCKOC			0.48	KOWWIN			434700	Merck		
Anilazine	101053	0.116	AOPWIN	1400	Lyman, 4-5			3.88	PHYS			8	PHYS	99	Assump.
Aniline	62533	0.3	AOPWIN; exp	240	CHMF			0.9	PHYS			36000	PHYS	99	Assump.
p-Anisidine	104949	0.254	AOPWIN	22	Lyman, 4-5			0.95	PHYS			15400	PHYS	99	Assump.
o-Anisidine hydrochloride	134292	0.0147	AOPWIN	104	Lyman, 4-8			-1.28	KOWWIN			845000	WSKOW	99	Assump.
o-Anisidine	90040	0.254	AOPWIN		Ion			1.18	PHYS			9598	PHYS	99	Assump.
Anthracene	120127	0.108	AOPWIN; exp	25000	CHMF	0.6	CHMF; photo	4.45	PHYS			0.0434	PHYS	99	Assump.
Antimony and antimony compounds	7440360			14	PCKOC			0.73	PHYS	9	Gerritse	22970	PHYS		

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Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Arsenic and arsenic compounds	7440382			14	PCKOC			0.68	PHYS	38	Gerritse	34710	PHYS	97.5	EPA, 92
Asbestos (friable)	1332214														
Atrazine	1912249	0.074	AOPWIN	570	CHMF	0.0000033	CHMF	2.61	PHYS			34.7	PHYS	99	Assump.
Barium and barium compounds	7440393			14	PCKOC			0.23	PHYS	31	Gerritse	54760	PHYS		
Bendiocarb	22781233	0.0644	AOPWIN	210	Lyman, 4-5	0.00233	HYDRO	1.7	PHYS			260	PHYS	99	Assump.
Benfluralin	1861401	0.06	AOPWIN	10700	CHMF			5.29	PHYS			0.1	PHYS	99	Assump.
Benomyl	17804352	0.575	AOPWIN	2100	Lyman, 4-5	9.43E-08	HYDRO	2.12	PHYS			3.8	PHYS	99	Assump.
Benzal chloride	98873	0.00619	AOPWIN		Fast Hyd	5.62	CHMF	2.97	PHYS			250	PHYS	99	Assump.
Benzamide	55210	0.0102	AOPWIN	23	Lyman, 4-5			0.64	PHYS			13500	PHYS	99	Assump.
Benzene	71432	0.00332	AOPWIN; exp	29	CHMF			2.13	PHYS			1790	PHYS	99	Assump.
Benzidine	92875	0.415	AOPWIN	174000	CHMF			1.34	PHYS			322	PHYS	99	Assump.
Benzo(g,h,i)perylene**	191242	0.235	AOPWIN			0.00026	PHYS					#REF!	#REF!	99	Assump.
Benzotrichloride	98077	0.000965	AOPWIN		Fast Hyd	130	CHMF	3.9	PHYS			53	PHYS	99	Assump.
Benzoyl chloride	98884	0.0048	AOPWIN		Fast Hyd	150	CHMF	1.44	PHYS			4941	PHYS	99	Assump.
Benzoyl peroxide	94360	0.0096	AOPWIN		Fast Hyd	19.6	HYDRO	3.46	PHYS			9.1	PHYS	99	Assump.
Benzyl chloride	100447	0.00783	AOPWIN; exp	139	CHMF	0.0461	CHMF	2.3	PHYS			525	PHYS	99	Assump.
Beryllium and beryllium compounds	7440417			14	PCKOC			-0.57	PHYS	170	Gerritse	148900	PHYS	97.3	EPA, 92
Bifenthrin	82657043	0.08	AOPWIN	15000	Lyman, 4-5	0.0000145	HYDRO	6	PHYS			0.1	PHYS	99	Assump.
Biphenyl	92524	0.0194	AOPWIN; exp	12000	CHMF			3.98	PHYS			6.94	PHYS	99	Assump.
Bis(2-chloro-1-methethyl)ether	108601	0.00703	AOPWIN	52	CHMF			2.48	PHYS			1700	PHYS	99	Assump.

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Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Bis(2-chloroethoxy)methane	111911	0.0203	AOPWIN	32	Lyman, 4-5			1.3	PHYS			7800	PHYS	99	Assump.
Bis(2-chloroethyl)ether	111444	0.00852	AOPWIN	79	CHMF	0.000026	CHMF	1.29	PHYS			17200	PHYS	99	Assump.
2,2-Bis(Bromomethyl)-1,3-propanediol	329600							0.411	ACD			38000	PHYS	99	Assump.
Bis(chloromethyl)ether	542881	0.00192	AOPWIN		Fast Hyd	4.2	CHMF*	0.57	PHYS			22000	PHYS	99	Assump.
Bis(tributyltin) oxide	56359	0.231	AOPWIN	300	Lyman, 4-5			4.05	PHYS			100	PHYS		
Boron trichloride	10294345			35	PCKOC			1.16	PHYS			10510	PHYS		
Boron trifluoride	7637072			35	PCKOC			0.22	PHYS			3320000	PHYS		
Bromacil	314409	0.0525	AOPWIN	69	CHMF			2.11	PHYS			815	PHYS	99	Assump.
Bromacil lithium salt	53404196			120	Lyman, 4-5			1.87	HL			700	HL	99	Assump.
Bromine	7726956			14	PCKOC			1.03	PHYS			35000	PHYS		
1-Bromo-1-(bromomethyl)-1,3-propanedicarbonitrile	35691657	0.0016	AOPWIN	184	Lyman, 4-8			1.63	PHYS			424	WSKOW	99	Assump.
Bromochlorodifluoro-methane	353593	0.0000054	AOPWIN	198	Lyman, 4-5			1.9	PHYS			276.5	PHYS	99	Assump.
Bromoform (Tribromomethane)	75252	0.000115	AOPWIN	52	CHMF	1.31E-08	HYDRO	2.4	PHYS			3100	PHYS	99	Assump.
Bromomethane (Methyl bromide)	74839	0.000109	AOPWIN; exp	9.9	CHMF	0.00147	CHMF	1.19	PHYS			15200	PHYS	99	Assump.
Bromotrifluoromethane (Halon 1301)	75638	5.4E-07	AOPWIN	180	Lyman, 4-5			1.86	PHYS			320	PHYS	99	Assump.
Bromoxynil	1689845	0.000566	AOPWIN	300	Lyman, 4-5			2.8	PHYS			130	PHYS	99	Assump.
Bromoxynil octanoate	1689992	0.02	AOPWIN	18000	Lyman, 4-5	0.00183	HYDRO	6.1	PHYS			0.08	PHYS	99	Assump.
Brucine	357573	0.866	AOPWIN	52	Lyman, 4-5	2.1E-08	CHMF	0.98	PHYS			3200	PHYS	99	Assump.
1,3-Butadiene	106990	0.18	AOPWIN; exp	116	CHMF			1.99	PHYS			735	PHYS	99	Assump.
2,4-D butoxyethyl ester	1929733	0.067	AOPWIN	1100	Lyman, 4-5	0.0033	HYDRO	4.1	PHYS			12	PHYS	99	Assump.

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Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Butyl acrylate	141322	0.0372	AOPWIN	67	CHMF	7.46E-06	HYDRO	2.36	PHYS			2000	PHYS	99	Assump.
n-Butyl alcohol	71363	0.023	AOPWIN; exp	10	Lyman, 4-5			0.88	PHYS			63200	PHYS	99	Assump.
sec-Butyl alcohol	78922	0.0259	AOPWIN; exp	5.6	CHMF			0.61	PHYS			181000	PHYS	99	Assump.
tert-Butyl alcohol	75650	0.00302	AOPWIN; exp	2	Lyman, 4-5			0.35	PHYS			1000000	PHYS	99	Assump.
2,4-D butyl ester	94804	0.022	AOPWIN	530	Lyman, 4-5	0.00128	HYDRO	4.38	PHYS			46	PHYS	99	Assump.
1,2-Butylene oxide	106887	0.00516	AOPWIN; exp	8	CHMF	0.000026	HYDRO	0.86	PHYS			95000	PHYS	99	Assump.
Butyraldehyde	123728	0.0635	AOPWIN; exp	9.4	CHMF	0.049	CHMF; photo	0.88	PHYS			71000	PHYS	99	Assump.
C.I. Acid Green 3	4680788	1.11	AOPWIN	3.45E+09	PCKOC			-3.2	PHYS			217	WSKOW	99	Assump.
C.I. Acid Red 114	6459945	0.0492	AOPWIN	450000	Lyman, 4-8; C.I.			7.86	PHYS			2.517E-06	PHYS	99	Assump.
C.I. Basic Green 4	569642	1.19	AOPWIN	13	Lyman, 4-5			0.62	PHYS			40000	PHYS	99	Assump.
C.I. Basic Red 1	989388	0.803	AOPWIN	38100	Lyman, 4-8	0.0000136	HYDRO	0.72	KOWWIN			238	WSKOW	99	Assump.
C.I. Direct Black 38	1937377	0.546	AOPWIN	53	Lyman, 4-5			4.9	PHYS			3000	PHYS	99	Assump.
C.I. Direct Blue 218	28407376	0.168	AOPWIN	1E+10	PCKOC			3.39	KOWWIN			3.15E-06	WSKOW	99	Assump.
C.I. Direct Blue 6	2602462	0.04	AOPWIN	620	Lyman, 4-8			2.6	PHYS			0.0001366	PHYS	99	Assump.
C.I. Direct Brown 95	16071866	0.13	AOPWIN	1080000	PCKOC			-6.53	KOWWIN			1000000	WSKOW	99	Assump.
C.I. Disperse Yellow 3	2832408	0.058	AOPWIN	3990	Lyman, 4-5			3.98	PHYS			1.18	PHYS	99	Assump.
C.I. Food Red 15	81889	0.64	AOPWIN	25	Lyman, 4-5			1.95	PHYS			12000	PHYS	99	Assump.
C.I. Food Red 5	3761533	0.0175	AOPWIN	550	Lyman, 4-8			2.5	HL			1580	WSKOW	99	Assump.
C.I. Solvent Orange 7	3118976	0.0622	AOPWIN	21600	Lyman, 4-5			6.6	PHYS			0.05445	PHYS	99	Assump.
C.I. Solvent Yellow 14	842079	0.0494	AOPWIN	5400	Lyman, 4-5			5.51	PHYS			0.6738	PHYS	99	Assump.

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Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
C.I. Solvent Yellow 3	97563	0.147	AOPWIN	1500	Lyman, 4-5			4.29	PHYS			7	PHYS	99	Assump.
Auramine	492808	0.554	AOPWIN	489	Lyman, 4-5	0.00039	CHMF	2.98	PHYS			53.54	PHYS	99	Assump.
C.I. Vat Yellow 4	128665	0.0445	AOPWIN	114000	Lyman, 4-5			6.28	PHYS			0.002637	PHYS	99	Assump.
Cadmium and cadmium compounds	7440439			14	PCKOC			-0.07	PHYS	32	Gerritse	122800	PHYS	88.5	EPA, 92
Calcium cyanamide	156627			5.4	Lyman, 4-5			-0.2	PHYS			193400	PHYS		
Captan	133062	0.239	AOPWIN	200	CHMF	0.23	CHMF	2.8	PHYS			5.1	PHYS	99	Assump.
Carbaryl	63252	0.0702	AOPWIN	210	CHMF	0.0021	CHMF	2.36	PHYS			110	PHYS	99	Assump.
Carbofuran	1563662	0.0715	AOPWIN	62	CHMF	0.000726	HYDRO	2.32	PHYS			320	PHYS	99	Assump.
Carbon disulfide	75150			89	Lyman, 4-5			1.94	PHYS			1180	PHYS	99	Assump.
Carbon tetrachloride	56235	3.24E-07	AOPWIN	71	CHMF			2.83	PHYS			793	PHYS	99	Assump.
Carbonyl sulfide	463581			88	CHMF			-1.33	PHYS			1220	PHYS	99	Assump.
Carboxin	5234684	0.343	AOPWIN	237	Lyman, 4-5			2.14	PHYS			199	PHYS	99	Assump.
Catechol	120809	0.0627	AOPWIN	118	CHMF			0.88	PHYS			461000	PHYS	99	Assump.
CFC 114 (1,2-dichloro,1,1,2,2-tetrafluoroethane)	76142			300	Lyman, 4-5			2.82	PHYS			130	PHYS	99	Assump.
CFC 115 (chloropenta-fluoroethane)	76153			470	Lyman, 4-5			2.47	PHYS			58	PHYS	99	Assump.
CFC-11 (trichlorofluoromethane)	75694	0.000003	AOPWIN	93	CHMF			2.53	PHYS			1100	PHYS	99	Assump.
CFC-12 (dichlorodi-fluoromethane)	75718	0.00018	AOPWIN	200	CHMF			2.16	PHYS			280	PHYS	99	Assump.
Chinomethionat (6-methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one)	2439012	0.00905	AOPWIN	4400	Lyman, 4-5			3.78	PHYS			1	PHYS	99	Assump.
Chloramben	133904	0.0177	AOPWIN	130	CHMF			1.9	PHYS			700	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Chlordane	57749	0.0143	AOPWIN	38000	CHMF	4.3E-10	CHMF	6.16	PHYS			0.056	PHYS	99	Assump.
Chlorendic acid	115286	0.0221	AOPWIN	49	Lyman, 4-5			3.14	PHYS			3500	PHYS	99	Assump.
Chlorimuron ethyl*	90982324	0.115	AOPWIN	88	Lyman, 4-5	0.0000136	HYDRO	2.5	PHYS			1200	PHYS	99	Assump.
Chlorine	7782505			14	PCKOC			0.85	PHYS			6300	PHYS		
Chlorine dioxide	10049044			24	PCKOC			-3.22	KOWWIN			1000000	WSKOW		
2-Chloro-1,1,1,2-tetrafluoroethane	2837890	0.0000257	AOPWIN; exp	245	Lyman, 4-8	3.82E-06	HYDRO	1.86	PHYS			404	WSKOW	99	Assump.
2-Chloro-1,1,1-trifluoroethane	75887	0.0000437	AOPWIN; exp	29	Lyman, 4-5	1.47E-11	HYDRO	1.99	PHYS			9203	PHYS	99	Assump.
3-Chloro-1,1,1-trifluoropropane (HCFC-253fb)	460355	0.00124	AOPWIN	532	Lyman, 4-8	1.33E-11	HYDRO	2.48	PHYS			123	WSKOW	99	Assump.
1-Chloro-1,1,2,2-tetrafluoroethane	354256	1.43E-06	AOPWIN	245	Lyman, 4-8	0.0569	HYDRO	1.86	PHYS			404	WSKOW	99	Assump.
1-Chloro-1,1-difluoroethane	75683	0.0000083	AOPWIN; exp	81	Lyman, 4-5	8.44E-13	HYDRO	2.05	PHYS			1400	PHYS	99	Assump.
3-Chloro-2-methyl-1-propene	563473	0.107	AOPWIN	81	Lyman, 4-5			2.48	PHYS			1400	PHYS	99	Assump.
Chloroacetic acid	79118	0.00212	AOPWIN		Ion			0.22	PHYS			858000	PHYS	99	Assump.
2-Chloroacetophenone	532274	0.00552	AOPWIN	75	Lyman, 4-5			1.93	PHYS			1635	PHYS	99	Assump.
1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride	4080313	1.43	AOPWIN; ave	2	Lyman, 4-5			-5.92	PHYS			1000000	PHYS	99	Assump.
p-Chloroaniline	106478	0.115	AOPWIN; exp	410	CHMF	0.047	CHMF; photo	1.83	PHYS			3900	PHYS	99	Assump.
Chlorobenzene	108907	0.00208	AOPWIN; exp	430	CHMF	9E-08	CHMF	2.84	PHYS			498	PHYS	99	Assump.
Chlorobenzilate	510156	0.0138	AOPWIN	1100	CHMF	9.66E-08	HYDRO	4.74	PHYS			13	PHYS	99	Assump.
2,4-D chlorocrotyl ester	2971382	0.0788	AOPWIN; ave	6050	Lyman, 4-8	0.00434	HYDRO	4.42	KOWWIN			1.83	WSKOW	99	Assump.
Chlorodifluoromethane (HCFC-22)	75456	0.0000126	AOPWIN; exp	56	Lyman, 4-5	0.000325	HYDRO	1.08	PHYS			2770	PHYS	99	Assump.
Chloroethane (Ethyl chloride)	75003	0.00105	AOPWIN; exp	38	CHMF	4.22E-15	HYDRO	1.43	PHYS			5680	PHYS	99	Assump.
Chloroform	67663	0.000278	AOPWIN; exp	45	CHMF	2.48E-08	CHMF	1.97	PHYS			7950	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013

Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Chloromethane	74873	0.000118	AOPWIN; exp	39	Lyman, 4-5	0.0000853	CHMF	0.91	PHYS			5320	PHYS	99	Assump.
Chloromethyl methyl ether	107302	0.00621	AOPWIN		Fast Hyd	21	CHMF	0.32	PHYS			69440	PHYS	99	Assump.
p-Chloro-o-toluidine	95692	0.104	AOPWIN	100	Lyman, 4-5			2.27	PHYS			953.9	PHYS	99	Assump.
Chlorophenols	N084	0.0015	PHYS; penta	4800	CHMF; penta			5.12	PHYS; penta			14	PHYS; penta	99	Assump.
Chloropicrin	76062	0.000351	AOPWIN	81	CHMF	0.000007	CHMF	2.09	PHYS			1620	PHYS	99	Assump.
Chloroprene	126998	0.0595	AOPWIN	105	Lyman, 4-5	0	CHMF	2.53	PHYS			874.9	PHYS	99	Assump.
3-Chloropropionitrile	542767	0.000288	AOPWIN	12	Lyman, 4-5	0.0013	CHMF	0.18	PHYS			47590	PHYS	99	Assump.
Chlorotetrafluoroethane	63938103	0.0136	AOPWIN	245	Lyman, 4-8	0.0569	HYDRO	1.86	HL			0.00917	WSKOW	99	Assump.
Chlorothalonil	1897456	0.0000167	AOPWIN	1820	CHMF			3.05	PHYS			0.6	PHYS	99	Assump.
Chlorotrifluoromethane	75729	3.78E-06	AOPWIN	370	Lyman, 4-5			1.65	PHYS			90	PHYS	99	Assump.
Chlorpyrifos methyl	5598130	0.159	AOPWIN	3311	CHMF			4.31	PHYS			4.76	PHYS	99	Assump.
Chlorsulfuron	64902723	0.0068	AOPWIN	16	Lyman, 4-5			2	PHYS			28000	PHYS	99	Assump.
Chromium and chromium compounds	7440473			14	PCKOC			0.23	PHYS	340	Gerritse	86670	PHYS	99	EPA, 92
Cobalt and cobalt compounds	7440484			14	PCKOC			0.23	PHYS	10	Gerritse	87450	PHYS		
Copper and copper compounds	7440508	0.0264	AOPWIN	14	PCKOC			-0.57	PHYS	150	Gerritse	420800	PHYS	99.9	EPA, 92
Creosote, coal tar	8001589											0	Merck	99	Assump.
p-Cresidine	120718	0.543	AOPWIN	55	Lyman, 4-5			1.74	PHYS			2810	PHYS	99	Assump.
Cresol (mixed isomers)	1319773	0.113	AOPWIN	29	Lyman, 4-5			1.95	PHYS			9066	PHYS	99	Assump.
m-Cresol	108394	0.173	AOPWIN; exp	35	CHMF			1.96	PHYS			22700	PHYS	99	Assump.
o-Cresol	95487	0.113	AOPWIN; exp	47	CHMF			1.95	PHYS			25900	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
p-Cresol	106445	0.127	AOPWIN; exp	940	CHMF			1.94	PHYS			21500	PHYS	99	Assump.
Crotonaldehyde	4170303	0.095	AOPWIN; exp	5.6	Lyman, 4-5			0.6	PHYS			181000	PHYS	99	Assump.
Cumene	98828	0.0176	AOPWIN; exp	454	CHMF			3.66	PHYS			61.3	PHYS	99	Assump.
Cumene hydroperoxide	80159	0.0233	AOPWIN	23	CHMF			2.16	PHYS			13900	PHYS	99	Assump.
Cupferron	135206	0.0902	AOPWIN	2.9	Lyman, 4-5			-1.73	PHYS			608000	PHYS	99	Assump.
Cyanazine	21725462	0.0252	AOPWIN	191	CHMF			2.22	PHYS			170	PHYS	99	Assump.
Cyanide compounds	N106	0.000081	AOPWIN; HCN	4.5	PCKOC; Cu(CN)2			-1.49	PHYS; Cu(CN)2			1000000	WSKOW; Cu(CN)2		
Cycloate	1134232	0.0955	AOPWIN; exp	347	CHMF			3.88	PHYS			85	PHYS	99	Assump.
Cyclohexane	110827	0.0202	AOPWIN	480	Lyman, 4-5			3.44	PHYS			55	PHYS	99	Assump.
Cyclohexanol	108930	0.0472	AOPWIN	13	Lyman, 4-5			1.23	PHYS			42000	PHYS	99	Assump.
Cyfluthrin	68359375	0.037	AOPWIN	110000	Lyman, 4-5	2.21E-06	HYDRO	5.95	PHYS			0.003	PHYS	99	Assump.
Cyhalothrin	68085858	0.085	AOPWIN	80000	Lyman, 4-5	2.21E-06	HYDRO	6.8	PHYS			0.005	PHYS	99	Assump.
Dazomet	533744	0.77	AOPWIN	53	Lyman, 4-5			1.4	PHYS			3000	PHYS	99	Assump.
Dazomet, sodium salt	53404607			53	Lyman, 4-5			1.4	HL			3000	HL	99	Assump.
2,4-DB	94826	0.0385	AOPWIN	530	CHMF			3.53	PHYS			46	PHYS	99	Assump.
Decabromodiphenyl ether	1163195	0.000248	AOPWIN	33000	Lyman, 4-5			12.11	PHYS			0.025	PHYS	99	Assump.
Desmedipham	13684565	0.247	AOPWIN	1500	Lyman, 4-5	0.0894	HYDRO	3.39	PHYS			7	PHYS	99	Assump.
Di(2-ethylhexyl) phthalate	117817	0.0593	AOPWIN	87400	CHMF	0.0000148	HYDRO	7.6	PHYS			0.27	PHYS	99	Assump.
Diallate	2303164	0.0976	AOPWIN	720	CHMF	0.000012	CHMF	4.49	PHYS			14	PHYS	99	Assump.
2,4-Diaminoanisole sulfate	39156417	0.0564	AOPWIN	16	Lyman, 4-8			-4.2	KOWWIN			1000000	WSKOW	99	Assump.

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Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
2,4-Diaminoanisole	615054	0.542	AOPWIN	19	Lyman, 4-5			-0.31	PHYS			19500	PHYS	99	Assump.
4,4'-Diaminodiphenylether	101804	0.54	AOPWIN	134	Lyman, 4-5			1.36	PHYS			559.7	PHYS	99	Assump.
Diaminotoluene (mixed isomers)	25376458	0.518	AOPWIN	9.1	Lyman, 4-5			0.16	PHYS			74820	PHYS	99	Assump.
2,4-Diaminotoluene	95807	0.518	AOPWIN; exp	9.1	Lyman, 4-5			0.14	PHYS			74820	PHYS	99	Assump.
Diazinon	333415	0.261	AOPWIN	534	CHMF			3.81	PHYS			40	PHYS	99	Assump.
Diazomethane	334883	0.00252	AOPWIN	58	Lyman, 4-5			2	PHYS			2549	PHYS	99	Assump.
Dibenzofuran	132649	0.0105	AOPWIN; exp	8100	CHMF			4.12	PHYS			3.1	PHYS	99	Assump.
1,2-Dibromo-3-chloropropane (DBCP)	96128	0.00117	AOPWIN; exp	130	CHMF	2.06E-06	CHMF	2.96	PHYS			1230	PHYS	99	Assump.
1,2-Dibromoethane	106934	0.000675	AOPWIN; exp	58	CHMF	0.0000099	CHMF	1.96	PHYS			4150	PHYS	99	Assump.
1,2-Dibromotetrafluoroethane	124732	7.02E-07	AOPWIN	1200	Lyman, 4-5			2.96	PHYS			11.19	PHYS	99	Assump.
Dibutyl phthalate	84742	0.025	AOPWIN	3400	CHMF	0.0000079	CHMF	4.5	PHYS			11.2	PHYS	99	Assump.
Dicamba	1918009	0.00805	AOPWIN	5.5	CHMF			2.21	PHYS			8310	PHYS	99	Assump.
Dichloran	99309	0.000373	AOPWIN	5000	CHMF			2.8	PHYS			7	PHYS	99	Assump.
3,3-Dichloro-1,1,1,2,2-pentafluoropropane (HCFC-225ca)	422560	0.0000135	AOPWIN	1220	Lyman, 4-8	1.87E-07	HYDRO	3.14	KOWWIN			15.9	WSKOW	99	Assump.
2,3-Dichloro-1,1,1,2,3-pentafluoropropane (HCFC-225ba)	422480			1220	Lyman, 4-8			3.14	HL					99	Assump.
2,2-Dichloro-1,1,1,3,3-pentafluoropropane (HCFC-225aa)	128903219	0.0000116	AOPWIN	1220	Lyman, 4-8	0.0223	HYDRO	3.14	KOWWIN			15.9	WSKOW	99	Assump.
2,2-Dichloro-1,1,1-trifluoroethane	306832	0.0000983	AOPWIN; exp	79	Lyman, 4-5	5.88E-07	HYDRO	2.17	PHYS			1488	PHYS	99	Assump.
1,3-Dichloro-1,1,2,2,3-pentafluoropropane	507551	3.37E-06	AOPWIN	1220	Lyman, 4-8	4.34E-07	HYDRO	3.14	KOWWIN			15.9	WSKOW	99	Assump.

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Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
1,2-Dichloro-1,1,2,3,3-pentafluoropropane (HCFC-225bb)	422446	0.0000116	AOPWIN	1220	Lyman, 4-8	0.0223	HYDRO	3.14	KOWWIN			15.9	WSKOW	99	Assump.
1,3-Dichloro-1,1,2,3,3-pentafluoropropane (HCFC-225ea)	136013791	4.73E-07	AOPWIN	1220	Lyman, 4-8	0.0000879	HYDRO	3.14	HL			15.9	WSKOW	99	Assump.
Dichloro-1,1,2-trifluoroethane	90454185			361	Lyman, 4-8			2.17	HL					99	Assump.
1,2-Dichloro-1,1,2-trifluoroethane	354234	0.0000332	AOPWIN; exp	361	Lyman, 4-8	0.00877	HYDRO	2.17	PHYS			186	WSKOW	99	Assump.
1,2-Dichloro-1,1,3,3,3-pentafluoropropane (HCFC-225da)	431867			1220	Lyman, 4-8			3.14	HL					99	Assump.
1,2-Dichloro-1,1-difluoroethane	1649087	0.0000432	AOPWIN; exp	98	Lyman, 4-5	3.38E-08	HYDRO	2.31	PHYS			999	PHYS	99	Assump.
1,1-Dichloro-1,2,2,3,3-pentafluoropropane (HCFC-225cc)	13474889	8.34E-07	AOPWIN	1220	Lyman, 4-8	2.82E-06	HYDRO	3.14	KOWWIN			15.9	WSKOW	99	Assump.
1,1-Dichloro-1,2,2-trifluoroethane (HCFC-123b)	812044			361	Lyman, 4-8			2.17	HL					99	Assump.
1,1-Dichloro-1,2,3,3,3-pentafluoropropane (HCFC-225eb)	111512562	1.54E-06	AOPWIN	1220	Lyman, 4-8	0.00219	HYDRO	3.14	KOWWIN			15.9	WSKOW	99	Assump.
1,1-Dichloro-1-fluoroethane	1717006	0.0000189	AOPWIN; exp	57	Lyman, 4-5	2.68E-12	HYDRO	2.37	PHYS			2632	PHYS	99	Assump.
1,4-Dichloro-2-butene	764410	0.096	AOPWIN	130	Lyman, 4-5	0.009	CHMF	2.6	PHYS			580	PHYS	99	Assump.
Dichlorobenzene (mixed isomers)	25321226	0.00113	AOPWIN	390	Lyman, 4-5			3.28	PHYS			80	PHYS	99	Assump.
1,2-Dichlorobenzene	95501	0.00113	AOPWIN; exp	290	CHMF	9E-08	CHMF	3.43	PHYS			156	PHYS	99	Assump.
1,3-Dichlorobenzene	541731	0.00194	AOPWIN; exp	375	CHMF	9E-09	CHMF	3.53	PHYS			125	PHYS	99	Assump.
1,4-Dichlorobenzene	106467	0.000864	AOPWIN; exp	900	CHMF	9E-08	CHMF	3.44	PHYS			81.3	PHYS	99	Assump.
3,3'-Dichlorobenzidine dihydrochloride	612839	0.00151	AOPWIN	1930	Lyman, 4-8			0.45	KOWWIN			3590	WSKOW	99	Assump.
3,3'-Dichlorobenzidine sulfate	64969342	0.107	AOPWIN	1930	Lyman, 4-8			3.21	KOWWIN			22.9	WSKOW	99	Assump.
3,3'-Dichlorobenzidine	91941	0.107	AOPWIN	47000	CHMF			3.51	PHYS			3.1	PHYS	99	Assump.
Dichlorobromomethane	75274	0.000212	AOPWIN	53	Lyman, 4-5	5.8E-07	CHMF	2	PHYS			3032	PHYS	99	Assump.

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1,2-Dichloroethane	107062	0.00067	AOPWIN; exp	37	CHMF	1.69E-10	HYDRO	1.48	PHYS			8520	PHYS	99	Assump.
1,2-Dichloroethylene	540590	0.00717	AOPWIN; ave	49	Lyman, 4-5			1.86	PHYS			3500	PHYS	99	Assump.
Dichlorofluoromethane	75434	0.0000818	AOPWIN; exp	19	Lyman, 4-5	6.49E-06	HYDRO	1.55	PHYS			18800	PHYS	99	Assump.
Dichloromethane	75092	0.000383	AOPWIN; exp	28	CHMF	1.2E-07	CHMF	1.25	PHYS			13000	PHYS	99	Assump.
Dichloropentafluoro-propane	127564925			1220	Lyman, 4-8			3.14	HL					99	Assump.
Dichlorophene	97234	0.0673	AOPWIN	670	Lyman, 4-5			4.26	PHYS			30	PHYS	99	Assump.
2,4-Dichlorophenol	120832	0.00286	AOPWIN; exp	1570	CHMF			3.06	PHYS			4500	PHYS	99	Assump.
1,2-Dichloropropane	78875	0.00119	AOPWIN	27	CHMF	0.000005	CHMF	1.98	PHYS			2800	PHYS	99	Assump.
2,3-Dichloropropene	78886	0.0231	AOPWIN	64	Lyman, 4-5			2.42	PHYS			2150	PHYS	99	Assump.
1,3-Dichloropropylene	542756	0.0269	AOPWIN; ave	110	CHMF			2.29	PHYS			2800	PHYS	99	Assump.
Dichlorotrifluoroethane	34077877			361	Lyman, 4-8			2.17	HL					99	Assump.
Dichlorvos	62737	0.0254	AOPWIN	47	CHMF	0.0027	CHMF	1.47	PHYS			8000	PHYS	99	Assump.
Diclofop methyl	51338273	0.0716	AOPWIN	4900	Lyman, 4-5	0.0000456	HYDRO	4.62	PHYS			0.8	PHYS	99	Assump.
Dicofol	115322	0.00925	AOPWIN	4900	Lyman, 4-5			5.02	PHYS			0.8	PHYS	99	Assump.
Dicyclopentadiene	77736	0.326	AOPWIN	720	Lyman, 4-5			3.16	PHYS			26.47	PHYS	99	Assump.
Diepoxybutane	1464535	0.00269	AOPWIN	2	Lyman, 4-5	7.4E-07	HYDRO	-0.28	PHYS			1000000	PHYS	99	Assump.
Diethanolamine	111422	0.25	AOPWIN	2	Lyman, 4-5			-1.43	PHYS			1000000	PHYS	99	Assump.
Diethatyl ethyl	38727558	0.0641	AOPWIN	338	Lyman, 4-5	0.000207	HYDRO	3.6	PHYS			105	PHYS	99	Assump.
Diethyl sulfate	64675	0.00486	AOPWIN; exp	34	CHMF			1.14	PHYS			7000	PHYS	99	Assump.
Diflubenzuron	35367385	0.0439	AOPWIN	6760	CHMF			3.88	PHYS			0.08	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Diglycidyl resorcinol ether	101906	0.581	AOPWIN	111	Lyman, 4-8	6.33E-07	HYDRO	1.23	PHYS			2960	WSKOW	99	Assump.
Dihydrosafrole	94586	0.139	AOPWIN	470	Lyman, 4-5			3.58	PHYS			56.87	PHYS	99	Assump.
Diisocyanates	N120														
Dimethipin	55290647	0.346	AOPWIN	42	Lyman, 4-5			-0.17	PHYS			4600	PHYS	99	Assump.
Dimethoate	60515	0.214	AOPWIN	11	CHMF	0.0000756	CHMF	0.78	PHYS			25000	PHYS	99	Assump.
3,3'-Dimethoxybenzidine dihydrochloride	20325400	0.364	AOPWIN	93	Lyman, 4-8			2.08	KOWWIN			724	WSKOW	99	Assump.
3,3'-Dimethoxybenzidine hydrochloride	111984099													99	Assump.
3,3'-Dimethoxybenzidine	119904	0.364	AOPWIN	460	Lyman, 4-5			1.81	PHYS			60	PHYS	99	Assump.
Dimethyl chlorothiophosphate	2524030	0.16	AOPWIN; exp	43	Lyman, 4-5			1.39	PHYS			4400	PHYS	99	Assump.
1,1-Dimethyl hydrazine	57147	0.00683	AOPWIN	2	Lyman, 4-5			-1.19	PHYS			1000000	PHYS	99	Assump.
Dimethyl phthalate	131113	0.00155	AOPWIN	40	CHMF	0.0000288	HYDRO	1.6	PHYS			4000	PHYS	99	Assump.
Dimethyl sulfate	77781	0.000514	AOPWIN	16	CHMF	0.6	CHMF	0.16	PHYS			28000	PHYS	99	Assump.
Dimethylamine	124403	0.177	AOPWIN; exp	435	CHMF			-0.38	PHYS			1630000	PHYS	99	Assump.
Dimethylamine dicamba	2300665	0.0199	AOPWIN	2.6	Lyman, 4-5	0.00331	HYDRO	1.13	KOWWIN			720000	HL	99	Assump.
4-Dimethyl-aminoazobenzene	60117	0.405	AOPWIN	9800	Lyman, 4-5			4.58	PHYS			0.23	PHYS	99	Assump.
N,N-Dimethylaniline	121697	0.4	AOPWIN; exp	80	CHMF			2.31	PHYS			1450	PHYS	99	Assump.
3,3'-Dimethylbenzidine dihydrochloride	612828	0.51	AOPWIN	1050	Lyman, 4-8			3.02	KOWWIN			379	WSKOW	99	Assump.
3,3'-Dimethylbenzidine dihydrofluoride	41766750			447	Lyman, 4-8			2.34	HL					99	Assump.
3,3'-Dimethylbenzidine	119937	0.51	AOPWIN	85	Lyman, 4-5			2.34	PHYS			1300	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Dimethylcarbamyl chloride	79447	0.0435	AOPWIN		Fast Hyd	4.2	HYDRO	-0.72	PHYS			458500	PHYS	99	Assump.
N,N-Dimethylformamide	68122	0.0474	AOPWIN	2	Lyman, 4-5			-1.01	PHYS			1000000	PHYS	99	Assump.
2,4-Dimethylphenol	105679	0.193	AOPWIN; exp	31	Lyman, 4-5			2.3	PHYS			7870	PHYS	99	Assump.
m-Dinitrobenzene	99650	0.0000824	AOPWIN	138	Lyman, 4-5			1.49	PHYS			533	PHYS	99	Assump.
o-Dinitrobenzene	528290	0.0000575	AOPWIN	296	Lyman, 4-5			1.69	PHYS			133	PHYS	99	Assump.
p-Dinitrobenzene	100254	0.0000575	AOPWIN	430	Lyman, 4-5			1.46	PHYS			69	PHYS	99	Assump.
Dinitrobutyl phenol (Dinoseb)	88857	0.0109	AOPWIN	124	CHMF			3.56	PHYS			52	PHYS	99	Assump.
4,6-Dinitro-o-cresol	534521	0.000818	AOPWIN	257	CHMF			2.12	PHYS			198	PHYS	99	Assump.
2,4-Dinitrophenol	51285	0.00178	AOPWIN		Ion			1.67	PHYS			2790	PHYS	99	Assump.
Dinitrotoluene (mixed isomers)	25321146	0.000517	AOPWIN	200	Lyman, 4-5			2.18	PHYS			270	PHYS	99	Assump.
2,4-Dinitrotoluene	121142	0.000582	AOPWIN	200	Lyman, 4-5			1.98	PHYS			270	PHYS	99	Assump.
2,6-Dinitrotoluene	606202	0.000582	AOPWIN	100	CHMF			2.1	PHYS			182	PHYS	99	Assump.
Dinocap	39300453	0.0831	AOPWIN; ave	2000	Lyman, 4-5	0.0000223	HYDRO	5.98	PHYS			4	PHYS	99	Assump.
Dioxane	123911	0.0294	AOPWIN; exp	2	Lyman, 4-5			-0.27	PHYS			1000000	PHYS	99	Assump.
Dioxin and dioxin-like compounds	N150	0.00203	AOPWIN									0.0002	PHYS	99.9999	by law
Diphenamid	957517	0.0724	AOPWIN	210	Lyman, 4-5			2.17	PHYS			260	PHYS	99	Assump.
Diphenylamine	122394	0.525	AOPWIN; exp	600	CHMF			3.5	PHYS			53	PHYS	99	Assump.
1,2-Diphenylhydrazine	122667	0.23	AOPWIN	224	Lyman, 4-5			2.94	PHYS			221	PHYS	99	Assump.
Dipotassium endothall	2164070	0.0772	AOPWIN	330	Lyman, 4-5			1.89	KOWWIN			110	HL	99	Assump.
Dipropyl isocinchomeronate	136458	0.0171	AOPWIN	822	Lyman, 4-5	0.0000231	HYDRO	3.57	PHYS			20.8	PHYS	99	Assump.

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Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Disodium cyanodithio-imidocarbonate	138932	0.0878	AOPWIN	35	Lyman, 4-8			0.31	KOWWIN			2740	WSKOW	99	Assump.
2,4-Dithiobiuret	541537	0.284	AOPWIN	57	Lyman, 4-5	0.0071	CHMF	-1.52	PHYS			2700	PHYS	99	Assump.
Diuron	330541	0.0294	AOPWIN	350	CHMF			2.68	PHYS			42	PHYS	99	Assump.
Dodine	2439103	0.294	AOPWIN	130	Lyman, 4-5	0.00177	HYDRO	-0.88	PHYS			630	PHYS	99	Assump.
2,4-DP (Dichlorprop)	120365	0.0308	AOPWIN	170	Lyman, 4-5			3.43	PHYS			350	PHYS	99	Assump.
D-trans-allethrin (D-trans-chrysanthemic acid of D-allethrone)	28057489			9490	Lyman, 4-8			4.78	HL					99	Assump.
Epichlorohydrin	106898	0.00119	AOPWIN; exp	10	CHMF	0.0035	CHMF	0.45	PHYS			65900	PHYS	99	Assump.
Ethoprop	13194484	0.187	AOPWIN	110	Lyman, 4-5			3.59	PHYS			750	PHYS	99	Assump.
2-Ethoxyethanol	110805	0.0416	AOPWIN	2	Lyman, 4-5			-0.32	PHYS			1000000	PHYS	99	Assump.
Ethyl acrylate	140885	0.0432	AOPWIN; exp	22	CHMF	0.000023	CHMF	1.32	PHYS			15000	PHYS	99	Assump.
Ethyl chloroformate	541413	0.00449	AOPWIN	15	Lyman, 4-5			0.63	PHYS			32060	PHYS	99	Assump.
Ethyl dipropylthiocarbamate	759944	0.086	AOPWIN; exp	200	CHMF			3.21	PHYS			375	PHYS	99	Assump.
2,4-D 2-ethyl-4-methylpentyl ester	53404378			24900	Lyman, 4-5			5.55	HL					99	Assump.
Ethylbenzene	100414	0.0192	AOPWIN; exp	190	CHMF			3.15	PHYS			169	PHYS	99	Assump.
Ethylene	74851	0.023	AOPWIN; exp	299	Lyman, 4-5			1.13	PHYS			131	PHYS	99	Assump.
Ethylene glycol	107211	0.0208	AOPWIN; exp	2	Lyman, 4-5			-1.36	PHYS			1000000	PHYS	99	Assump.
Ethylene oxide	75218	0.000205	AOPWIN; exp	2	Lyman, 4-5	0.0025	CHMF	-0.3	PHYS			1000000	PHYS	99	Assump.
Ethylene thiourea	96457	0.386	AOPWIN	19	Lyman, 4-5	0	CHMF	-0.66	PHYS			20000	PHYS	99	Assump.
Ethylenebisdithiocarbamic acid, salts and esters (EBDCs)	N171	0.971	AOPWIN; met	22	Lyman, 4-5; met			0.3	PHYS; met			14530	PHYS; met	99	Assump.; met

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Ethyleneimine (Aziridine)	151564	0.0165	AOPWIN; exp	2	Lyman, 4-5	0.000188	CHMF	-0.28	PHYS			1000000	PHYS	99	Assump.
2,4-D 2-ethylhexyl ester	1928434	0.0392	AOPWIN	61400	Lyman, 4-8	0.000825	HYDRO	6.27	KOWWIN			0.0347	WSKOW	99	Assump.
Ethylidene dichloride	75343	0.00074	AOPWIN; exp	40	CHMF	3.3E-13	HYDRO	1.79	PHYS			5060	PHYS	99	Assump.
Famphur	52857	0.167	AOPWIN	332	Lyman, 4-5	0.00025	CHMF	2.23	PHYS			108.5	PHYS	99	Assump.
Fenarimol	60168889	0.0107	AOPWIN	1000	Lyman, 4-5			3.6	PHYS			14	PHYS	99	Assump.
Fenbutatin oxide (Vendex)	13356086	1.64	AOPWIN	48000	Lyman, 4-5			5.2	PHYS			0.0127	PHYS		
Fenoxaprop ethyl	66441234	0.0904	AOPWIN	4600	Lyman, 4-5	0.0000431	HYDRO	4.95	PHYS			0.9	PHYS	99	Assump.
Fenoxycarb	72490018	0.176	AOPWIN	1600	Lyman, 4-5	6.33E-09	HYDRO	4.3	PHYS			6	PHYS	99	Assump.
Fenpropathrin	39515418	0.0483	AOPWIN	8000	Lyman, 4-5	2.21E-06	HYDRO	5.7	PHYS			0.33	PHYS	99	Assump.
Fenthion	55389	0.192	AOPWIN	1400	Lyman, 4-5	0.000251	HYDRO	4.09	PHYS			7.5	PHYS	99	Assump.
Fenvalerate	51630581	0.0602	AOPWIN	34000	Lyman, 4-5	1.65E-06	HYDRO	6.2	PHYS			0.024	PHYS	99	Assump.
Ferbam (Tris(dimethylcarba-modithioato-S,S')iron)	14484641	0.555	AOPWIN	300	Lyman, 4-5			-1.6	PHYS			130	PHYS	99	Assump.
Fluazifop butyl	69806504	0.0813	AOPWIN	4400	Lyman, 4-5	0.0000366	HYDRO	4.5	PHYS			1	PHYS	99	Assump.
Fluometuron	2164172	0.0205	AOPWIN	175	CHMF			2.42	PHYS			110	PHYS	99	Assump.
Fluorine	7782414			14	PCKOC			0.22	PHYS			1.69	PHYS		
Fluorouracil (5-fluorouracil)	51218	0.0157	AOPWIN	26	Lyman, 4-5			-0.89	PHYS			11100	PHYS	99	Assump.
Fluvalinate	69409945	0.0791	AOPWIN	80000	Lyman, 4-5	5.97E-09	HYDRO	6.81	PHYS			0.005	PHYS	99	Assump.
Folpet	133073	0.0425	AOPWIN	1860	CHMF			2.85	PHYS			1	PHYS	99	Assump.
Fomesafen	72178020	0.00434	AOPWIN	510	Lyman, 4-5			2.9	PHYS			50	PHYS	99	Assump.
Formaldehyde	50000	0.0253	AOPWIN; exp	3.6	Lyman, 4-5			0.35	PHYS			400000	PHYS	99	Assump.

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Formic acid	64186	0.00122	AOPWIN; exp		Ion			-0.54	PHYS			1000000	PHYS	99	Assump.
Freon 113	76131	0.000001	AOPWIN	260	Lyman, 4-5			3.16	PHYS			170	PHYS	99	Assump.
Furan	110009							1.32	Reaxys			1000	PHYS	99	Assump.
Glycidol	556525							-0.96	Reaxys			1000000	PHYS	99	Assump.
Glycol ethers	N230	0.034	PHYS; methoxy	2	Lyman, 4-5; methoxy			-0.77	PHYS; methoxy			1000000	PHYS; methoxy	99	Assump.
Heptachlor	76448	0.166	AOPWIN	11000	Lyman, 4-5	0.00536	EPA, 99	6.1	PHYS			0.18	PHYS	99	Assump.
Hexachloro-1,3-butadiene	87683	0.000081	AOPWIN	2300	CHMF			4.78	PHYS			3.2	PHYS	99	Assump.
Hexachlorobenzene	118741	0.0000456	AOPWIN	16300	CHMF	0	CHMF	5.73	PHYS			0.0062	PHYS	99	Assump.
alpha-Hexachlorocyclohexane	319846	0.00155	AOPWIN	2000	CHMF	2.22E-15	HYDRO	3.8	PHYS			2	PHYS	99	Assump.
Hexachlorocyclo-pentadiene	77474	0.00106	AOPWIN	2000	CHMF	0.002	CHMF	5.04	PHYS			1.8	PHYS	99	Assump.
Hexachloroethane	67721			2188	CHMF	0	CHMF	4.14	PHYS			50	PHYS	99	Assump.
Hexachloronaphthalene	1335871	0.000505	AOPWIN	160000	Lyman, 4-5			7.04	PHYS			0.0015	PHYS	99	Assump.
Hexachlorophene	70304	0.00588	AOPWIN	5000	CHMF			7.54	PHYS			140	PHYS	99	Assump.
Hexamethyl-phosphoramide	680319	0.243	AOPWIN	2	Lyman, 4-5			0.28	PHYS			1000000	PHYS	99	Assump.
n-Hexane	110543	0.0152	AOPWIN; exp	1300	Lyman, 4-5			3.9	PHYS			9.5	PHYS	99	Assump.
Hexazinone	51235042	0.244	AOPWIN	14	Lyman, 4-5			1.85	PHYS			33000	PHYS	99	Assump.
Hydramethylnon	67485294	0.386	AOPWIN; ave	73000	Lyman, 4-5			2.31	PHYS			0.006	PHYS	99	Assump.
Hydrazine	302012	0.18	PHYS		Ion			-2.07	PHYS			1000000	PHYS	99	Assump.
Hydrazine sulfate	10034932	0.171	AOPWIN	15	Lyman, 4-5			-4.05	KOWWIN			30303	Merck		
Hydrochloric acid	7647010			14	PCKOC	3.52E-09	HYDRO	0.54	KOWWIN			823000	CRC; 0 degrees C		

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Hydrogen cyanide	74908	0.000081	AOPWIN; exp	2	Lyman, 4-5			-0.25	PHYS			1000000	PHYS	99	Assump.
Hydrogen fluoride	7664393			14	PCKOC			0.23	PHYS			922	PHYS		
Hydroquinone	123319	0.0627	AOPWIN	9.3	CHMF			0.59	PHYS			72000	PHYS	99	Assump.
Imazalil	35554440	0.229	AOPWIN	250	Lyman, 4-5			3.82	PHYS			180	PHYS	99	Assump.
3-Iodo-2-propynyl butylcarbamate	55406536	0.069	AOPWIN	513	Lyman, 4-8	0.00507	HYDRO	2.45	KOWWIN			127	WSKOW	99	Assump.
Iron pentacarbonyl	13463406													99	Assump.
Isobutyraldehyde	78842	0.071	AOPWIN; exp	8	CHMF			0.74	PHYS			89000	PHYS	99	Assump.
Isodrin	465736	0.18	AOPWIN	45400	Lyman, 4-5	0.0000017	CHMF	6.75	PHYS			0.01415	PHYS	99	Assump.
Isofenphos	25311711	0.745	AOPWIN	795	Lyman, 4-5	0.0000102	HYDRO	4.12	PHYS			22.1	PHYS	99	Assump.
Isoprene	78795							2.3	Reaxys			642	PHYS	99	Assump.
Isopropyl alcohol	67630	0.0137	AOPWIN; exp	2	Lyman, 4-5			0.05	PHYS			1000000	PHYS	99	Assump.
2,4-D isopropyl ester	94111	0.019	AOPWIN	600	Lyman, 4-5	0.00114	HYDRO	3.81	PHYS			37.34	PHYS	99	Assump.
4,4'-Isopropylidenediphenol	80057	0.218	AOPWIN	310	Lyman, 4-5			3.32	PHYS			120	PHYS	99	Assump.
Isosafrole	120581	0.218	AOPWIN; ave	283	Lyman, 4-5			3.37	PHYS			144.3	PHYS	99	Assump.
Lactofen	77501634	0.009	AOPWIN	15000	Lyman, 4-5	0.0000773	HYDRO	4.81	PHYS			0.1	PHYS	99	Assump.
Lead and lead compounds	7439921			14	PCKOC			0.73	PHYS	580	Gerritse	9581	PHYS	91.6	EPA, 92
Lindane	58899	0.00155	AOPWIN	1290	CHMF	0.00012	CHMF	3.72	PHYS			7.3	PHYS	99	Assump.
Linuron	330552	0.028	AOPWIN	1510	CHMF			3.2	PHYS			75	PHYS	99	Assump.
Lithium carbonate	554132			24	Lyman, 4-5			-6.19	PHYS			12800	PHYS		
Malathion	121755	0.209	AOPWIN	1800	CHMF	0.0000218	HYDRO	2.36	PHYS			143	PHYS	99	Assump.

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Maleic anhydride	108316	0.00392	AOPWIN; exp		Fast Hyd	113	CHMF	1.62	PHYS			4912	PHYS	99	Assump.
Malonitrile	109773	0.000091	AOPWIN	6.6	Lyman, 4-5	0.00135	CHMF	-0.6	PHYS			133000	PHYS	99	Assump.
Maneb	12427382	0.575	AOPWIN	550	CHMF			0.62	PHYS			6	PHYS	99	Assump.
Manganese and manganese compounds	7439965			14	PCKOC			0.23	PHYS	5	Gerritse	87170	PHYS		
Mecoprop	93652	0.0939	AOPWIN	130	Lyman, 4-5			3.13	PHYS			620	PHYS	99	Assump.
2-Mercaptobenzothiazole	149304	0.11	AOPWIN	310	Lyman, 4-5			2.42	PHYS			120	PHYS	99	Assump.
Mercury and mercury compounds	7439976			14	PCKOC			0.62	PHYS	4100	Gerritse	0.06	PHYS		
Merphos	150505	0.213	AOPWIN	98000	Lyman, 4-5			7.67	PHYS			0.0035	PHYS	99	Assump.
Methacrylonitrile	126987	0.0226	AOPWIN	16	Lyman, 4-5			0.68	PHYS			25400	PHYS	99	Assump.
Metham sodium	137428	0.174	AOPWIN	2.6	Lyman, 4-5			-2.62	PHYS			722000	PHYS	99	Assump.
Methanol	67561	0.00255	AOPWIN; exp	2	Lyman, 4-5			-0.77	PHYS			1000000	PHYS	99	Assump.
Methazole	20354261	0.0111	AOPWIN	2630	CHMF			3.22	PHYS			1.5	PHYS	99	Assump.
Methiocarb	2032657	0.0364	AOPWIN	209	CHMF	0.000775	HYDRO	2.92	PHYS			27	PHYS	99	Assump.
Methoxone (MCPA)	94746	0.0341	AOPWIN	130	Lyman, 4-5			3.25	PHYS			630	PHYS	99	Assump.
Methoxone sodium salt	3653483	0.0341	AOPWIN	4.5	Lyman, 4-5			-1.29	PHYS			270000	PHYS	99	Assump.
Methoxychlor	72435	0.145	AOPWIN	63000	CHMF	0.0000787	PRNA	5.08	PHYS			0.1	PHYS	99	Assump.
2-Methoxyethanol	109864	0.034	PHYS	2	Lyman, 4-5			-0.77	PHYS			1000000	PHYS	99	Assump.
Methyl acrylate	96333	0.0254	AOPWIN	11	CHMF	9.31E-06	HYDRO	0.8	PHYS			49400	PHYS	99	Assump.
Methyl chlorocarbonate	79221	0.000588	AOPWIN		Fast Hyd	2.03	CHMF	0.14	PHYS			92750	PHYS	99	Assump.
Methyl ethyl ketone	78933	0.00311	AOPWIN; exp	5	Lyman, 4-5			0.29	PHYS			223000	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Methyl hydrazine	60344	0.176	AOPWIN; exp	2	Lyman, 4-5	0	CHMF	-1.05	PHYS			1000000	PHYS	99	Assump.
Methyl iodide	74884	0.000194	AOPWIN; exp	23	Lyman, 4-5	0.000262	CHMF	1.51	PHYS			13800	PHYS	99	Assump.
Methyl isobutyl ketone	108101	0.0381	AOPWIN; exp	19	CHMF			1.31	PHYS			19000	PHYS	99	Assump.
Methyl isocyanate	624839	0.000367	AOPWIN		Fast Hyd	4.2	HYDRO	0.79	PHYS			29200	PHYS	99	Assump.
Methyl isothiocyanate	556616	0.000367	AOPWIN	6	CHMF	0.000676	HYDRO	0.94	PHYS			7600	PHYS	99	Assump.
Methyl methacrylate	80626	0.0702	AOPWIN; exp	22	CHMF	0.00002	CHMF	1.38	PHYS			15000	PHYS	99	Assump.
Methyl parathion	298000	0.16	AOPWIN	5100	CHMF	0.0004	CHMF	2.86	PHYS			37.7	PHYS	99	Assump.
Methyl tert-butyl ether	1634044	0.00794	AOPWIN; exp	11	CHMF			0.94	PHYS			51000	PHYS	99	Assump.
Methylene bromide	74953	0.000305	AOPWIN; exp	25	CHMF	8.94E-12	HYDRO	1.7	PHYS			11900	PHYS	99	Assump.
4,4'-Methylenebis(2-chloroaniline)	101144	0.209	AOPWIN	8000	CHMF	9E-08	CHMF	3.91	PHYS			13.9	PHYS	99	Assump.
4,4'-Methylenebis(N,N-dimethylbenzenamine)	101611	0.556	AOPWIN	2000	Lyman, 4-5			4.37	PHYS			4.14	PHYS	99	Assump.
Methylenebis(phenyl-isocyanate) (MDI)	101688	0.0312	AOPWIN		Fast Hyd	4.2	HYDRO	5.22	PHYS			0.8288	PHYS	99	Assump.
4,4'-Methylenedianiline	101779	0.543	AOPWIN; exp	98	CHMF			1.59	PHYS			1000	PHYS	99	Assump.
Methyleugenol	93152							2.97	Reaxys			500	PHYS	99	Assump.
2-Methyllactonitrile	75865	0.00317	AOPWIN		Fast Hyd	4.47	CHMF	-0.03	PHYS			1000000	PHYS	99	Assump.
2-Methylpyridine	109068	0.00298	AOPWIN	2	Lyman, 4-5			1.11	PHYS			1000000	PHYS	99	Assump.
Metiram	9006422	0.971	AOPWIN	22	Lyman, 4-5			0.3	PHYS			14530	PHYS	99	Assump.
Metribuzin	21087649	0.0493	AOPWIN	95	CHMF			1.7	PHYS			1050	PHYS	99	Assump.
Mevinphos	7786347	0.0981	AOPWIN	200	CHMF	2.38E-06	HYDRO	0.13	PHYS			600000	PHYS	99	Assump.
Michlers Ketone	90948	0.554	AOPWIN	162	CHMF			3.87	PHYS			400	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Molinate	2212671	0.0835	AOPWIN	83	CHMF			3.21	PHYS			970	PHYS	99	Assump.
Molybdenum trioxide	1313275			35	PCKOC			2.23	KOWWIN			490	Merck		
Monuron	150685	0.0393	AOPWIN	110	CHMF			1.94	PHYS			230	PHYS	99	Assump.
Mustard gas	505602	0.0211	AOPWIN	120	CHMF			2.41	PHYS			684	PHYS	99	Assump.
Myclobutanil	88671890	0.019	AOPWIN	286	Lyman, 4-5			2.94	PHYS			142	PHYS	99	Assump.
Nabam	142596	0.398	AOPWIN	5.3	Lyman, 4-5	0.693	PRNA	-4.24	PHYS			200000	PHYS	99	Assump.
Naled	300765	0.0172	AOPWIN	3500	Lyman, 4-5	0.021	HYDRO	1.38	PHYS			1.5	PHYS	99	Assump.
Naphthalene	91203	0.0583	AOPWIN; exp	1500	CHMF	0.0019	CHMF; photo	3.3	PHYS			31	PHYS	99	Assump.
beta-Naphthylamine	91598	0.54	AOPWIN	1600	Lyman, 4-5			2.28	PHYS			6.4	PHYS	99	Assump.
alpha-Naphthylamine	134327	0.54	AOPWIN	3210	CHMF			2.25	PHYS			1700	PHYS	99	Assump.
Nickel and nickel compounds	7440020			14	PCKOC			-0.57	PHYS	27	Gerritse	421600	PHYS	99	EPA, 92
Nicotine and salts	N503	0.25	AOPWIN; nic	2	Lyman, 4-5; nic			1.17	PHYS; nic			1000000	PHYS; nic	99	Assump.
Nitrapyrin	1929824	0.0000945	AOPWIN	321	CHMF			3.41	PHYS			72	PHYS	99	Assump.
Nitrate compounds (water dissociable)	N511	0.000972	AOPWIN									90900	PHYS		
Nitric acid	7697372	0.000972	AOPWIN	14	PCKOC			0.21	PHYS			90900	PHYS		
Nitrilotriacetic acid	139139	0.235	AOPWIN	280	CHMF			-3.81	PHYS			59060	PHYS	99	Assump.
o-Nitroanisole	91236							1.73	Reaxys			1690	PHYS	99	Assump.
Nitrobenzene	98953	0.000402	AOPWIN; exp	150	CHMF			1.85	PHYS			2090	PHYS	99	Assump.
4-Nitrobiphenyl	92933	0.00788	AOPWIN	1240	Lyman, 4-5			3.82	PHYS			9.835	PHYS	99	Assump.
Nitrofen	1836755	0.00427	AOPWIN	4400	CHMF			4.64	PHYS			1	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Nitrogen mustard	51752	0.0227	AOPWIN	25	Lyman, 4-5			0.91	PHYS			12000	PHYS	99	Assump.
Nitroglycerin	55630	0.00297	AOPWIN	468	CHMF	0.0000077	CHMF	1.62	PHYS			1380	PHYS	99	Assump.
Nitromethane	75525							-0.284	Reaxys			11100	Physprop	99	Assump.
5-Nitro-o-anisidine	99592	0.0242	AOPWIN	321	Lyman, 4-5			1.47	PHYS			115	PHYS	99	Assump.
5-Nitro-o-toluidine	99558	0.0315	AOPWIN	69	Lyman, 4-5			1.87	PHYS			1878	PHYS	99	Assump.
2-Nitrophenol	88755	0.00243	AOPWIN; exp	113	CHMF			1.79	PHYS			2500	PHYS	99	Assump.
4-Nitrophenol	100027	0.0116	AOPWIN	141	CHMF	0.0021	CHMF; photo	1.91	PHYS			11600	PHYS	99	Assump.
2-Nitropropane	79469	0.000702	AOPWIN; exp	21	Lyman, 4-5			0.93	PHYS			17000	PHYS	99	Assump.
N-Nitrosodiethylamine	55185	0.0478	AOPWIN	7.5	Lyman, 4-5			0.48	PHYS			106000	PHYS	99	Assump.
N-Nitrosodimethylamine	62759	0.00683	AOPWIN; exp	2	Lyman, 4-5			-0.57	PHYS			1000000	PHYS	99	Assump.
N-Nitrosodi-n-butylamine	924163	0.0724	AOPWIN	86	CHMF			2.63	PHYS			1270	PHYS	99	Assump.
N-Nitrosodi-n-propylamine	621647	0.0648	AOPWIN	24	Lyman, 4-5			1.36	PHYS			13000	PHYS	99	Assump.
N-Nitrosodiphenylamine	86306	0.067	AOPWIN	620	Lyman, 4-5			3.13	PHYS			35	PHYS	99	Assump.
p-Nitrosodiphenylamine	156105	0.54	AOPWIN	910	Lyman, 4-5			3.16	PHYS			17.3	PHYS	99	Assump.
N-Nitrosomethylvinylamine	4549400	0.046	AOPWIN	15	Lyman, 4-5			-0.28	PHYS			30000	PHYS	99	Assump.
N-Nitrosomorpholine	59892	0.202	AOPWIN	2	Lyman, 4-5			-0.44	PHYS			1000000	PHYS	99	Assump.
N-Nitroso-N-ethylurea	759739	0.0135	AOPWIN	24	Lyman, 4-5	0.0000063	CHMF	0.23	PHYS			13000	PHYS	99	Assump.
N-Nitroso-N-methylurea	684935	0.00421	AOPWIN	23	Lyman, 4-5			-0.03	PHYS			14400	PHYS	99	Assump.
Nitrosonornicotine	16543558	0.0795	AOPWIN	2	Lyman, 4-5			0.32	PHYS			1000000	PHYS	99	Assump.
N-Nitrosopiperidine	100754	0.0691	AOPWIN	9	CHMF			0.36	PHYS			76500	PHYS	99	Assump.

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N-methyl-2-pyrrolidone	872504	0.0637	AOPWIN	2	Lyman, 4-5			-0.38	PHYS			1000000	PHYS	99	Assump.
N-methylolacrylamide	924425	0.0763	AOPWIN	1	PCKOC			-1.81	KOWWIN			1000000	WSKOW	99	Assump.
Norflurazon	27314132	0.0268	AOPWIN	1905	CHMF			2.3	PHYS			33.7	PHYS	99	Assump.
Octachloronaphthalene	2234131	0.000104	AOPWIN	780000	CHMF; octa			8.24	PHYS			0.00008	PHYS	99	Assump.
Octochlorostyrene	29082744	0.00305	AOPWIN									0.00174	WSKOW	99	Assump.
Oryzalin (4-(dipropylamino)-3,5-dinitro-benzenesulfonamide)	19044883	0.0648	AOPWIN	2600	Lyman, 4-5			2.73	PHYS			2.5	PHYS	99	Assump.
Osmium tetroxide	20816120			49	PCKOC			2.23	KOWWIN			72400	Merck		
Oxadiazon	19666309	0.0657	AOPWIN	1480	CHMF			4.8	PHYS			0.7	PHYS	99	Assump.
Oxydemeton methyl	301122	0.285	AOPWIN	2	Lyman, 4-5			-0.74	PHYS			1000000	PHYS	99	Assump.
Oxyfluorfen	42874033	0.0358	AOPWIN	14300	Lyman, 4-5			4.73	PHYS			0.116	PHYS	99	Assump.
Ozone	10028156			2.6	Lyman, 4-5			-0.87	PHYS			744100	PHYS		
Paraldehyde	123637	0.0589	AOPWIN	7.3	Lyman, 4-5			0.67	PHYS			112000	PHYS	99	Assump.
Paraquat dichloride	1910425	0.0575	AOPWIN	2.7	Lyman, 4-5			-2.71	PHYS			700000	PHYS	99	Assump.
Parathion	56382	0.249	AOPWIN	1900	CHMF	0.000355	HYDRO	3.83	PHYS			11	PHYS	99	Assump.
p-Chlorophenyl isocyanate	104121	0.00406	AOPWIN	306	Lyman, 4-5	4.2	HYDRO	3.24	PHYS			125.7	PHYS	99	Assump.
Pebulate	1114712	0.0795	AOPWIN	631	CHMF			3.83	PHYS			100	PHYS	99	Assump.
Pendimethalin	40487421	0.082	AOPWIN	8880	Lyman, 4-5			5.18	PHYS			0.275	PHYS	99	Assump.
Pentachlorobenzene	608935	0.000156	PHYS	8800	CHMF	9E-08	CHMF	5.17	PHYS			0.831	PHYS	99	Assump.
Pentachloroethane	76017	0.0000521	AOPWIN	146	CHMF	0.00429	HYDRO	3.22	PHYS			480	PHYS	99	Assump.

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Pentachlorophenol	87865	0.0015	PHYS	2400	CHMF	0.0032	CHMF; photo	5.12	PHYS			14	PHYS	99	Assump.
Pentobarbital sodium	57330	0.0486	AOPWIN	330	Lyman, 4-8			2	KOWWIN			513	WSKOW	99	Assump.
Perchloromethyl mercaptan	594423			475	Lyman, 4-5			3.47	PHYS			56.32	PHYS	99	Assump.
Permethrin	52645531	0.062	AOPWIN	63100	CHMF	0.0000145	HYDRO	6.5	PHYS			0.006	PHYS	99	Assump.
Peroxyacetic acid	79210	0.0109	AOPWIN	2	Lyman, 4-5	0.0836	HYDRO	-1.07	PHYS			1000000	PHYS	99	Assump.
Phenanthrene	85018	0.0351	AOPWIN; exp	8300	CHMF			4.46	PHYS			1.15	PHYS	99	Assump.
Phenol	108952	0.071	AOPWIN; exp	160	CHMF			1.46	PHYS			82800	PHYS	99	Assump.
Phenolphthalein	77098							3.06	EPI			400	PHYS	99	Assump.
Phenothrin	26002802	0.287	AOPWIN	56000	Lyman, 4-5	0.0000145	HYDRO	7.54	PHYS			0.0097	PHYS	99	Assump.
1,2-Phenylenediamine dihydrochloride	615281	0.476	AOPWIN	29	Lyman, 4-8			0.16	KOWWIN			82200	WSKOW	99	Assump.
1,4-Phenylenediamine dihydrochloride	624180	0.476	AOPWIN	16	Lyman, 4-8			-0.39	KOWWIN			199000	WSKOW	99	Assump.
1,2-Phenylenediamine	95545	0.476	AOPWIN	13	Lyman, 4-5			0.15	PHYS			40400	PHYS	99	Assump.
1,3-Phenylenediamine	108452	0.54	AOPWIN	4.8	Lyman, 4-5			-0.33	PHYS			238000	PHYS	99	Assump.
p-Phenylenediamine	106503	0.476	AOPWIN	13	Lyman, 4-5			-0.3	PHYS			37000	PHYS	99	Assump.
2-Phenylphenol	90437	0.0738	AOPWIN	119	CHMF			3.09	PHYS			700	PHYS	99	Assump.
Phenytoin	57410	0.0286	AOPWIN	650	Lyman, 4-5			2.47	PHYS			32	PHYS	99	Assump.
Phosgene	75445	0.0000027	AOPWIN		Fast Hyd	4.2	HYDRO	-0.71	PHYS			475100	PHYS	99	Assump.
Phosphine	7803512				Gas			-0.27	PHYS			204800	PHYS		
Phosphorus (yellow or white)	7723140			14	PCKOC			-0.27	PHYS			204800	PHYS		
Phthalic anhydride	85449	0.00202	AOPWIN		Fast Hyd	1.23	CHMF	1.6	PHYS			6200	PHYS	99	Assump.

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Picloram	1918021	0.00231	AOPWIN	21	CHMF			0.3	PHYS			430	PHYS	99	Assump.
Picric acid	88891	0.00038	AOPWIN		Ion			1.33	PHYS			12700	PHYS	99	Assump.
Piperonyl butoxide	51036	0.291	AOPWIN	1010	Lyman, 4-5			4.75	PHYS			14.3	PHYS	99	Assump.
Pirimiphos methyl	29232937	0.432	AOPWIN	1300	Lyman, 4-5			4.2	PHYS			8.6	PHYS	99	Assump.
p-Nitroaniline	100016	0.0363	AOPWIN	76	CHMF			1.39	PHYS			728	PHYS	99	Assump.
Polybrominated biphenyls (PBBs)	N575	0.00076	AOPWIN; hex	363	CHMF; hex			6.39	PHYS; hex			0.011	PHYS; hex	99	Assump.
Polychlorinated alkanes	N583													99	Assump.
Polychlorinated biphenyls (PCBs)	1336363	0.0027	AOPWIN; exp	48000	CHMF			7.1	PHYS			0.7	PHYS	99.9999	By law
Polycyclic aromatic compounds	N590	0.29	EPA, 99; B(a)p	2130000	CHMF; B(a)p			6.13	PHYS; B(a)p			0.00162	PHYS; B(a)p	99	Assump.
Potassium bromate	7758012			35	PCKOC			-7.18	PHYS			69000	PHYS		
Potassium dimethyldithiocarbamate	128030	0.314	AOPWIN	57	Lyman, 4-8			1.67	KOWWIN			29000	WSKOW	99	Assump.
Potassium N-methyldithiocarbamate	137417	0.261	AOPWIN	43	Lyman, 4-8			0.48	KOWWIN			440000	WSKOW	99	Assump.
Profenofos	41198087	0.121	AOPWIN	700	Lyman, 4-5			4.68	PHYS			28	PHYS	99	Assump.
Prometryn	7287196	0.103	AOPWIN	708	CHMF			3.51	PHYS			33	PHYS	99	Assump.
Pronamide	23950585	0.0358	AOPWIN	200	CHMF	7.4E-09	CHMF	3.43	PHYS			15	PHYS	99	Assump.
Propachlor	1918167	0.0565	AOPWIN	263	CHMF			2.18	PHYS			700	PHYS	99	Assump.
Propane sultone	1120714	0.00727	AOPWIN	5.8	Lyman, 4-5	0.082	CHMF	-0.28	PHYS			170700	PHYS	99	Assump.
Propanil	709988	0.0102	AOPWIN	275	Lyman, 4-5	0.0011	CHMF; photo	3.07	PHYS			152	PHYS	99	Assump.
Propargite	2312358	0.161	AOPWIN	6400	Lyman, 4-5			5	PHYS			0.5	PHYS	99	Assump.
Propargyl alcohol	107197	0.0281	AOPWIN	2	Lyman, 4-5			-0.38	PHYS			1000000	PHYS	99	Assump.

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Propetamphos	31218834	0.745	AOPWIN	330	Lyman, 4-5	1.69E-06	HYDRO	3.82	PHYS			110	PHYS	99	Assump.
Propiconazole	60207901	0.0735	AOPWIN	330	Lyman, 4-5			3.72	PHYS			110	PHYS	99	Assump.
beta-Propiolactone	57578	0.00166	AOPWIN	3.8	Lyman, 4-5			-0.8	PHYS			370000	PHYS	99	Assump.
Propionaldehyde	123386	0.0529	AOPWIN; exp	4	CHMF			0.59	PHYS			306000	PHYS	99	Assump.
Propoxur	114261	0.0855	AOPWIN	47	CHMF	0.00168	HYDRO	1.52	PHYS			1860	PHYS	99	Assump.
Propylene (Propene)	115071	0.071	AOPWIN; exp	240	Lyman, 4-5			1.77	PHYS			200	PHYS	99	Assump.
2,4-D, propylene glycol butylether ester	1320189	0.03	AOPWIN	5400	Lyman, 4-8	0.00331	HYDRO	4.34	KOWWIN			1.24	WSKOW	99	Assump.
Propylene oxide	75569	0.0014	AOPWIN; exp	2.9	Lyman, 4-5	0.002	CHMF	0.03	PHYS			590000	PHYS	99	Assump.
Propyleneimine	75558	0.0184	AOPWIN	2	Lyman, 4-5	0.008	CHMF	0.13	PHYS			1000000	PHYS	99	Assump.
Pyridine	110861	0.000999	AOPWIN	14	CHMF			0.65	PHYS			1000000	PHYS	99	Assump.
Quinoline	91225	0.0313	AOPWIN; exp	320	CHMF	0.0014	CHMF; photo	2.03	PHYS			6110	PHYS	99	Assump.
Quinone	106514	0.0122	AOPWIN	26	CHMF			0.2	PHYS			11100	PHYS	99	Assump.
Quintozene	82688	0.0000194	AOPWIN	26600	CHMF	0.000028	CHMF	4.64	PHYS			0.44	PHYS	99	Assump.
Quizalofop-ethyl	76578148	0.0768	AOPWIN	8500	Lyman, 4-5	0.0000431	HYDRO	4.28	PHYS			0.3	PHYS	99	Assump.
Resmethrin	10453868	0.783	AOPWIN	26000	Lyman, 4-5	0.0000614	HYDRO	7.11	PHYS			0.0379	PHYS	99	Assump.
Saccharin (manufacturing)	81072	0.0159	AOPWIN	46	CHMF			0.91	PHYS			4000	PHYS	99	Assump.
Safrole	94597	0.206	AOPWIN	310	Lyman, 4-5	0	CHMF	3.45	PHYS			121	PHYS	99	Assump.
Selenium and selenium compounds	7782492	0.176	AOPWIN	14	PCKOC			0.24	PHYS	22	Gerritse	2063	PHYS	99.8	EPA, 92
Sethoxydim	74051802	0.392	AOPWIN	740	Lyman, 4-5			4.38	PHYS			25	PHYS	99	Assump.
Silver and silver compounds	7440224			14	PCKOC			0.23	PHYS	540	Gerritse	70480	PHYS		

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Simazine	122349	0.0482	AOPWIN	120	CHMF			2.18	PHYS			6.2	PHYS	99	Assump.
Sodium azide	26628228			13	Lyman, 4-5			0.16	KOWWIN			36700	WSKOW	99	Assump.
Sodium dicamba	1982690	0.0131	AOPWIN	3.8	Lyman, 4-5			-0.9	KOWWIN			360000	HL	99	Assump.
Sodium dimethyldithiocarbamate	128041	0.185	AOPWIN	2	Lyman, 4-5			-2.41	PHYS			1000000	PHYS	99	Assump.
Sodium fluoroacetate	62748	0.0000734	AOPWIN	1.2	PCKOC			-3.78	PHYS			1110000	PHYS	99	Assump.
Sodium nitrite	7632000	0.000351	AOPWIN	24	PCKOC			-2.37	KOWWIN			1000000	WSKOW		
Sodium o-phenylphenoxide	132274	0.0506	AOPWIN	2	Lyman, 4-5			0.59	PHYS			1000000	PHYS	99	Assump.
Sodium pentachlorophenate	131522	0.00715	AOPWIN	4	Lyman, 4-5			2.05	PHYS			330000	PHYS	99	Assump.
2,4-D sodium salt	2702729	0.00972	AOPWIN	4	Lyman, 4-5			-1.19	PHYS			335000	PHYS	99	Assump.
Strychnine and salts	N746	0.6	AOPWIN; str		Ion; str			1.93	PHYS; str			160	PHYS; str	99	Assump.
Styrene	100425	0.157	AOPWIN; exp	920	CHMF			2.95	PHYS			310	PHYS	99	Assump.
Styrene oxide	96093	0.0137	AOPWIN	53	CHMF	0.00322	HYDRO	1.61	PHYS			3000	PHYS	99	Assump.
Sulfuric acid	7664939	0.000756	AOPWIN	6.1	PCKOC			-2.2	PHYS			1000000	PHYS		
Sulfuryl fluoride (Vikane)	2699798			110	Lyman, 4-5			0.41	PHYS			750	PHYS	99	Assump.
Sulprofos	35400432	0.29	AOPWIN	8300	Lyman, 4-5			5.48	PHYS			0.31	PHYS	99	Assump.
Tebuthiuron	34014181	0.00895	AOPWIN	617	CHMF			1.79	PHYS			2500	PHYS	99	Assump.
Temephos	3383968	0.366	AOPWIN	9000	Lyman, 4-5			5.96	PHYS			0.27	PHYS	99	Assump.
Terbacil	5902512	0.0202	AOPWIN	48	CHMF			1.89	PHYS			710	PHYS	99	Assump.
Tetrabromobisphenol A (TBBPA)	79947	0.00799	AOPWIN									0.001	WSKOW	99	Assump.
1,1,2,2-Tetrachloro-1-fluoroethane (HCFC-121)	354143	0.0000332	AOPWIN	790	Lyman, 4-8	0.00429	HYDRO	2.8	PHYS			209	WSKOW	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
1,1,1,2-Tetrachloro-2-fluoroethane (HCFC-121a)	354110	0.0000129	AOPWIN	790	Lyman, 4-8	0.0279	HYDRO	2.8	PHYS			209	WSKOW	99	Assump.
1,1,1,2-Tetrachloroethane	630206	0.0000486	AOPWIN; exp	93	CHMF	1.07E-07	HYDRO	2.93	PHYS			1100	PHYS	99	Assump.
1,1,2,2-Tetrachloroethane	79345	0.000675	AOPWIN; exp	79	CHMF	0.000529	HYDRO	2.39	PHYS			2960	PHYS	99	Assump.
Tetrachloroethylene (Perchloroethylene)	127184	0.000451	AOPWIN; exp	230	CHMF			3.4	PHYS			200	PHYS	99	Assump.
Tetrachlorvinphos	961115	0.065	AOPWIN	1200	CHMF	0.000351	HYDRO	3.53	PHYS			11	PHYS	99	Assump.
Tetracycline hydrochloride	64755	0.525	AOPWIN	4.7	Lyman, 4-8			-3.7	KOWWIN			249000	WSKOW	99	Assump.
Tetrafluoroethylene	116143							1.35	ACD			159	PHYS	99	Assump.
Tetramethrin	7696120	0.405	AOPWIN	3100	Lyman, 4-5	0.0000318	HYDRO	4.73	PHYS			1.83	PHYS	99	Assump.
Tetranitromethane	509148							8.49	ACD			900	PHYS	99	Assump.
Thallium and thallium compounds	7440280			14	PCKOC			0.23	PHYS			26480	PHYS		
Thiabendazole	148798	0.176	AOPWIN	1738	CHMF			2.47	PHYS			50	PHYS	99	Assump.
Thioacetamide	62555	0.0572	AOPWIN	5.9	Lyman, 4-5	0.000086	CHMF	-0.26	PHYS			163000	PHYS	99	Assump.
Thiobencarb	28249776	0.0685	AOPWIN	1840	CHMF			3.4	PHYS			28	PHYS	99	Assump.
4,4'-Thiodianiline	139651	0.357	AOPWIN	190	Lyman, 4-5			2.18	PHYS			310	PHYS	99	Assump.
Thiodicarb	59669260	0.0359	AOPWIN	620	Lyman, 4-5	2.54E-12	HYDRO	1.7	PHYS			35	PHYS	99	Assump.
Thiophanate ethyl	23564069	0.228	AOPWIN	322	Lyman, 4-8	3.55E-09	HYDRO	2.08	PHYS			5.47	WSKOW	99	Assump.
Thiophanate-methyl	23564058	0.207	AOPWIN	154	Lyman, 4-5	3.55E-09	HYDRO	1.4	PHYS			438.9	PHYS	99	Assump.
Thiosemicarbazide	79196	0.227	AOPWIN	28	Lyman, 4-5			-1.67	PHYS			10020	PHYS	99	Assump.
Thiourea	62566	0.113	AOPWIN	6.4	Lyman, 4-5	5.3E-07	CHMF	-1.08	PHYS			142000	PHYS	99	Assump.
Thiram	137268	0.98	AOPWIN	670	CHMF	0.006	CHMF	1.73	PHYS			30	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Thorium dioxide	1314201			24	PCKOC			2.23	KOWWIN			0	Merck		
Titanium tetrachloride	7550450	276	Assump.; TiCl4	49	PCKOC	276	Assump.; TiCl4	1.47	KOWWIN			2740	WSKOW		
Toluene	108883	0.0161	AOPWIN; exp	110	CHMF			2.73	PHYS			526	PHYS	99	Assump.
Toluenediisocyanate	26471625	0.0191	AOPWIN; exp		Fast Hyd	4.2	HYDRO	3.74	PHYS			37.57	PHYS	99	Assump.
Toluene-2,4-diisocyanate	584849	0.0191	AOPWIN; exp		Fast Hyd	4.2	HYDRO	3.74	PHYS			37.57	PHYS	99	Assump.
Toluene-2,6-diisocyanate	91087	0.019	AOPWIN; exp		Fast Hyd	4.2	HYDRO	3.74	PHYS			37.57	PHYS	99	Assump.
o-Toluidine hydrochloride	636215	0.357	AOPWIN	31	Lyman, 4-5			1.62	PHYS			8292	PHYS	99	Assump.
o-Toluidine	95534	0.357	AOPWIN	100	CHMF			1.32	PHYS			16600	PHYS	99	Assump.
Toxaphene	8001352	0.00674	AOPWIN	210000	CHMF	0.000008	CHMF	5.9	PHYS			0.55	PHYS	99	Assump.
trans-1,3-Dichloropropene	10061026	0.0269	AOPWIN; ave	67	Lyman, 4-5			2.03	PHYS			1994	PHYS	99	Assump.
trans-1,4-Dichloro-2-butene	110576	0.0958	AOPWIN; ave	110	Lyman, 4-5	0.009	CHMF	2.6	PHYS			850	PHYS	99	Assump.
Triadimefon	43121433	0.0455	AOPWIN	417	Lyman, 4-5			2.77	PHYS			71.5	PHYS	99	Assump.
Triallate	2303175	0.09	AOPWIN	2239	CHMF			4.6	PHYS			4	PHYS	99	Assump.
Triaziquone	68768	0.0824	AOPWIN	3.7	Lyman, 4-5			-0.13	PHYS			394100	PHYS	99	Assump.
Tribenuron methyl	101200480	0.008	AOPWIN	510	Lyman, 4-5	0.0000144	HYDRO	-0.44	PHYS			50	PHYS	99	Assump.
Tributyltin fluoride	1983104	0.115	AOPWIN	15000	PCKOC			4.39	PHYS			1.945	PHYS		
Tributyltin methacrylate	2155706	0.164	AOPWIN	16400	PCKOC			4.14	KOWWIN			1.27	WSKOW		
S,S,S-tributyltrithiophosphate	78488	0.213	AOPWIN	2800	Lyman, 4-5	0.0000506	HYDRO	5.7	PHYS			2.3	PHYS	99	Assump.
Trichlorfon	52686	0.0167	AOPWIN	79	CHMF	0.01	CHMF	0.51	PHYS			120000	PHYS	99	Assump.
Trichloroacetyl chloride	76028				Fast Hyd	4.2	HYDRO	0.88	PHYS			9493	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
1,2,4-Trichlorobenzene	120821	0.00149	AOPWIN; exp	2200	CHMF	0.000023	CHMF	4.02	PHYS			49	PHYS	99	Assump.
1,1,1-Trichloroethane	71556	0.0000252	AOPWIN	90	CHMF	2.68E-12	HYDRO	2.49	PHYS			1490	PHYS	99	Assump.
1,1,2-Trichloroethane	79005	0.000529	AOPWIN; exp	79	CHMF	6.76E-06	HYDRO	1.89	PHYS			4420	PHYS	99	Assump.
Trichloroethylene	79016	0.00637	AOPWIN; exp	87	CHMF			2.42	PHYS			1100	PHYS	99	Assump.
2,4,5-Trichlorophenol	95954	0.00577	AOPWIN	1100	CHMF			3.72	PHYS			1200	PHYS	99	Assump.
2,4,6-Trichlorophenol	88062	0.00164	AOPWIN	604	CHMF	2.3E-07	CHMF	3.69	PHYS			800	PHYS	99	Assump.
1,2,3-Trichloropropane	96184	0.00095	AOPWIN	72	CHMF	0.0000018	CHMF	2.27	PHYS			1750	PHYS	99	Assump.
Triclopyr triethylammonium salt	57213691	0.08	AOPWIN	160	Lyman, 4-8	0.0615	HYDRO	1.5	KOWWIN			299	WSKOW	99	Assump.
Triethylamine	121448	0.25	AOPWIN	9.2	Lyman, 4-5			1.45	PHYS			73670	PHYS	99	Assump.
Trifluralin	1582098	0.217	EPA, 99	7080	CHMF	0	PRNA	5.34	PHYS			0.184	PHYS	99	Assump.
Triforine	26644462	0.178	AOPWIN	670	Lyman, 4-5			2.2	PHYS			30	PHYS	99	Assump.
1,2,4-Trimethylbenzene	95636	0.0878	AOPWIN; exp	470	Lyman, 4-5			3.63	PHYS			57	PHYS	99	Assump.
2,3,5-trimethylphenyl methylcarbamate	2655154	0.0565	AOPWIN	470	Lyman, 4-5	0.000775	HYDRO	2.56	KOWWIN			58	HL	99	Assump.
Triphenyltin chloride	639587	0.0158	AOPWIN	4380	Lyman, 4-5			4.19	PHYS			0.9941	PHYS		
Triphenyltin hydroxide	76879	0.0161	AOPWIN	7200	Lyman, 4-5			3.53	PHYS			0.4	PHYS		
Tris(2,3-dibromopropyl)-phosphate	126727	0.0748	AOPWIN	1400	CHMF	0.000018	CHMF	4.29	PHYS			8	PHYS	99	Assump.
Trypan blue	72571	0.061	AOPWIN	20	Lyman, 4-8			-0.12	PHYS			0.0835	WSKOW	99	Assump.
Urethane (Ethyl carbamate)	51796	0.0198	AOPWIN	3.3	Lyman, 4-5	2.6E-07	CHMF	-0.15	PHYS			480000	PHYS	99	Assump.
Vanadium and vanadium compounds	7440622			14	PCKOC			0.23	KOWWIN	68	Gerritse; el	0	Merck	90	EPA, 92
Vinclozolin	50471448	0.089	AOPWIN	2600	Lyman, 4-5			3.1	PHYS			2.6	PHYS	99	Assump.

Table B-6. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013															
Chemical Name	CAS Number	Air Decay	Air Decay Ref.	Koc	Koc Ref.	H2O Decay	H2O Decay Ref.	LOG Kow	LOG Kow Ref.	Kd	Kd Ref.	Water Solubility	Water Solubility Ref.	Inciner. DRE	Inciner. DRE Ref.
Vinyl acetate	108054	0.07	AOPWIN; exp	19	CHMF	0.004	CHMF	0.73	PHYS			20000	PHYS	99	Assump.
Vinyl bromide	593602	0.0184	AOPWIN; exp	38	Lyman, 4-5			1.57	PHYS			5679	PHYS	99	Assump.
Vinyl chloride	75014	0.0188	AOPWIN; exp	30	CHMF			1.62	PHYS			8800	PHYS	99	Assump.
Vinyl Fluoride	75025							1.62	ACD Labs			5480	EPI	99	Assump.
Vinylidene chloride (1,1-dichloroethylene)	75354	0.0294	AOPWIN; exp	63	Lyman, 4-5			2.13	PHYS			2250	PHYS	99	Assump.
Warfarin and salts	N874	0.14	AOPWIN; wrf	920	CHMF; wrf	0.0000049	CHMF; wrf	2.6	PHYS; wrf			17	PHYS; wrf	99	Assump.
Xylene (mixed isomers)	1330207	0.037	AOPWIN	336	Lyman, 4-5			3.16	PHYS			106	PHYS	99	Assump.
m-Xylene	108383	0.0637	AOPWIN; exp	178	CHMF			3.2	PHYS			161	PHYS	99	Assump.
o-Xylene	95476	0.037	AOPWIN; exp	93	CHMF			3.12	PHYS			178	PHYS	99	Assump.
p-Xylene	106423	0.0386	AOPWIN; exp	260	CHMF			3.15	PHYS			162	PHYS	99	Assump.
2,6-Xylidine	87627	0.437	AOPWIN		Ion			1.84	PHYS			8240	PHYS	99	Assump.
Zinc and zinc compounds	7440666			14	PCKOC			-0.47	PHYS	31	Gerritse	343700	PHYS	99.9	EPA, 92
Zineb	12122677	0.398	AOPWIN	1200	CHMF			1.3	PHYS			10	PHYS	99	Assump.

* When chlorine dioxide dissolves in water, it rapidly reacts to form chlorate, chlorite, and chloride ions. The IRIS oral toxicity data for chlorine dioxide is largely based on the toxicity of sodium chlorite. The water decay term for chlorine dioxide used in the RSEI model reflects rapid hydrolysis to sodium chlorite, which is toxic and does not decay rapidly in water.

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Abamectin	71751412	98.23	RREL	44.67	EFDB	0	EFDB	55.33	EFDB	3600	Lyman, 5-2	2.26E-10	HL			870.29	Merck; calc.
Acephate	30560191	45.42	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	3.2	BCFWIN	5.01E-13	PHYS			183.17	PHYS
Acetaldehyde	75070	92.13	EPI	0.36	EPI	0.61	EPI	99.03	EPI	3.2	BCFWIN	0.0000667	PHYS			44.05	PHYS
Acetamide	60355	92.06	RREL	0.36	EFDB	0	EFDB	99.63	EFDB	3.2	BCFWIN	1.12E-08	PHYS			59.07	PHYS
2,4-D ((2,4-dichlorophenoxy)acetic acid)	94757	93.8	RREL	1.71	EFDB	0	EFDB	98.29	EFDB	10	CHMF	3.54E-08	PHYS	0.07	NPDWS	221.04	PHYS
Acetonitrile	75058	75.27	RREL	0.82	EFDB	0.82	EFDB	98.35	EFDB	3.2	BCFWIN	0.0000345	PHYS			41.05	PHYS
Acetophenone	98862	92.2	RREL	0.44	EFDB	0.11	EFDB	99.44	EFDB	9.3	Lyman, 5-2	0.0000104	PHYS			120.15	PHYS
2-Acetylaminofluorene	53963	57.53	RREL	8.26	EFDB	0	EFDB	91.76	EFDB	140	Lyman, 5-2	1.92E-10	PHYS			223.28	PHYS
Acifluorfen, sodium salt	62476599	74.69	SUM	16.43	EFDB	0.013	EFDB	83.56	EFDB	3.2	BCFWIN	2.97E-07	HL			384.65	PHYS
Acrolein	107028	92.18	EPI	0.36	EPI	1.01	EPI	98.62	EPI	350	CHMF	0.000122	PHYS			56.06	PHYS
Acrylamide	79061	92.06	EPI	0.36	EPI	0	EPI	99.64	EPI	1	CHMF	1E-09	PHYS		NPDWS; TTreq.	71.08	PHYS
Acrylic acid	79107	92.07	RREL	0.37	EFDB	0.011	EFDB	99.62	EFDB	3.2	BCFWIN	3.7E-07	PHYS			72.06	PHYS
Acrylonitrile	107131	92.19	RREL	0.36	EFDB	1.12	EFDB	98.51	EFDB	48	CHMF	0.000138	PHYS			53.06	PHYS
Alachlor	15972608	88.75	RREL	8.17	EFDB	0	EFDB	91.83	EFDB	280	Lyman, 5-2	2.23E-08	HENRY WIN	0.002	NPDWS	269.77	PHYS
Aldicarb	116063	45.58	RREL	2.46	EFDB	0	EFDB	97.52	EFDB	42	CHMF	1.44E-09	PHYS	0.003	NPDWS	190.27	PHYS
Aldrin	309002	98.96	RREL	62.16	EFDB	0.03	EFDB	37.81	EFDB	3715	EPA, 99	0.000044	PHYS			364.92	PHYS
Allyl alcohol	107186	92.07	RREL	0.37	EFDB	0.054	EFDB	99.59	EFDB	3.2	BCFWIN	4.99E-06	PHYS			58.08	PHYS
Allyl chloride	107051	84.36	RREL	0.83	EFDB	81.86	EFDB	17.31	EFDB	17	Lyman, 5-2	0.011	PHYS			76.53	PHYS
Allylamine	107119	75.18	RREL	0.82	EFDB	0.43	EFDB	98.74	EFDB	3.2	BCFWIN	0.0000182	PHYS			57.1	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013

		POTW Partition Rates														
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Aluminum (fume or dust)	7429905	66.39	RREL	100	Assump.	0	Assump.	0	Assump.	231	EPA, 97	0.0245	HENRY WIN			26.98	Merck
Aluminum oxide (fibrous forms)	1344281	1.85	EPI	95.14	EPI	0	EPI	4.86	EPI	3.2	BCFWIN					101.96	AOPWIN
Aluminum phosphide	20859738	1.85	EPI	95.14	EPI	0	EPI	4.86	EPI	3.2	BCFWIN					57.96	PHYS
Ametryn	834128	54.71	RREL	6.96	EFDB	0	EFDB	93.04	EFDB	110	Lyman, 5-2	2.43E-09	PHYS			227.33	PHYS
1-Amino-2,4-dibromoanthraquinone	81492									12000	Lyman, 5-2	1.78E-13	ChemSpider			381.02	Reaxys
1-Amino-2-methyl-anthraquinone	82280	86.22	RREL	24.3	EFDB	0	EFDB	75.7	EFDB	730	Lyman, 5-2	1.24E-12	PHYS			237.26	PHYS
2-Aminoanthraquinone	117793	48.36	RREL	3.91	EFDB	0	EFDB	96.09	EFDB	190	Lyman, 5-2	9.19E-11	PHYS			223.23	PHYS
4-Aminoazobenzene	60093	65.22	RREL	11.73	EFDB	0	EFDB	88.27	EFDB	230	Lyman, 5-2	8.7E-11	PHYS			197.24	PHYS
4-Aminodiphenyl	92671	52.74	RREL	6.05	EFDB	0	EFDB	93.95	EFDB	88	Lyman, 5-2	1.46E-07	PHYS			169.23	PHYS
Amitraz	33089611	99.3	RREL	50.05	EFDB	0	EFDB	49.95	EFDB	8900	Lyman, 5-2	9.87E-06	PHYS			293.42	PHYS
Amitrole	61825	45.42	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	3.2	BCFWIN	2.21E-13	PHYS			84.08	PHYS
Ammonia	7664417	59.9	RREL	0	Assump.	0	Assump.	100	Assump.	3.2	BCFWIN	0.0000161	PHYS			17.03	PHYS
Ammonium Nitrate	6484522	1.85	EPI	94.59	EPI	0	EPI	4.86	EPI	3.2	BCFWIN	1.23E-14	HENRY WIN			80.04	AOPWIN
Ammonium sulfate	7783202	1.86	EPI	95.16	EPI	0	EPI	4.84	EPI	3.2	BCFWIN	5.87E-22	HENRY WIN			132.14	Merck
Anilazine	101053	80.63	RREL	20	EFDB	0	EFDB	80	EFDB	520	Lyman, 5-2	2.81E-10	PHYS			275.53	PHYS
Aniline	62533	92.09	RREL	0.38	EFDB	0.022	EFDB	99.6	EFDB	9.3	CHMF	2.02E-06	PHYS			93.13	PHYS
p-Anisidine	104949	92.09	RREL	0.38	EFDB	0	EFDB	99.61	EFDB	3.1	CHMF	6.6E-08	PHYS			123.16	PHYS
o-Anisidine hydrochloride	134292	45.63	RREL	2.48	EFDB	0.13	EFDB	97.39	EFDB	4.6	Lyman, 5-2	1.04E-14	HENRY WIN			159.62	AOPWIN
o-Anisidine	90040	75.19	RREL	0.88	EFDB	0	EFDB	99.12	EFDB	4.6	CHMF	1.77E-06	PHYS			123.16	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Anthracene	120127	94.15	RREL	33.45	EFDB	2.19	EFDB	64.37	EFDB	1900	CHMF	0.0000556	PHYS			178.24	PHYS
Antimony and antimony compounds	7440360	31.51	RREL	100	Assump.	0	Assump.	0	Assump.	1	EPA, 97	0.0245	PHYS	0.006	NPDWS	124.77	PHYS
Arsenic and arsenic compounds	7440382	48.57	RREL	100	Assump.	0	Assump.	0	Assump.	44	EPA, 97	0.773	PHYS	0.05	NPDWS	77.95	PHYS
Asbestos (friable)	1332214													7	NPDWS; fpl	554.22	Merck; est.
Atrazine	1912249	25.68	RREL	11.21	EFDB	0	EFDB	88.79	EFDB	8.8	CHMF	2.36E-09	PHYS	0.003	NPDWS	215.69	PHYS
Barium and barium compounds	7440393	69.02	RREL	100	Assump.	0	Assump.	0	Assump.	3.2	BCFWIN			2	NPDWS	139.36	PHYS
Bendiocarb	22781233	76.54	RREL	0.94	EFDB	0.026	EFDB	99.05	EFDB	12	Lyman, 5-2	3.9E-08	PHYS			223.23	PHYS
Benfluralin	1861401	97.2	RREL	57.94	EFDB	0.32	EFDB	41.74	EFDB	6200	Lyman, 5-2	0.000291	PHYS			335.29	PHYS
Benomyl	17804352	51.31	RREL	2.71	EFDB	0	EFDB	97.29	EFDB	24	Lyman, 5-2	4.93E-12	PHYS			290.32	PHYS
Benzal chloride	98873	99.99	RREL	0.1	EFDB	0.04	EFDB	99.86	EFDB		Fast Hyd	0.000398	PHYS			161.03	PHYS
Benzamide	55210	92.07	RREL	0.37	EFDB	0	EFDB	99.63	EFDB	2.9	Lyman, 5-3	2.45E-10	PHYS			121.14	PHYS
Benzene	71432	94.09	RREL	0.62	EFDB	18.34	EFDB	81.04	EFDB	5	CHMF	0.00555	PHYS	0.005	NPDWS	78.12	PHYS
Benzidine	92875	75.24	RREL	0.89	EFDB	0	EFDB	99.11	EFDB	93	CHMF	3.88E-11	PHYS			184.24	PHYS
Benzo(g,h,i)perylene**	191242									11000	BCFWIN						
Benzotrichloride	98077	100	RREL	0.03	EFDB	0	EFDB	99.97	EFDB		Fast Hyd	0.00026	PHYS			195.48	PHYS
Benzoyl chloride	98884	100	RREL	0.01	EFDB	0.01	EFDB	99.98	EFDB		Fast Hyd	0.000123	PHYS			140.57	PHYS
Benzoyl peroxide	94360	96.7	RREL	5.18	EFDB	0.021	EFDB	94.8	EFDB		Fast Hyd	3.54E-06	PHYS			242.23	PHYS
Benzyl chloride	100447	78.03	RREL	1.38	EFDB	6.43	EFDB	92.17	EFDB	33	CHMF	0.000412	PHYS			126.59	PHYS
Beryllium and beryllium compounds	7440417	37.44	RREL	100	Assump.	0	Assump.	0	Assump.	19	EPA, 97	0.0154	PHYS	0.004	NPDWS	9.01	CRC

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Bifenthrin	82657043	99.93	RREL	38.26	EFDB	0	EFDB	61.74	EFDB	21000	Lyman, 5-2	0.000001	PHYS			422.88	PHYS
Biphenyl	92524	98.86	RREL	10.67	EFDB	0.62	EFDB	88.71	EFDB	377	CHMF	0.000308	PHYS			154.21	PHYS
Bis(2-chloro-1-methethyl)ether	108601	50.47	RREL	3.86	EFDB	6.2	EFDB	89.93	EFDB	45	CHMF	0.0000742	PHYS			171.07	PHYS
Bis(2-chloroethoxy)methane	111911	22.57	RREL	6.69	EFDB	2.26	EFDB	91.05	EFDB	5.7	Lyman, 5-2	1.7E-07	PHYS			173.04	PHYS
Bis(2-chloroethyl)ether	111444	22.77	RREL	6.59	EFDB	3.38	EFDB	90.03	EFDB	11	CHMF	0.000017	PHYS			143.01	PHYS
2,2-Bis(Bromomethyl)-1,3-propanediol	329600									1.6	Lyman, 5-3	4.06E-09	ACD			261.94	Reaxys
Bis(chloromethyl)ether	542881	100	RREL	0	EFDB	0	EFDB	100	EFDB		Fast Hyd	0.00436	PHYS			114.96	PHYS
Bis(tributyltin) oxide	56359	91.16	EPI	98.74	EPI	0.43	EPI	0.83	EPI	700	Lyman, 5-2	94.5	HENRY WIN			596.08	PHYS
Boron trichloride	10294345	1.9	EPI	95.26	EPI	0	EPI	4.74	EPI	1.6	BCFWIN	0.0183	PHYS			117.17	PHYS
Boron trifluoride	7637072	1.85	EPI	94.59	EPI	0	EPI	4.86	EPI	3.2	BCFWIN					67.81	PHYS
Bromacil	314409	46.87	RREL	3.14	EFDB	0	EFDB	96.84	EFDB	24	Lyman, 5-2	1.05E-10	PHYS			261.12	PHYS
Bromacil lithium salt	53404196	46.26	RREL	2.83	EFDB	0	EFDB	97.17	EFDB	16	Lyman, 5-2	1.51E-16	HL				
Bromine	7726956	1.89	EPI	95.24	EPI	0	EPI	4.76	EPI	1.2	BCFWIN	0.0245	PHYS			159.82	PHYS
1-Bromo-1-(bromomethyl)-1,3-propanedicarbonitrile	35691657	45.91	RREL	2.64	EFDB	0	EFDB	97.34	EFDB	10	Lyman, 5-2	3.94E-10	HENRY WIN			265.94	PHYS
Bromochlorodifluoro-methane	353593	97.39	RREL	0.48	EFDB	98.18	EFDB	1.32	EFDB	16	Lyman, 5-2	0.094	PHYS			165.36	PHYS
Bromoform (Tribromomethane)	75252	54.51	RREL	3.14	EFDB	21.06	EFDB	75.8	EFDB	3.2	CHMF	0.000535	PHYS	0.1	NPDWS	252.73	PHYS
Bromomethane (Methyl bromide)	74839	77.45	RREL	0.81	EFDB	73.7	EFDB	25.49	EFDB	4.7	CHMF	0.00624	PHYS			94.94	PHYS
Bromotrifluoromethane (Halon 1301)	75638	99.46	RREL	0.42	EFDB	98.83	EFDB	0.74	EFDB	15	Lyman, 5-2	0.499	PHYS			148.91	PHYS
Bromoxynil	1689845	86.74	RREL	6.69	EFDB	0	EFDB	93.31	EFDB	79	Lyman, 5-2	1.32E-10	PHYS			276.92	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Bromoxynil octanoate	1689992	99.91	RREL	37.78	EFDB	0	EFDB	62.21	EFDB	25000	Lyman, 5-2	0.0000319	PHYS			403.12	PHYS
Brucine	357573	45.53	RREL	2.44	EFDB	0	EFDB	97.56	EFDB	3.3	Lyman, 5-2	2.09E-16	PHYS			394.47	PHYS
1,3-Butadiene	106990	97.32	RREL	0.5	EFDB	85.67	EFDB	13.83	EFDB	19	CHMF	0.0736	PHYS			54.09	PHYS
2,4-D butoxyethyl ester	1929733	99.15	RREL	12.17	EFDB	0	EFDB	87.84	EFDB	770	Lyman, 5-2	1.59E-07	PHYS			321.2	PHYS
Butyl acrylate	141322	93.02	RREL	0.85	EFDB	2.62	EFDB	96.52	EFDB	37	Lyman, 5-2	0.000657	PHYS			128.17	PHYS
n-Butyl alcohol	71363	92.09	RREL	0.38	EFDB	0.087	EFDB	99.53	EFDB	2.7	CHMF	8.81E-06	PHYS			74.12	PHYS
sec-Butyl alcohol	78922	92.08	RREL	0.37	EFDB	0.098	EFDB	99.54	EFDB	3.2	BCFWIN	9.06E-06	PHYS			74.12	PHYS
tert-Butyl alcohol	75650	45.74	RREL	2.36	EFDB	1.05	EFDB	96.57	EFDB	3.2	BCFWIN	9.05E-06	PHYS			74.12	PHYS
2,4-D butyl ester	94804	99.61	RREL	15.35	EFDB	0	EFDB	84.65	EFDB	1300	Lyman, 5-2	4.88E-07	PHYS			277.15	PHYS
1,2-Butylene oxide	106887	75.95	RREL	0.82	EFDB	3.54	EFDB	95.64	EFDB	3.2	BCFWIN	0.00018	PHYS			72.11	PHYS
Butyraldehyde	123728	92.2	RREL	0.38	EFDB	0.97	EFDB	98.66	EFDB	3.2	BCFWIN	0.000115	PHYS			72.11	PHYS
C.I. Acid Green 3	4680788	45.49	RREL	2.42	EFDB	0	EFDB	97.58	EFDB	3.2	BCFWIN	4.83E-29	HL			690.82	PHYS
C.I. Acid Red 114	6459945	99.93	RREL	0.25	EFDB	97.99	EFDB	1.76	EFDB	550000	Lyman, 5-2; C.I.	5.08E-31	PHYS			830.83	PHYS
C.I. Basic Green 4	569642	45.49	RREL	2.42	EFDB	0	EFDB	97.58	EFDB	1.6	Lyman, 5-3	1.93E-14	PHYS			364.92	PHYS
C.I. Basic Red 1	989388	99.54	RREL	51.71	EFDB	0	EFDB	48.29	EFDB	18000	Lyman, 5-2	2.56E-18	HENRY WIN			479.02	AOPWIN
C.I. Direct Black 38	1937377	97.89	RREL	43.38	EFDB	0	EFDB	56.62	EFDB	3100	Lyman, 5-2	8.23E-40	HENRY WIN			779.77	PHYS
C.I. Direct Blue 218	28407376									3.2	BCFWIN					876.82	AOPWIN
C.I. Direct Blue 6	2602462	54.18	RREL	6.72	EFDB	0	EFDB	93.28	EFDB	56	Lyman, 5-2	9.11E-44	PHYS			932.76	PHYS
C.I. Direct Brown 95	16071866	99.68	RREL	52.87	EFDB	0	EFDB	47.13	EFDB	3.2	BCFWIN	1E-24	HL			760.11	AOPWIN

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		POTW Partition Rates															
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C.I. Disperse Yellow 3	2832408	83.69	RREL	22.2	EFDB	0	EFDB	77.8	EFDB	620	Lyman, 5-2	1.5E-11	PHYS			269.31	PHYS
C.I. Food Red 15	81889	46.43	RREL	2.91	EFDB	0	EFDB	97.07	EFDB	18	Lyman, 5-2	2.4E-24	HL			480.03	PHYS
C.I. Food Red 5	3761533	48.85	RREL	4.16	EFDB	0	EFDB	95.84	EFDB	47	Lyman, 5-2	3.97E-23	HL			482.43	AOPWIN
C.I. Solvent Orange 7	3118976	99.66	RREL	52.69	EFDB	0	EFDB	47.31	EFDB	61000	Lyman, 5-2	2.74E-11	PHYS			276.34	PHYS
C.I. Solvent Yellow 14	842079	99.31	RREL	50.11	EFDB	0	EFDB	49.89	EFDB	9100	Lyman, 5-2	2.62E-11	PHYS			248.29	PHYS
C.I. Solvent Yellow 3	97563	91.29	RREL	29.73	EFDB	0	EFDB	70.28	EFDB	1100	Lyman, 5-2	3.18E-08	PHYS			225.3	PHYS
Auramine	492808	50.47	RREL	4.95	EFDB	0	EFDB	95.05	EFDB	110	Lyman, 5-2	3.64E-09	PHYS			267.38	PHYS
C.I. Vat Yellow 4	128665	98.89	RREL	61.97	EFDB	0	EFDB	38.03	EFDB	35000	Lyman, 5-2	8.31E-12	PHYS			332.36	PHYS
Cadmium and cadmium compounds	7440439	68.15	RREL	100	Assump.	0	Assump.	0	Assump.	64	EPA, 97	0.0308	PHYS	0.005	NPDWS	112.4	PHYS
Calcium cyanamide	156627	1.9	EPI	92.63	EPI	3.16	EPI	4.74	EPI	3.2	BCFWIN					82.12	PHYS
Captan	133062	76.84	RREL	1.52	EFDB	0.17	EFDB	98.31	EFDB	10	CHMF	7E-09	PHYS			300.59	PHYS
Carbaryl	63252	93.29	RREL	0.85	EFDB	5.79	EFDB	93.36	EFDB	300	CHMF	3.27E-09	PHYS			201.23	PHYS
Carbofuran	1563662	92.71	RREL	0.82	EFDB	0	EFDB	99.17	EFDB	34	Lyman, 5-2	3.09E-09	PHYS	0.04	NPDWS	221.26	PHYS
Carbon disulfide	75150	87.17	RREL	0.91	EFDB	84.73	EFDB	14.37	EFDB	18	Lyman, 5-2	0.0144	PHYS			76.14	PHYS
Carbon tetrachloride	56235	92.57	RREL	2.12	EFDB	87.58	EFDB	10.31	EFDB	23	CHMF	0.0276	PHYS	0.005	NPDWS	153.82	PHYS
Carbonyl sulfide	463581	96.18	RREL	0.3	EFDB	82.86	EFDB	16.84	EFDB	11	CHMF	0.61	PHYS			60.08	PHYS
Carboxin	5234684	76.16	RREL	1.26	EFDB	0	EFDB	98.74	EFDB	25	Lyman, 5-2	2.8E-10	PHYS			235.31	PHYS
Catechol	120809	92.08	RREL	0.38	EFDB	0	EFDB	99.62	EFDB	3.2	BCFWIN	3.14E-09	PHYS			110.11	PHYS
CFC 114 (1,2-dichloro,1,1,2,2-tetrafluoroethane)	76142	99.91	RREL	1.75	EFDB	97.51	EFDB	0.74	EFDB	82	Lyman, 5-2	2.8	PHYS			170.92	PHYS

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CFC 115 (chloropenta-fluoroethane)	76153	99.9	RREL	0.93	EFDB	98.41	EFDB	0.66	EFDB	44	Lyman, 5-2	5.58	PHYS			154.47	PHYS
CFC-11 (trichlorofluoromethane)	75694	97.48	RREL	1.11	EFDB	97.47	EFDB	1.43	EFDB	49	CHMF	0.097	PHYS			137.37	PHYS
CFC-12 (dichlorodi-fluoromethane)	75718	99.27	RREL	0.59	EFDB	98.58	EFDB	0.82	EFDB	26	CHMF	0.343	PHYS			120.91	PHYS
Chinomethionat (6-methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one)	2439012	77.37	RREL	17.95	EFDB	0	EFDB	82.05	EFDB	440	Lyman, 5-2	6.17E-08	PHYS			234.3	PHYS
Chloramben	133904	46.32	RREL	2.87	EFDB	0	EFDB	97.13	EFDB	16	Lyman, 5-2	3.87E-11	PHYS			206.03	PHYS
Chlordane	57749	98.72	RREL	61.52	EFDB	0.01	EFDB	38.48	EFDB	11050	EPA, 99	0.0000486	PHYS	0.002	NPDWS	409.78	PHYS
Chlorendic acid	115286	33.15	RREL	17.83	EFDB	0	EFDB	82.17	EFDB	140	Lyman, 5-2	1.12E-13	PHYS			388.85	PHYS
Chlorimuron ethyl	90982324	77.46	RREL	1.81	EFDB	0	EFDB	98.19	EFDB	47	Lyman, 5-2	1.82E-15	PHYS			414.83	PHYS
Chlorine	7782505	1.87	EPI	95.19	EPI	0	EPI	4.81	EPI	3.2	BCFWIN	0.0117	PHYS			70.91	PHYS
Chlorine dioxide	10049044	1.85	EPI	94.59	EPI	0	EPI	4.86	EPI	3.2	BCFWIN	0.0245	HENRY WIN			67.45	AOPWIN
2-Chloro-1,1,1,2-tetrafluoroethane	2837890	99.53	RREL	0.42	EFDB	98.85	EFDB	0.72	EFDB	15	Lyman, 5-2	0.54	HENRY WIN			136.48	PHYS
2-Chloro-1,1,1-trifluoroethane	75887	99.07	RREL	0.49	EFDB	98.66	EFDB	0.86	EFDB	19	Lyman, 5-2	0.271	PHYS			118.49	PHYS
3-Chloro-1,1,1-trifluoropropane (HCFC-253fb)	460355	99.3	RREL	0.97	EFDB	98.19	EFDB	0.85	EFDB	45	Lyman, 5-2	0.36	HENRY WIN			132.51	PHYS
1-Chloro-1,1,2,2-tetrafluoroethane	354256	99.53	RREL	0.42	EFDB	98.85	EFDB	0.72	EFDB	15	Lyman, 5-2	0.54	HENRY WIN			136.48	PHYS
1-Chloro-1,1-difluoroethane	75683	96.62	RREL	0.58	EFDB	97.85	EFDB	1.56	EFDB	21	Lyman, 5-2	0.0588	PHYS			100.5	PHYS
3-Chloro-2-methyl-1-propene	563473	95.78	RREL	1.06	EFDB	93.07	EFDB	5.88	EFDB	45	Lyman, 5-2	0.0087	PHYS			90.55	PHYS
Chloroacetic acid	79118	92.06	RREL	0.37	EFDB	0	EFDB	99.64	EFDB	3.2	BCFWIN	9.42E-09	PHYS			94.5	PHYS
2-Chloroacetophenone	532274	46.45	RREL	2.88	EFDB	0.26	EFDB	96.86	EFDB	17	Lyman, 5-2	3.46E-06	PHYS			154.6	PHYS

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		POTW Partition Rates														
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1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride	4080313	45.42	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	3.2	BCFWIN	1.76E-08	PHYS			251.16	PHYS
p-Chloroaniline	106478	46.22	RREL	2.79	EFDB	0.13	EFDB	97.1	EFDB	14	CHMF	1.16E-06	PHYS			127.57	PHYS
Chlorobenzene	108907	85.32	RREL	2.47	EFDB	28.63	EFDB	68.89	EFDB	79	CHMF	0.00311	PHYS	0.1	NPDWS	112.56	PHYS
Chlorobenzilate	510156	96.95	RREL	40.37	EFDB	0	EFDB	59.63	EFDB	2400	Lyman, 5-2	7.24E-08	PHYS			325.19	PHYS
2,4-D chlorocrotyl ester	2971382	99.65	RREL	15.76	EFDB	0	EFDB	84.24	EFDB	1300	Lyman, 5-2	2.14E-06	HENRY WIN			309.58	AOPWIN
Chlorodifluoromethane (HCFC-22)	75456	60.96	RREL	1.44	EFDB	80.87	EFDB	17.68	EFDB	3.9	Lyman, 5-2	0.0406	PHYS			86.47	PHYS
Chloroethane (Ethyl chloride)	75003	84.39	RREL	0.65	EFDB	82.45	EFDB	16.9	EFDB	7.2	CHMF	0.0111	PHYS			64.52	PHYS
Chloroform	67663	70.8	RREL	1.34	EFDB	62.23	EFDB	36.43	EFDB	4.8	CHMF	0.00367	PHYS	0.1	NPDWS	119.38	PHYS
Chloromethane	74873	87.66	RREL	0.5	EFDB	53.59	EFDB	45.92	EFDB	2.9	CHMF	0.00882	PHYS			50.49	PHYS
Chloromethyl methyl ether	107302	100	RREL	0	EFDB	0.01	EFDB	99.98	EFDB		Fast Hyd	0.000304	PHYS			80.51	PHYS
p-Chloro-o-toluidine	95692	47.52	RREL	3.47	EFDB	0.11	EFDB	96.42	EFDB	31	Lyman, 5-2	1.99E-06	PHYS			141.6	PHYS
Chlorophenols	N084	96.2	RREL; penta	56.27	EFDB; penta	0	EFDB; penta	43.73	EFDB; penta	46	CHMF; penta	2.45E-08	PHYS; penta			266.34	PHYS; penta
Chloropicrin	76062	61.7	RREL	1.94	EFDB	80.16	EFDB	17.89	EFDB	23	Lyman, 5-2	0.00205	PHYS			164.38	PHYS
Chloroprene	126998	95.71	RREL	1.16	EFDB	92.82	EFDB	6.02	EFDB	49	Lyman, 5-2	0.0561	PHYS			88.54	PHYS
3-Chloropropionitrile	542767	45.73	RREL	2.36	EFDB	1.05	EFDB	96.59	EFDB	1.4	Lyman, 5-3	0.0000143	PHYS			89.53	PHYS
Chlorotetrafluoroethane	63938103	99.53	RREL	0.42	EFDB	98.85	EFDB	0.72	EFDB	15	Lyman, 5-2	0.0000153	HENRY WIN			136.48	CRC; est
Chlorothalonil	1897456	82.03	SUM	3.93	EFDB	0.037	EFDB	96.04	EFDB	120	Lyman, 5-2	0.000002	PHYS			265.91	PHYS
Chlorotrifluoromethane	75729	99.82	RREL	0.35	EFDB	99.01	EFDB	0.63	EFDB	11	Lyman, 5-2	1.38	PHYS			104.46	PHYS
Chlorpyrifos methyl	5598130	97.73	RREL	22.19	EFDB	0.041	EFDB	77.78	EFDB	1100	Lyman, 5-2	3.75E-06	PHYS			322.54	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Chlorsulfuron	64902723	46.55	RREL	2.99	EFDB	0	EFDB	97.01	EFDB	19	Lyman, 5-2	3.9E-15	PHYS			357.78	PHYS
Chromium and chromium compounds	7440473	76.4	RREL	100	Assump.	0	Assump.	0	Assump.	16	EPA, 97			0.1	NPDWS	52	PHYS
Cobalt and cobalt compounds	7440484	32.06	RREL	100	Assump.	0	Assump.	0	Assump.	4430	Jorg					58.93	PHYS
Copper and copper compounds	7440508	72.47	RREL	100	Assump.	0	Assump.	0	Assump.	36	EPA, 97	0.0245	PHYS	1.3	NPDWS	63.55	PHYS
Creosote, coal tar	8001589																
p-Cresidine	120718	46.05	RREL	2.71	EFDB	0	EFDB	97.26	EFDB	10	CHMF	1.24E-07	PHYS			137.18	PHYS
Cresol (mixed isomers)	1319773	92.37	RREL	0.58	EFDB	0.011	EFDB	99.42	EFDB	18	Lyman, 5-2	6.19E-07	PHYS			324.42	PHYS
m-Cresol	108394	92.35	RREL	0.56	EFDB	0.011	EFDB	99.43	EFDB	20	CHMF	8.56E-07	PHYS			108.14	PHYS
o-Cresol	95487	92.35	RREL	0.56	EFDB	0.011	EFDB	99.43	EFDB	18	CHMF	0.0000012	PHYS			108.14	PHYS
p-Cresol	106445	92.34	RREL	0.56	EFDB	0.011	EFDB	99.44	EFDB	18	CHMF	0.000001	PHYS			108.14	PHYS
Crotonaldehyde	4170303	92.27	RREL	0.37	EFDB	1.81	EFDB	97.83	EFDB	3.2	BCFWIN	9.68E-06	PHYS			70.09	PHYS
Cumene	98828	98.07	RREL	6.93	EFDB	11.35	EFDB	81.71	EFDB	35	CHMF	0.0115	PHYS			120.2	PHYS
Cumene hydroperoxide	80159	76.21	RREL	1.29	EFDB	0	EFDB	98.71	EFDB	26	Lyman, 5-2	4.71E-08	PHYS			152.19	PHYS
Cupferron	135206	21.97	RREL	6.55	EFDB	0	EFDB	93.45	EFDB	3.2	BCFWIN	3.62E-09	PHYS			155.16	PHYS
Cyanazine	21725462	23.52	RREL	8.67	EFDB	0	EFDB	91.33	EFDB	29	Lyman, 5-2	2.96E-12	PHYS			240.7	PHYS
Cyanide compounds	N106	1.89	EPI; Cu(CN)2	92.59	EPI; Cu(CN)2	2.65	EPI; Cu(CN)2	4.76	EPI; Cu(CN)2	3.2	BCFWIN; Cu(CN)2	0.000122	Bodek; HCN	0.2	NPDWS; CN-	89.56	PHYS; Cu(CN)2
Cycloate	1134232	93.92	RREL	13.64	EFDB	0.44	EFDB	85.92	EFDB	520	Lyman, 5-2	0.0000067	PHYS			215.36	PHYS
Cyclohexane	110827	88.74	RREL	6.99	EFDB	9.14	EFDB	83.89	EFDB	240	CHMF	0.15	PHYS			84.16	PHYS
Cyclohexanol	108930	92.22	RREL	0.4	EFDB	0.87	EFDB	98.73	EFDB	5.1	Lyman, 5-2	0.0000044	PHYS			100.16	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
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Cyfluthrin	68359375	99.9	RREL	37.6	EFDB	0	EFDB	62.4	EFDB	20000	Lyman, 5-2	2.9E-08	PHYS			434.3	PHYS
Cyhalothrin	68085858	99.58	RREL	52.02	EFDB	0	EFDB	47.98	EFDB	87000	Lyman, 5-2	1.48E-06	PHYS			449.86	PHYS
Dazomet	533744	96.67	RREL	0.17	EFDB	0.01	EFDB	99.81	EFDB	6.8	Lyman, 5-2	4.98E-10	PHYS			162.28	PHYS
Dazomet, sodium salt	53404607	45.71	RREL	2.54	EFDB	0	EFDB	97.46	EFDB	6.8	Lyman, 5-2	1.97E-10	HL				
2,4-DB	94826	88.9	RREL	8.29	EFDB	0	EFDB	91.71	EFDB	71	CHMF	2.29E-09	PHYS			249.1	PHYS
Decabromodiphenyl ether	1163195	99.07	RREL	62.47	EFDB	0	EFDB	37.52	EFDB	4900	Lyman, 5-3	1.19E-08	PHYS			959.17	PHYS
Desmedipham	13684565	90.71	RREL	5.2	EFDB	0	EFDB	94.8	EFDB	220	Lyman, 5-2	1.69E-10	PHYS			300.32	PHYS
Di(2-ethylhexyl) phthalate	117817	99.93	RREL	38.25	EFDB	0	EFDB	61.75	EFDB	210	CHMF	2.7E-07	PHYS	0.006	NPDWS	390.57	PHYS
Diallate	2303164	86.49	RREL	24.52	EFDB	0.046	EFDB	75.43	EFDB	1500	Lyman, 5-2	0.0000038	PHYS			270.22	PHYS
2,4-Diaminoanisole sulfate	39156417	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	1.16E-24	HENRY WIN			234.23	AOPWIN
2,4-Diaminoanisole	615054	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	2.4	Lyman, 5-3	7.22E-10	PHYS			138.17	PHYS
4,4'-Diaminodiphenylether	101804	76.37	RREL	1.35	EFDB	0	EFDB	98.65	EFDB	6.4	Lyman, 5-2	1.5E-11	PHYS			200.24	PHYS
Diaminotoluene (mixed isomers)	25376458	22	EPI	4.55	EPI	0	EPI	95.45	EPI	3.2	BCFWIN	7.43E-10	PHYS			610.86	PHYS
2,4-Diaminotoluene	95807	45.44	RREL	2.4	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	7.92E-10	PHYS			122.17	PHYS
Diazinon	333415	92.99	RREL	12.44	EFDB	0	EFDB	87.56	EFDB	460	Lyman, 5-2	1.13E-07	PHYS			304.35	PHYS
Diazomethane	334883	92.38	RREL	0.58	EFDB	0	EFDB	99.42	EFDB	19	Lyman, 5-2	3.37E-08	PHYS			42.04	PHYS
Dibenzofuran	132649	96.39	RREL	18.29	EFDB	0.23	EFDB	81.49	EFDB	1350	CHMF	0.000213	PHYS			168.2	PHYS
1,2-Dibromo-3-chloropropane (DBCP)	96128	33.45	RREL	13.03	EFDB	15.22	EFDB	71.78	EFDB	100	Lyman, 5-2	0.000147	PHYS	0.0002	NPDWS	236.33	PHYS
1,2-Dibromoethane	106934	54.38	RREL	2.24	EFDB	25.78	EFDB	71.97	EFDB	10	CHMF	0.000667	PHYS	0.00005	NPDWS	187.86	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
1,2-Dibromotetrafluoroethane	124732	98.48	RREL	2.39	EFDB	96.3	EFDB	1.31	EFDB	100	Lyman, 5-2	0.162	PHYS			259.82	PHYS
Dibutyl phthalate	84742	99.22	RREL	29.61	EFDB	0	EFDB	70.38	EFDB	866	CHMF	1.81E-06	PHYS			278.35	PHYS
Dicamba	1918009	47.23	RREL	3.35	EFDB	0	EFDB	96.65	EFDB	28	Lyman, 5-2	2.18E-09	PHYS			221.04	PHYS
Dichloran	99309	51.39	RREL	5.39	EFDB	0	EFDB	94.59	EFDB	79	Lyman, 5-2	4.67E-08	PHYS			207.02	PHYS
3,3-Dichloro-1,1,1,2,2-pentafluoropropane (HCFC-225ca)	422560	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HENRY WIN			202.94	AOPWIN
2,3-Dichloro-1,1,1,2,3-pentafluoropropane (HCFC-225ba)	422480	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HL			202.94	AOPWIN; isom.
2,2-Dichloro-1,1,1,3,3-pentafluoropropane (HCFC-225aa)	128903219	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HENRY WIN			202.94	AOPWIN
2,2-Dichloro-1,1,1-trifluoroethane	306832	97.43	RREL	0.66	EFDB	98	EFDB	1.34	EFDB	26	Lyman, 5-2	0.0256	PHYS			152.93	PHYS
1,3-Dichloro-1,1,2,2,3-pentafluoropropane	507551	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HENRY WIN			202.94	AOPWIN
1,2-Dichloro-1,1,2,3,3-pentafluoropropane (HCFC-225bb)	422446	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HENRY WIN			202.94	AOPWIN
1,3-Dichloro-1,1,2,3,3-pentafluoropropane (HCFC-225ea)	136013791	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HL			202.94	AOPWIN
Dichloro-1,1,2-trifluoroethane	90454185	97.43	RREL	0.66	EFDB	98	EFDB	1.34	EFDB	26	Lyman, 5-2	0.0955	HL			152.93	AOPWIN; isom.
1,2-Dichloro-1,1,2-trifluoroethane	354234	97.43	RREL	0.66	EFDB	98	EFDB	1.34	EFDB	26	Lyman, 5-2	0.0955	HENRY WIN			152.93	PHYS
1,2-Dichloro-1,1,3,3,3-pentafluoropropane (HCFC-225da)	431867	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HL			202.94	AOPWIN; isom.
1,2-Dichloro-1,1-difluoroethane	1649087	95.06	RREL	0.85	EFDB	97.04	EFDB	2.1	EFDB	34	Lyman, 5-2	0.048	PHYS			134.94	PHYS
1,1-Dichloro-1,2,2,3,3-pentafluoropropane (HCFC-225cc)	13474889	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HENRY WIN			202.94	AOPWIN

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		POTW Partition Rates															
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1,1-Dichloro-1,2,2-trifluoroethane (HCFC-123b)	812044	97.43	RREL	0.66	EFDB	98	EFDB	1.34	EFDB	26	Lyman, 5-2	0.0955	HL			152.93	AOPWIN; isom.
1,1-Dichloro-1,2,3,3,3-pentafluoropropane (HCFC-225eb)	111512562	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HENRY WIN			202.94	AOPWIN
1,1-Dichloro-1-fluoroethane	1717006	90.83	RREL	1.07	EFDB	95.38	EFDB	3.56	EFDB	37	Lyman, 5-2	0.0241	PHYS			116.95	PHYS
1,4-Dichloro-2-butene	764410	90.12	RREL	1.49	EFDB	82.28	EFDB	16.22	EFDB	56	Lyman, 5-2	0.00851	PHYS			125	PHYS
Dichlorobenzene (mixed isomers)	25321226	75.23	RREL	10.46	EFDB	29.48	EFDB	60.06	EFDB	180	Lyman, 5-2	0.00355	PHYS			441.01	PHYS
1,2-Dichlorobenzene	95501	73.77	RREL	10	EFDB	28.37	EFDB	61.64	EFDB	150	CHMF	0.00192	PHYS	0.6	NPDWS	147	PHYS
1,3-Dichlorobenzene	541731	76.9	SUM	10.48	EFDB	31.64	EFDB	57.88	EFDB	575	CHMF	0.00263	PHYS			147	PHYS
1,4-Dichlorobenzene	106467	75.34	RREL	9.85	EFDB	32.51	EFDB	57.65	EFDB	150	CHMF	0.00241	PHYS	0.075	NPDWS	147	PHYS
3,3'-Dichlorobenzidine dihydrochloride	612839	68.37	RREL	13.21	EFDB	0	EFDB	86.78	EFDB	270	Lyman, 5-2	2.44E-19	HENRY WIN			326.05	AOPWIN
3,3'-Dichlorobenzidine sulfate	64969342	68.37	RREL	13.21	EFDB	0	EFDB	86.78	EFDB	270	Lyman, 5-2	2.84E-11	HENRY WIN			253.13	AOPWIN
3,3'-Dichlorobenzidine	91941	68.37	RREL	13.21	EFDB	0	EFDB	86.78	EFDB	329	CHMF	2.84E-11	PHYS			253.13	PHYS
Dichlorobromomethane	75274	64.24	RREL	1.68	EFDB	49.67	EFDB	48.63	EFDB	19	Lyman, 5-2	0.00212	PHYS	0.1	NPDWS	163.83	PHYS
1,2-Dichloroethane	107062	58.03	RREL	1.69	EFDB	37.34	EFDB	60.97	EFDB	2	CHMF	0.00118	PHYS	0.005	NPDWS	98.96	PHYS
1,2-Dichloroethylene	540590	72.25	RREL	1.4	EFDB	64.18	EFDB	34.42	EFDB	15	CHMF	0.00408	PHYS	0.1	NPDWS	96.94	PHYS
Dichlorofluoromethane	75434	71.35	RREL	1.09	EFDB	87.5	EFDB	11.41	EFDB	8.9	Lyman, 5-2	0.0108	PHYS			120.92	PHYS
Dichloromethane	75092	81.57	SUM	0.67	EFDB	31.68	EFDB	67.65	EFDB	5.2	CHMF	0.00325	PHYS	0.005	NPDWS	84.93	PHYS
Dichloropentafluoro-propane	127564925	99.51	RREL	3.34	EFDB	95.61	EFDB	1.05	EFDB	140	Lyman, 5-2	0.502	HL			202.94	AOPWIN; isom.
Dichlorophene	97234	78.05	RREL	40.23	EFDB	0	EFDB	59.77	EFDB	1000	Lyman, 5-2	1.15E-12	PHYS			269.13	PHYS

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2,4-Dichlorophenol	120832	94.76	RREL	2.63	EFDB	0.021	EFDB	97.34	EFDB	62	CHMF	5.51E-06	PHYS			163	PHYS
1,2-Dichloropropane	78875	67.88	RREL	1.83	EFDB	55.36	EFDB	42.81	EFDB	10	CHMF	0.00282	PHYS	0.005	NPDWS	112.99	PHYS
2,3-Dichloropropene	78886	65.86	RREL	2.31	EFDB	49.56	EFDB	48.15	EFDB	41	Lyman, 5-2	0.00416	PHYS			110.97	PHYS
1,3-Dichloropropylene	542756	82.99	RREL	0.92	EFDB	32.34	EFDB	66.73	EFDB	32	Lyman, 5-2	0.00355	PHYS			110.97	PHYS
Dichlorotrifluoroethane	34077877	97.43	RREL	0.66	EFDB	98	EFDB	1.34	EFDB	26	Lyman, 5-2	0.0955	HL			152.93	AOPWIN; isom.
Dichlorvos	62737	75.26	RREL	0.86	EFDB	0.35	EFDB	98.79	EFDB	7.7	Lyman, 5-2	5.74E-07	PHYS			220.98	PHYS
Diclofop methyl	51338273	95.96	RREL	37.78	EFDB	0	EFDB	62.21	EFDB	1900	Lyman, 5-2	1.97E-06	PHYS			341.19	PHYS
Dicofol	115322	98.37	RREL	45.27	EFDB	0	EFDB	54.73	EFDB	13900	CHMF	2.42E-07	PHYS			370.49	PHYS
Dicyclopentadiene	77736	96.68	RREL	7.24	EFDB	83.13	EFDB	9.63	EFDB	150	Lyman, 5-2	0.0625	PHYS			132.21	PHYS
Diepoxybutane	1464535	75.07	RREL	0.83	EFDB	0.027	EFDB	99.16	EFDB	3.2	BCFWIN	3.54E-08	PHYS			86.09	PHYS
Diethanolamine	111422	92.06	RREL	0.36	EFDB	0	EFDB	99.63	EFDB	3.2	BCFWIN	3.87E-11	PHYS			105.14	PHYS
Diethatyl ethyl	38727558	89.98	RREL	9.21	EFDB	0	EFDB	90.78	EFDB	320	Lyman, 5-2	6.03E-09	PHYS			311.81	PHYS
Diethyl sulfate	64675	95.12	RREL	0.22	EFDB	0.053	EFDB	99.73	EFDB	4.3	CHMF	6.14E-06	PHYS			154.19	PHYS
Diflubenzuron	35367385	93.88	RREL	13.68	EFDB	0	EFDB	86.33	EFDB	520	Lyman, 5-2	4.6E-09	PHYS			310.69	PHYS
Diglycidyl resorcinol ether	101906	75.2	RREL	0.88	EFDB	0	EFDB	99.12	EFDB	5.1	Lyman, 5-2	2.8E-10	HENRY WIN			222.24	PHYS
Dihydrosafrole	94586	70.75	RREL	14.3	EFDB	0.34	EFDB	85.36	EFDB	310	Lyman, 5-2	0.0000122	PHYS			164.21	PHYS
Diisocyanates	N120																
Dimethipin	55290647	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	5.3	Lyman, 5-3	2.3E-11	PHYS			210.27	PHYS
Dimethoate	60515	45.49	RREL	2.42	EFDB	0	EFDB	97.58	EFDB	2	Lyman, 5-3	1.05E-10	PHYS			229.26	PHYS

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3,3'-Dimethoxybenzidine dihydrochloride	20325400	45.56	RREL	2.46	EFDB	0	EFDB	97.54	EFDB	4	Lyman, 5-2	1.81E-13	HENRY WIN			244.3	AOPWIN
3,3'-Dimethoxybenzidine hydrochloride	111984099	46.15	RREL	2.77	EFDB	0	EFDB	97.23	EFDB								
3,3'-Dimethoxybenzidine	119904	46.15	RREL	2.77	EFDB	0	EFDB	97.23	EFDB	14	CHMF	4.7E-11	PHYS			244.3	PHYS
Dimethyl chlorothiophosphate	2524030	96.76	RREL	0.17	EFDB	0.99	EFDB	98.84	EFDB	6.7	Lyman, 5-2	0.00152	PHYS			160.56	PHYS
1,1-Dimethyl hydrazine	57147	75.12	RREL	0.83	EFDB	0.24	EFDB	98.94	EFDB	3.2	BCFWIN	0.0000124	PHYS			60.1	PHYS
Dimethyl phthalate	131113	92.18	RREL	0.44	EFDB	0	EFDB	99.56	EFDB	58	CHMF	1.97E-07	PHYS			194.19	PHYS
Dimethyl sulfate	77781	96.97	RREL	0.14	EFDB	0.021	EFDB	99.84	EFDB	1.9	CHMF	0.000004	PHYS			126.13	PHYS
Dimethylamine	124403	92.08	RREL	0.36	EFDB	0.17	EFDB	99.46	EFDB	3.2	BCFWIN	0.0000177	PHYS			45.08	PHYS
Dimethylamine dicamba	2300665	45.58	RREL	2.46	EFDB	0	EFDB	97.52	EFDB	4.3	Lyman, 5-2	5.55E-17	HENRY WIN			266.13	AOPWIN
4-Dimethyl-aminoazobenzene	60117	95.55	RREL	36.86	EFDB	0	EFDB	63.14	EFDB	1800	CHMF	4E-10	PHYS			225.3	PHYS
N,N-Dimethylaniline	121697	48.68	RREL	3.45	EFDB	3.53	EFDB	93	EFDB	10	CHMF	0.0000568	PHYS			121.18	PHYS
3,3'-Dimethylbenzidine dihydrochloride	612828	55.46	RREL	7.3	EFDB	0	EFDB	92.7	EFDB	120	Lyman, 5-2	6.29E-11	HENRY WIN			212.3	AOPWIN
3,3'-Dimethylbenzidine dihydrofluoride	41766750	47.84	RREL	3.64	EFDB	0	EFDB	96.34	EFDB	35	Lyman, 5-2	8.1E-11	HL				
3,3'-Dimethylbenzidine	119937	76.76	RREL	1.51	EFDB	0	EFDB	98.49	EFDB	35	CHMF	6.29E-11	PHYS			212.3	PHYS
Dimethylcarbamyl chloride	79447	100	RREL	0	EFDB	0	EFDB	100	EFDB		Fast Hyd	7.23E-07	PHYS			107.54	PHYS
N,N-Dimethylformamide	68122	92.06	RREL	0.36	EFDB	0	EFDB	99.63	EFDB	3.2	BCFWIN	7.39E-08	PHYS			73.1	PHYS
2,4-Dimethylphenol	105679	76.63	RREL	1.46	EFDB	0.052	EFDB	98.5	EFDB	48	CHMF	9.51E-07	PHYS			122.17	PHYS
m-Dinitrobenzene	99650	45.78	RREL	2.58	EFDB	0.022	EFDB	97.4	EFDB	74	CHMF	4.9E-08	PHYS			168.11	PHYS
o-Dinitrobenzene	528290	45.98	RREL	2.68	EFDB	0	EFDB	97.3	EFDB	11	Lyman, 5-2	8.39E-08	PHYS			168.11	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
p-Dinitrobenzene	100254	45.75	RREL	2.56	EFDB	0	EFDB	97.44	EFDB	7.6	Lyman, 5-2	8.39E-08	PHYS			168.11	PHYS
Dinitrobutyl phenol (Dinoseb)	88857	46.36	RREL	25.39	EFDB	0.3	EFDB	74.29	EFDB	30	CHMF	4.56E-07	PHYS	0.007	NPDWS	240.22	PHYS
4,6-Dinitro-o-cresol	534521	46.93	RREL	3.15	EFDB	0.11	EFDB	96.74	EFDB	24	CHMF	0.0000014	PHYS			198.14	PHYS
2,4-Dinitrophenol	51285	75.45	RREL	0.98	EFDB	0.013	EFDB	99.01	EFDB	11	Lyman, 5-2	8.6E-08	PHYS			184.11	PHYS
Dinitrotoluene (mixed isomers)	25321146	47.12	RREL	3.27	EFDB	0.042	EFDB	96.69	EFDB	27	Lyman, 5-2	9.26E-08	PHYS			546.41	PHYS
2,4-Dinitrotoluene	121142	46.5	RREL	2.95	EFDB	0	EFDB	97.03	EFDB	204	CHMF	5.4E-08	PHYS			182.14	PHYS
2,6-Dinitrotoluene	606202	46.85	RREL	3.14	EFDB	0.064	EFDB	96.82	EFDB	23	Lyman, 5-2	7.47E-07	PHYS			182.14	PHYS
Dinocap	39300453	99.57	RREL	51.93	EFDB	0	EFDB	48.07	EFDB	21000	Lyman, 5-2	4.79E-09	PHYS			364.4	PHYS
Dioxane	123911	45.53	RREL	2.37	EFDB	0.35	EFDB	97.25	EFDB	3.2	BCFWIN	0.0000048	PHYS			88.11	PHYS
Dioxin and dioxin-like compounds	N150								EPI	14200	BCFWIN			3E-08	NPDWS	321.98	PHYS
Diphenamid	957517	52.74	RREL	6.05	EFDB	0	EFDB	93.97	EFDB	26	Lyman, 5-2	3.63E-11	PHYS			239.32	PHYS
Diphenylamine	122394	88.44	RREL	7.93	EFDB	0.045	EFDB	92.04	EFDB	30	CHMF	3.39E-06	PHYS			169.23	PHYS
1,2-Diphenylhydrazine	122667	54.01	RREL	6.63	EFDB	0	EFDB	93.37	EFDB	100	CHMF	4.39E-09	PHYS			184.24	PHYS
Dipotassium endothall	2164070	75.72	RREL	1.08	EFDB	0	EFDB	98.92	EFDB	17	Lyman, 5-2	3.62E-15	HENRY WIN			186.17	AOPWIN
Dipropyl isocinchomeronate	136458	97.24	RREL	6.16	EFDB	0	EFDB	93.84	EFDB	300	Lyman, 5-2	9.09E-10	PHYS			251.28	PHYS
Disodium cyanodithio-imidocarbonate	138932	77.6	RREL	0.75	EFDB	11.33	EFDB	87.93	EFDB	3.2	BCFWIN	0.000776	HENRY WIN			118.17	AOPWIN
2,4-Dithiobiuret	541537	48.65	RREL	2.12	EFDB	0	EFDB	97.88	EFDB	7.2	Lyman, 5-3	7.23E-09	HENRY WIN			135.21	PHYS
Diuron	330541	50.51	RREL	4.95	EFDB	0.18	EFDB	94.89	EFDB	64	Lyman, 5-2	5.04E-10	PHYS			233.1	PHYS
Dodine	2439103	75.06	RREL	0.83	EFDB	0	EFDB	99.17	EFDB	16	Lyman, 5-3	9.01E-11	PHYS			287.45	PHYS

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		POTW Partition Rates															
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2,4-DP (Dichlorprop)	120365	65.84	RREL	12.01	EFDB	0	EFDB	87.97	EFDB	240	CHMF	8.68E-11	PHYS			235.07	PHYS
D-trans-allethrin (D-trans-chrysanthemic acid of D-allethrone)	28057489	99.33	RREL	30.47	EFDB	0	EFDB	69.52	EFDB	2500	Lyman, 5-2	6.12E-07	HL				
Epichlorohydrin	106898	46.05	RREL	2.35	EFDB	2.17	EFDB	95.5	EFDB	3.2	BCFWIN	0.0000304	PHYS		NPDWS; TTreq.	92.53	PHYS
Ethoprop	13194484	71	RREL	14.51	EFDB	0	EFDB	85.49	EFDB	320	Lyman, 5-2	1.62E-07	PHYS			242.34	PHYS
2-Ethoxyethanol	110805	92.06	RREL	0.36	EFDB	0.011	EFDB	99.63	EFDB			4.7E-07	PHYS			90.12	PHYS
Ethyl acrylate	140885	92.4	RREL	0.4	EFDB	2.51	EFDB	97.08	EFDB	5.9	CHMF	0.000339	PHYS			100.12	PHYS
Ethyl chloroformate	541413	81.95	RREL	0.63	EFDB	30.76	EFDB	68.6	EFDB	1.8	Lyman, 5-3	0.00312	PHYS			108.53	PHYS
Ethyl dipropylthiocarbamate	759944	59.92	RREL	9.15	EFDB	0.95	EFDB	89.9	EFDB	160	Lyman, 5-2	0.0000159	PHYS			189.32	PHYS
2,4-D 2-ethyl-4-methylpentyl ester	53404378	99.97	RREL	21.23	EFDB	0	EFDB	78.77	EFDB	9700	Lyman, 5-2	0.000029	HL				
Ethylbenzene	100414	89.8	RREL	3.93	EFDB	38.24	EFDB	57.82	EFDB	8.4	CHMF	0.00788	PHYS	0.7	NPDWS	106.17	PHYS
Ethylene	74851	99.06	RREL	0.28	EFDB	91.49	EFDB	8.23	EFDB	4.3	CHMF	0.228	PHYS			28.05	PHYS
Ethylene glycol	107211	92.06	RREL	0.36	EFDB	0	EFDB	99.63	EFDB	10	CHMF	6E-08	PHYS			62.07	PHYS
Ethylene oxide	75218	92.2	RREL	0.36	EFDB	1.18	EFDB	98.45	EFDB	3.2	BCFWIN	0.000148	PHYS			44.05	PHYS
Ethylene thiourea	96457	45.43	RREL	2.38	EFDB	0.022	EFDB	97.6	EFDB	2.3	Lyman, 5-3	1.36E-11	PHYS			102.16	PHYS
Ethylenebisdithiocarbamic acid, salts and esters (EBDCs)	N171	1.85	EPI; met	95.14	EPI; met	0	EPI; met	4.86	EPI; met	2.8	Lyman, 5-3; met	5.33E-08	PHYS; met			504.13	PHYS; met
Ethyleneimine (Aziridine)	151564	45.67	RREL	2.36	EFDB	0.9	EFDB	96.76	EFDB	3.2	BCFWIN	0.0000121	PHYS			43.07	PHYS
2,4-D 2-ethylhexyl ester	1928434	99.99	RREL	21.72	EFDB	0	EFDB	78.28	EFDB	34000	Lyman, 5-2	0.0000214	HENRY WIN			333.26	AOPWIN
Ethylidene dichloride	75343	76.2	RREL	1.01	EFDB	71.3	EFDB	27.69	EFDB	14	CHMF	0.00562	PHYS			98.96	PHYS

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Famphur	52857	76.4	RREL	1.36	EFDB	0	EFDB	98.64	EFDB	29	Lyman, 5-2	1.61E-08	PHYS			325.34	PHYS
Fenarimol	60168889	71.33	RREL	14.66	EFDB	0	EFDB	85.34	EFDB	320	Lyman, 5-2	7E-09	PHYS			331.2	PHYS
Fenbutatin oxide (Vendex)	13356086	94.04	EPI	99.17	EPI	0	EPI	0.83	EPI	5300	Lyman, 5-2	0.028	PHYS			1052.7	PHYS
Fenoxaprop ethyl	66441234	99.55	RREL	32.6	EFDB	0	EFDB	67.4	EFDB	3400	Lyman, 5-2	1.96E-11	HENRY WIN			361.78	PHYS
Fenoxycarb	72490018	97.67	RREL	21.99	EFDB	0	EFDB	78.01	EFDB	1100	Lyman, 5-2	4.3E-10	PHYS			301.35	PHYS
Fenpropathrin	39515418	99.88	RREL	37.09	EFDB	0	EFDB	62.9	EFDB	13000	Lyman, 5-2	7.64E-06	PHYS			349.43	PHYS
Fenthion	55389	96.12	RREL	17.71	EFDB	0.01	EFDB	82.28	EFDB	760	Lyman, 5-2	1.46E-06	PHYS			278.33	PHYS
Fenvalerate	51630581	99.62	RREL	52.32	EFDB	0	EFDB	47.67	EFDB	30000	Lyman, 5-2	3.45E-08	PHYS			419.91	PHYS
Ferbam (Tris(dimethylcarba-modithioato-S,S')iron)	14484641	45.48	RREL	2.42	EFDB	0	EFDB	97.58	EFDB	40	Lyman, 5-3	1E-24	HL			416.49	PHYS
Fluazifop butyl	69806504	99.8	RREL	35.71	EFDB	0	EFDB	64.29	EFDB	1500	Lyman, 5-2	2.08E-07	PHYS			383.37	PHYS
Fluometuron	2164172	48.3	RREL	3.89	EFDB	0	EFDB	96.13	EFDB	41	Lyman, 5-2	2.61E-09	PHYS			232.21	PHYS
Fluorine	7782414	1.85	EPI	95.14	EPI	0	EPI	4.86	EPI	3.2	BCFWIN	0.0245	HENRY WIN	4	NPDWS	38	PHYS
Fluorouracil (5-fluorouracil)	51218	45.42	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	3.2	Lyman, 5-3	1.66E-10	PHYS			130.08	PHYS
Fluvalinate	69409945	99.93	RREL	38.17	EFDB	0	EFDB	61.83	EFDB	88000	Lyman, 5-2	1.45E-08	PHYS			502.93	PHYS
Folpet	133073	79.92	RREL	2.89	EFDB	0.075	EFDB	97.03	EFDB	86	Lyman, 5-2	3.81E-06	PHYS			296.56	PHYS
Fomesafen	72178020	53.36	RREL	6.33	EFDB	0	EFDB	93.67	EFDB	94	Lyman, 5-2	7.53E-13	PHYS			438.77	PHYS
Formaldehyde	50000	92.07	RREL	0.37	EFDB	0	EFDB	99.62	EFDB	0	CHMF	3.37E-07	PHYS			30.03	PHYS
Formic acid	64186	92.06	RREL	0.36	EFDB	0	EFDB	99.63	EFDB	3.2	BCFWIN	1.67E-07	PHYS			46.03	PHYS
Freon 113	76131	99.53	RREL	3.48	EFDB	95.47	EFDB	1.05	EFDB	150	CHMF	0.526	PHYS			187.38	PHYS

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Furan	110009									5.9	Lyman, 5-2	0.00538	Reaxys			68.075	Reaxys
Glycidol	556525									0.9	BCFWIN	5.84E-09	Reaxys			74.079	Reaxys
Glycol ethers	N230	92.06	RREL; methoxy	0.36	EFDB; methoxy	0.01	EFDB; methoxy	99.63	EFDB; methoxy			3.3E-07	PHYS; methoxy			76.1	PHYS; methoxy
Heptachlor	76448	99.3	RREL	50	EFDB	0.28	EFDB	49.72	EFDB	19953	EPA, 99	0.000294	PHYS	0.0004	NPDWS	373.32	PHYS
Hexachloro-1,3-butadiene	87683	94.82	RREL	47.54	EFDB	18.49	EFDB	33.97	EFDB	11400	CHMF	0.0103	PHYS			260.76	PHYS
Hexachlorobenzene	118741	98.43	RREL	60.63	EFDB	0.46	EFDB	38.91	EFDB	66000	EPA/ OPPT, 98; high	0.0017	PHYS	0.001	NPDWS	284.78	PHYS
alpha-Hexachlorocyclohexane	319846	78.08	RREL	18.33	EFDB	0.2	EFDB	81.45	EFDB	1950	CHMF	0.0000122	PHYS			290.83	PHYS
Hexachlorocyclo-pentadiene	77474	98.78	RREL	44.83	EFDB	9.86	EFDB	45.31	EFDB	120	CHMF	0.027	PHYS	0.05	NPDWS	272.77	PHYS
Hexachloroethane	67721	77.49	RREL	23.01	EFDB	43.8	EFDB	33.19	EFDB	440	CHMF	0.00389	PHYS			236.74	PHYS
Hexachloronaphthalene	1335871	99.04	RREL	62.38	EFDB	0	EFDB	37.61	EFDB	24000	Lyman, 5-3	0.000087	PHYS			334.85	PHYS
Hexachlorophene	70304	99.06	RREL	62.45	EFDB	0	EFDB	37.55	EFDB	320000	CHMF; hexa	5.48E-13	PHYS			406.91	PHYS
Hexamethyl-phosphoramide	680319	45.44	RREL	2.4	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	2E-08	PHYS			179.2	PHYS
n-Hexane	110543	99.94	RREL	9.37	EFDB	52.66	EFDB	37.96	EFDB	540	Lyman, 5-2	1.8	PHYS			86.18	PHYS
Hexazinone	51235042	84.56	RREL	22.88	EFDB	0	EFDB	77.11	EFDB	15	Lyman, 5-2	2.26E-12	PHYS			252.32	PHYS
Hydramethylnon	67485294	99.69	RREL	52.93	EFDB	0	EFDB	47.07	EFDB	34	Lyman, 5-2	0.0000022	PHYS			494.49	PHYS
Hydrazine	302012	85	Howard	0	Assump.; hydr	0	Assump.; hydr	100	Assump.; hydr		Ion	6.07E-07	PHYS			32.05	PHYS
Hydrazine sulfate	10034932	1.85	EPI	94.59	EPI	0	EPI	4.86	EPI	1.8	Lyman, 5-3	8.72E-14	HENRY WIN			128.1	AOPWIN
Hydrochloric acid	7647010	100	Assump.; neu	0	Assump.; neu	0	Assump.; neu	100	Assump.; neu	3.2	BCFWIN	0.0245	HENRY WIN			36.45	AOPWIN
Hydrogen cyanide	74908	7.28	EPI	22.94	EPI	75.82	EPI	1.24	EPI			0.000133	PHYS			27.03	PHYS

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Hydrogen fluoride	7664393	1.85	EPI	95.14	EPI	0	EPI	4.86	EPI	3.2	BCFWIN					20.01	PHYS
Hydroquinone	123319	92.07	RREL	0.37	EFDB	0	EFDB	99.63	EFDB	40	CHMF	4.73E-11	PHYS			110.11	PHYS
Imazalil	35554440	78.69	RREL	18.76	EFDB	0	EFDB	81.24	EFDB	470	Lyman, 5-2	2.59E-09	PHYS			297.19	PHYS
3-Iodo-2-propynyl butylcarbamate	55406536	77.22	RREL	1.71	EFDB	0	EFDB	98.29	EFDB	43	Lyman, 5-2	8.93E-09	HENRY WIN			281.09	AOPWIN
Iron pentacarbonyl	13463406															195.9	PHYS
Isobutyraldehyde	78842	92.23	RREL	0.37	EFDB	1.39	EFDB	98.24	EFDB	3.2	BCFWIN	0.00018	PHYS			72.11	PHYS
Isodrin	465736	98.96	RREL	62.16	EFDB	0.02	EFDB	37.82	EFDB	20180	EPA, 99	0.000387	PHYS			364.92	PHYS
Isofenphos	25311711	96.38	RREL	18.31	EFDB	0	EFDB	81.69	EFDB	800	Lyman, 5-2	6.17E-08	PHYS			345.4	PHYS
Isoprene	78795									33	Lyman, 5-2	0.122	Reaxys			68.119	Reaxys
Isopropyl alcohol	67630	92.07	RREL	0.37	EFDB	0.087	EFDB	99.55	EFDB	3.2	BCFWIN	0.0000081	PHYS			60.1	PHYS
2,4-D isopropyl ester	94111	98.28	RREL	8.7	EFDB	0.02	EFDB	91.28	EFDB	460	Lyman, 5-2	2.15E-06	PHYS			263.12	PHYS
4,4'-Isopropylidenediphenol	80057	85.68	RREL	6	EFDB	0	EFDB	94	EFDB	100	CHMF	1E-11	PHYS			228.29	PHYS
Isosafrole	120581	64.08	RREL	11.17	EFDB	0.19	EFDB	88.64	EFDB	210	Lyman, 5-2	0.036	PHYS			162.19	PHYS
Lactofen	77501634	99.37	RREL	30.89	EFDB	0	EFDB	69.12	EFDB	2700	Lyman, 5-2	5.73E-10	PHYS			461.78	PHYS
Lead and lead compounds	7439921	63.48	RREL	100	Assump.	0	Assump.	0	Assump.	42	EPA/ OPPT, 99	0.0245	PHYS	0.015	NPDWS	209.21	PHYS
Lindane	58899	75.38	RREL	16.79	EFDB	0.04	EFDB	83.15	EFDB	1300	CHMF	5.14E-06	PHYS	0.0002	NPDWS	290.83	PHYS
Linuron	330552	59.41	RREL	9.09	EFDB	0	EFDB	90.91	EFDB	160	CHMF	6.25E-09	PHYS			249.1	PHYS
Lithium carbonate	554132	1.85	EPI	94.59	EPI	0	EPI	4.86	EPI	3	Lyman, 5-3					73.89	PHYS

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Malathion	121755	92.76	RREL	0.86	EFDB	0	EFDB	99.14	EFDB	36	CHMF	4.89E-09	PHYS			330.36	PHYS
Maleic anhydride	108316	100	RREL	0	EFDB	0	EFDB	100	EFDB		Fast Hyd	3.93E-06	PHYS			98.06	PHYS
Malonitrile	109773	45.42	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	3.2	BCFWIN	1.27E-08	PHYS			66.06	PHYS
Maneb	12427382	1.86	EPI	95.16	EPI	0	EPI	4.84	EPI	220	Lyman, 5-3	4.86E-09	PHYS			295.37	PHYS
Manganese and manganese compounds	7439965	38.85	RREL	100	Assump.	0	Assump.	0	Assump.	3.2	BCFWIN					54.94	PHYS
Mecoprop	93652	57.76	RREL	8.34	EFDB	0	EFDB	91.66	EFDB	140	Lyman, 5-2	1.82E-08	PHYS			214.65	PHYS
2-Mercaptobenzothiazole	149304	48.3	RREL	3.89	EFDB	0	EFDB	96.13	EFDB	41	Lyman, 5-2	3.63E-08	PHYS			167.25	PHYS
Mercury and mercury compounds	7439976	68.57	RREL	100	Assump.	0	Assump.	0	Assump.	36000	EPA, 99; methyl	0.008622	PHYS	0.002	NPDWS	200.59	PHYS
Merphos	150505	99.99	RREL	21.83	EFDB	0	EFDB	78.16	EFDB	15000	Lyman, 5-3	0.0000227	PHYS			298.51	PHYS
Methacrylonitrile	126987	76.17	RREL	0.8	EFDB	4.59	EFDB	94.59	EFDB	2	Lyman, 5-3	0.000247	PHYS			67.09	PHYS
Metham sodium	137428	75.91	RREL	0.8	EFDB	3.5	EFDB	95.69	EFDB	3.2	BCFWIN	0.000177	HL			129.18	PHYS
Methanol	67561	92.07	RREL	0.36	EFDB	0.043	EFDB	99.59	EFDB	3	CHMF	4.55E-06	PHYS			32.04	PHYS
Methazole	20354261	59.91	RREL	9.31	EFDB	0.017	EFDB	90.67	EFDB	160	Lyman, 5-2	2.29E-07	PHYS			261.07	PHYS
Methiocarb	2032657	80.58	RREL	3.21	EFDB	0	EFDB	96.79	EFDB	98	Lyman, 5-2	1.18E-09	PHYS			225.31	PHYS
Methoxone (MCPA)	94746	60.68	RREL	9.67	EFDB	0	EFDB	90.34	EFDB	170	Lyman, 5-2	1.33E-09	PHYS			200.62	PHYS
Methoxone sodium salt	3653483	75.23	RREL	0.89	EFDB	0	EFDB	99.11	EFDB	3.2	BCFWIN	1.38E-08	PHYS			222.61	PHYS
Methoxychlor	72435	98.56	RREL	46.1	EFDB	0	EFDB	53.91	EFDB	8128	EPA, 99	2.03E-07	PHYS	0.04	NPDWS	345.66	PHYS
2-Methoxyethanol	109864	92.06	RREL	0.36	EFDB	0.011	EFDB	99.63	EFDB			3.3E-07	PHYS			76.1	PHYS
Methyl acrylate	96333	92.25	RREL	0.37	EFDB	1.49	EFDB	98.14	EFDB	1.4	Lyman, 5-3	0.000199	PHYS			86.09	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Methyl chlorocarbonate	79221	99.63	RREL	0.05	EFDB	0.82	EFDB	99.13	EFDB		Fast Hyd	0.00235	PHYS			94.5	PHYS
Methyl ethyl ketone	78933	92.13	RREL	0.37	EFDB	0.53	EFDB	99.11	EFDB	3.2	BCFWIN	0.0000569	PHYS			72.11	PHYS
Methyl hydrazine	60344	75.08	RREL	0.83	EFDB	0.08	EFDB	99.11	EFDB	3.2	BCFWIN	3.03E-06	PHYS			46.07	PHYS
Methyl iodide	74884	75.27	RREL	0.94	EFDB	70.35	EFDB	28.71	EFDB	8.3	CHMF	0.00526	PHYS			141.94	PHYS
Methyl isobutyl ketone	108101	92.25	RREL	0.4	EFDB	1.12	EFDB	98.48	EFDB	5.8	Lyman, 5-2	0.000138	PHYS			100.16	PHYS
Methyl isocyanate	624839	99.95	RREL	0.02	EFDB	0.14	EFDB	99.84	EFDB		Fast Hyd	0.000926	PHYS			57.05	PHYS
Methyl isothiocyanate	556616	99.96	RREL	0.02	EFDB	0.23	EFDB	99.75	EFDB	3.1	Lyman, 5-2	0.0000448	PHYS			73.12	PHYS
Methyl methacrylate	80626	92.38	RREL	0.41	EFDB	2.23	EFDB	97.36	EFDB	6.6	CHMF	0.000319	PHYS			100.12	PHYS
Methyl parathion	298000	93.97	RREL	1.86	EFDB	0	EFDB	98.14	EFDB	40	CHMF	0.0000001	PHYS			263.21	PHYS
Methyl tert-butyl ether	1634044	52.94	RREL	1.87	EFDB	24.35	EFDB	73.78	EFDB	1.5	CHMF	0.000587	PHYS			88.15	PHYS
Methylene bromide	74953	55.71	RREL	1.94	EFDB	30.77	EFDB	67.29	EFDB	12	Lyman, 5-2	0.000822	PHYS			173.84	PHYS
4,4'-Methylenebis(2-chloroaniline)	101144	81.57	RREL	20.64	EFDB	0	EFDB	79.36	EFDB	550	Lyman, 5-2	4.06E-11	PHYS			267.16	PHYS
4,4'-Methylenebis(N,N-dimethylbenzenamine)	101611	92.73	RREL	31.74	EFDB	0	EFDB	68.25	EFDB	1200	Lyman, 5-2	1.07E-09	PHYS			254.38	PHYS
Methylenebis(phenyl-isocyanate) (MDI)	101688	99.99	RREL	3.18	EFDB	0	EFDB	96.82	EFDB		Fast Hyd	8.95E-07	PHYS			250.26	PHYS
4,4'-Methylenedianiline	101779	75.38	RREL	0.96	EFDB	0	EFDB	99.04	EFDB	9.5	CHMF	5.6E-11	PHYS			198.27	PHYS
Methyleugenol	93152									110	Lyman, 5-2	0.0000056	Reaxys			178.23	Reaxys
2-Methyllactonitrile	75865	99.95	RREL	0.02	EFDB	0	EFDB	99.98	EFDB		Fast Hyd	1.97E-09	PHYS			85.11	PHYS
2-Methylpyridine	109068	92.11	RREL	0.39	EFDB	0.098	EFDB	99.51	EFDB	4.1	Lyman, 5-2	9.96E-06	PHYS			93.13	PHYS
Metiram	9006422	1.85	EPI	95.14	EPI	0	EPI	4.86	EPI	2.8	Lyman, 5-3	5.33E-08	PHYS			504.13	PHYS

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Metribuzin	21087649	45.99	RREL	2.7	EFDB	0	EFDB	97.33	EFDB	12	Lyman, 5-2	1.17E-10	PHYS			214.29	PHYS
Mevinphos	7786347	92.06	RREL	0.37	EFDB	0	EFDB	99.64	EFDB	3.2	BCFWIN	6.39E-11	PHYS			224.15	PHYS
Michlers Ketone	90948	60.21	RREL	31.74	EFDB	0	EFDB	68.28	EFDB	510	Lyman, 5-2	4.91E-10	PHYS			268.36	PHYS
Molinate	2212671	59.71	RREL	9.19	EFDB	0.18	EFDB	90.62	EFDB	160	Lyman, 5-2	0.0000041	PHYS			187.31	PHYS
Molybdenum trioxide	1313275	2.52	EPI	96.03	EPI	0	EPI	3.97	EPI	10	BCFWIN					143.95	Merck
Monuron	150685	22.77	RREL	7.69	EFDB	0	EFDB	92.31	EFDB	18	Lyman, 5-2	5.72E-10	PHYS			198.65	PHYS
Mustard gas	505602	99.99	RREL	0.03	EFDB	0.01	EFDB	99.97	EFDB	40	Lyman, 5-2	0.0000275	PHYS			159.08	PHYS
Myclobutanil	88671890	68.04	RREL	13.07	EFDB	0	EFDB	86.95	EFDB	100	Lyman, 5-2	4.28E-09	PHYS			274.76	PHYS
Nabam	142596	90	RREL; NAB	0	Assump.	0	Assump.	100	Assump.	3.2	BCFWIN	1.6E-18	PHYS			256.34	PHYS
Naled	300765	75.26	RREL	0.9	EFDB	0	EFDB	99.1	EFDB	6.6	Lyman, 5-2	0.0000651	PHYS			380.79	PHYS
Naphthalene	91203	95.99	RREL	3.94	EFDB	1.71	EFDB	94.35	EFDB	60	CHMF	0.00044	PHYS			128.18	PHYS
beta-Naphthylamine	91598	76.56	RREL	1.42	EFDB	0	EFDB	98.56	EFDB	32	CHMF	8.1E-08	PHYS			143.19	PHYS
alpha-Naphthylamine	134327	76.46	RREL	1.39	EFDB	0.013	EFDB	98.6	EFDB	30	CHMF	1.11E-07	PHYS			143.19	PHYS
Nickel and nickel compounds	7440020	38.28	RREL	100	Assump.	0	Assump.	0	Assump.	47	EPA, 97	0.0245	PHYS	0.1	NPDWS	58.71	PHYS
Nicotine and salts	N503	1.91	EPI; nic	94.76	EPI; nic	0	EPI; nic	4.71	EPI; nic	4.6	CHMF; nic	3E-09	PHYS; nic			162.24	PHYS; nic
Nitrapyrin	1929824	65.8	RREL	11.57	EFDB	2.2	EFDB	86.25	EFDB	230	Lyman, 5-2	0.0000203	PHYS			230.91	PHYS
Nitrate compounds (water dissociable)	N511									3.2	BCFWIN			10	NPDWS		
Nitric acid	7697372	100	Assump; neu	0	Assump; neu	0	Assump; neu	100	Assump; neu	3.2	BCFWIN	0.0245	PHYS			63.01	PHYS
Nitrilotriacetic acid	139139	92.06	RREL	0.36	EFDB	0	EFDB	99.63	EFDB	3.2	BCFWIN	1.3E-10	PHYS			191.14	PHYS

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o-Nitroanisole	91236									12	Lyman, 5-2	4.29E-07	Reaxys			153.14	Reaxys
Nitrobenzene	98953	92.32	RREL	0.52	EFDB	0.23	EFDB	99.24	EFDB	13	CHMF	0.000024	PHYS			123.11	PHYS
4-Nitrobiphenyl	92933	93.12	RREL	12.62	EFDB	0.011	EFDB	87.37	EFDB	470	Lyman, 5-2	3.54E-06	PHYS			199.21	PHYS
Nitrofen	1836755	96.14	RREL	38.23	EFDB	0	EFDB	61.77	EFDB	1550	CHMF	2.55E-07	PHYS			284.1	PHYS
Nitrogen mustard	51752	99.1	RREL	0.071	EFDB	0.01	EFDB	99.92	EFDB	2.9	Lyman, 5-2	8.48E-08	PHYS			156.06	PHYS
Nitroglycerin	55630	75.4	RREL	0.95	EFDB	0	EFDB	99.05	EFDB	10	CHMF	9.87E-08	PHYS			227.09	PHYS
Nitromethane	75525									3.2	Lyman, 5-3	0.0000286	Reaxys			61.04	Reaxys
5-Nitro-o-anisidine	99592	45.76	RREL	2.56	EFDB	0	EFDB	97.44	EFDB	7.7	CHMF	1.25E-08	PHYS			168.15	PHYS
5-Nitro-o-toluidine	99558	46.26	RREL	2.83	EFDB	0	EFDB	97.17	EFDB	16	Lyman, 5-2	1.77E-08	PHYS			152.15	PHYS
2-Nitrophenol	88755	53.42	RREL	2.15	EFDB	23.96	EFDB	73.89	EFDB	14	Lyman, 5-2	0.0000128	PHYS			139.11	PHYS
4-Nitrophenol	100027	99.48	RREL	0.42	EFDB	92.39	EFDB	7.18	EFDB	110	CHMF	4.15E-10	PHYS			139.11	PHYS
2-Nitropropane	79469	75.73	RREL	0.83	EFDB	2.5	EFDB	96.66	EFDB	10	CHMF	0.000119	PHYS			89.1	PHYS
N-Nitrosodiethylamine	55185	22.14	RREL	6.55	EFDB	0.77	EFDB	92.68	EFDB	3.2	BCFWIN	3.63E-06	PHYS			102.14	PHYS
N-Nitrosodimethylamine	62759	45.46	RREL	2.38	EFDB	0.13	EFDB	97.49	EFDB	3.2	BCFWIN	1.82E-06	PHYS			74.08	PHYS
N-Nitrosodi-n-butylamine	924163	46.62	RREL	2.85	EFDB	0.94	EFDB	96.2	EFDB	59	Lyman, 5-2	0.0000132	PHYS			158.25	PHYS
N-Nitrosodi-n-propylamine	621647	45.79	RREL	2.51	EFDB	0.39	EFDB	97.1	EFDB	6.4	CHMF	5.38E-06	PHYS			130.19	PHYS
N-Nitrosodiphenylamine	86306	57.77	RREL	8.34	EFDB	0.052	EFDB	91.6	EFDB	219	CHMF	1.21E-06	PHYS			198.23	PHYS
p-Nitrosodiphenylamine	156105	58.45	RREL	8.66	EFDB	0	EFDB	91.34	EFDB	150	Lyman, 5-2	1.1E-08	PHYS			198.23	PHYS
N-Nitrosomethylvinylamine	4549400	59.08	SUM	15.22	EFDB	16.49	EFDB	68.3	EFDB	1.8	Lyman, 5-3	0.0000036	PHYS			86.09	PHYS

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N-Nitrosomorpholine	59892	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	2.45E-08	PHYS			116.12	PHYS
N-Nitroso-N-ethylurea	759739	45.44	RREL	2.4	EFDB	0	EFDB	97.6	EFDB	3	Lyman, 5-3	1.32E-10	PHYS			117.11	PHYS
N-Nitroso-N-methylurea	684935	45.43	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	2.8	Lyman, 5-3	9.91E-11	PHYS			103.08	PHYS
Nitrosonornicotine	16543558	45.44	RREL	2.4	EFDB	0	EFDB	97.62	EFDB	3.2	BCFWIN	1.69E-10	PHYS			177.21	PHYS
N-Nitrosopiperidine	100754	45.46	RREL	2.4	EFDB	0.066	EFDB	97.56	EFDB	3.2	BCFWIN	8.44E-07	PHYS			114.15	PHYS
N-methyl-2-pyrrolidone	872504	92.06	RREL	0.36	EFDB	0	EFDB	99.64	EFDB	3.2	BCFWIN	4.46E-08	PHYS			99.13	PHYS
N-methylolacrylamide	924425	92.06	RREL	0.36	EFDB	0	EFDB	99.63	EFDB	3.2	BCFWIN	9.45E-12	HENRY WIN			101.11	AOPWIN
Norflurazon	27314132	47.63	RREL	3.55	EFDB	0	EFDB	96.45	EFDB	33	Lyman, 5-2	3.43E-10	PHYS			303.67	PHYS
Octachloronaphthalene	2234131	99.07	RREL	62.47	EFDB	0	EFDB	37.53	EFDB	100000	Lyman, 5-4	0.000102	PHYS			403.74	PHYS
Octochlorostyrene	29082744									7921	BCFWIN					379.71	PHYS
Oryzalin (4-(dipropylamino)-3,5-dinitro-benzenesulfonamide)	19044883	51.02	RREL	5.23	EFDB	0	EFDB	94.79	EFDB	70	Lyman, 5-2	1.91E-09	PHYS			346.36	PHYS
Osmium tetroxide	20816120	2.52	EPI	96.03	EPI	0	EPI	3.97	EPI	10	BCFWIN					254.1	Merck
Oxadiazon	19666309	97.35	RREL	41.56	EFDB	0	EFDB	58.44	EFDB	2600	Lyman, 5-2	7.27E-08	PHYS			345.23	PHYS
Oxydemeton methyl	301122	75.06	RREL	0.83	EFDB	0	EFDB	99.17	EFDB	3.2	BCFWIN	1.62E-13	PHYS			246.29	PHYS
Oxyfluorfen	42874033	96.88	RREL	40.16	EFDB	0.01	EFDB	59.84	EFDB	2300	Lyman, 5-2	1.18E-06	PHYS			361.71	PHYS
Ozone	10028156	1.85	EPI	94.59	EPI	0	EPI	4.86	EPI	3.2	BCFWIN					48	PHYS
Paraldehyde	123637	45.48	RREL	2.42	EFDB	0.044	EFDB	97.56	EFDB	3.2	BCFWIN	0.0000171	PHYS			132.16	PHYS
Paraquat dichloride	1910425	45.42	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	3.2	BCFWIN	3.22E-13	HENRY WIN			257.16	PHYS

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Parathion	56382	98.36	RREL	8.93	EFDB	0	EFDB	91.06	EFDB	480	CHMF	2.98E-07	PHYS			291.26	PHYS
p-Chlorophenyl isocyanate	104121	98.53	RREL	1.18	EFDB	0.28	EFDB	98.54	EFDB	170	Lyman, 5-2	0.000172	PHYS			153.57	PHYS
Pebulate	1114712	98.37	RREL	8.91	EFDB	0.4	EFDB	90.69	EFDB	480	Lyman, 5-2	0.000237	PHYS			203.35	PHYS
Pendimethalin	40487421	98.82	RREL	47.3	EFDB	0.081	EFDB	52.62	EFDB	1944	EPA, 99	8.56E-07	PHYS			281.31	PHYS
Pentachlorobenzene	608935	83.63	EPI	95.097	EPI	4.0894	EPI	0.801148	EPI	7500	CHMF	0.000703	PHYS			250.34	PHYS
Pentachloroethane	76017	57.89	RREL	9.85	EFDB	57.59	EFDB	32.56	EFDB	67	CHMF	0.00194	PHYS			202.3	PHYS
Pentachlorophenol	87865	96.2	RREL	56.27	EFDB	0	EFDB	43.73	EFDB	110	CHMF	2.45E-08	PHYS	0.001	NPDWS	266.34	PHYS
Pentobarbital sodium	57330	46.83	RREL	3.14	EFDB	0	EFDB	96.88	EFDB	23	Lyman, 5-2	8.44E-13	HENRY WIN			248.26	Merck
Perchloromethyl mercaptan	594423	88.26	RREL	7.49	EFDB	2.13	EFDB	90.38	EFDB	260	Lyman, 5-2	0.000241	PHYS			185.89	PHYS
Permethrin	52645531	99.92	RREL	38.07	EFDB	0	EFDB	61.93	EFDB	51000	Lyman, 5-2	1.87E-06	PHYS			391.3	PHYS
Peroxyacetic acid	79210	92.06	RREL	0.36	EFDB	0.022	EFDB	99.62	EFDB	3.2	BCFWIN	2.14E-06	PHYS			76.05	PHYS
Phenanthrene	85018	94.11	RREL	33.95	EFDB	0.18	EFDB	65.87	EFDB	2160	CHMF	0.0000423	PHYS			178.24	PHYS
Phenol	108952	92.15	RREL	0.42	EFDB	0	EFDB	99.58	EFDB	45	CHMF	3.33E-07	PHYS			94.11	PHYS
Phenolphthalein	77098									130	Lyman, 5-2	8.98E-16	EPI			318.33	Reaxys
Phenothrin	26002802	99.93	RREL	38.25	EFDB	0	EFDB	61.76	EFDB	8400	Lyman, 5-3	0.0000068	PHYS			350.46	PHYS
1,2-Phenylenediamine dihydrochloride	615281	45.44	RREL	2.4	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	6.73E-10	HENRY WIN			108.14	AOPWIN
1,4-Phenylenediamine dihydrochloride	624180	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	6.73E-10	HENRY WIN			108.14	AOPWIN
1,2-Phenylenediamine	95545	45.44	RREL	2.4	EFDB	0	EFDB	97.6	EFDB	1.6	Lyman, 5-3	7.2E-09	PHYS			108.14	PHYS
1,3-Phenylenediamine	108452	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	1.25E-09	PHYS			108.14	PHYS

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p-Phenylenediamine	106503	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	1.6	Lyman, 5-3	6.73E-10	PHYS			108.14	PHYS
2-Phenylphenol	90437	94.89	RREL	2.76	EFDB	0.011	EFDB	97.22	EFDB	130	Lyman, 5-2	1.05E-06	PHYS			170.21	PHYS
Phenytoin	57410	48.63	RREL	4.05	EFDB	0	EFDB	95.95	EFDB	44	Lyman, 5-2	1.02E-11	PHYS			252.28	PHYS
Phosgene	75445	100	RREL	0	EFDB	0	EFDB	100	EFDB		Fast Hyd	0.00892	PHYS			98.92	PHYS
Phosphine	7803512	1.85	EPI	95.14	EPI	0	EPI	4.86	EPI		Gas	0.0244	PHYS			34	PHYS
Phosphorus (yellow or white)	7723140	59.8	RREL	100	Assump.	0	Assump.	0	Assump.	3.2	BCFWIN	0.0244	PHYS			34	PHYS
Phthalic anhydride	85449	99.3	RREL	0.081	EFDB	0	EFDB	99.91	EFDB		Fast Hyd	1.63E-08	PHYS			148.12	PHYS
Picloram	1918021	9.6	RREL	17.81	EFDB	0	EFDB	82.19	EFDB	20	Lyman, 5-3	5.33E-14	PHYS	0.5	NPDWS	241.46	PHYS
Picric acid	88891	22.17	RREL	6.86	EFDB	0	EFDB	93.14	EFDB	1	CHMF	1.7E-11	PHYS			229.11	PHYS
Piperonyl butoxide	51036	97.02	RREL	40.57	EFDB	0	EFDB	59.43	EFDB	2400	Lyman, 5-2	8.89E-11	PHYS			338.45	PHYS
Pirimiphos methyl	29232937	97.02	RREL	19.94	EFDB	0	EFDB	80.05	EFDB	920	Lyman, 5-2	7.01E-07	PHYS			305.34	PHYS
p-Nitroaniline	100016	45.7	RREL	2.54	EFDB	0	EFDB	97.46	EFDB	6.7	CHMF	1.26E-09	PHYS			138.13	PHYS
Polybrominated biphenyls (PBBs)	N575	94.03	EPI; hex	99.18	EPI; hex	0	EPI; hex	0.83	EPI; hex	18200	CHMF; hex	4.29E-06	PHYS; hex			627.59	PHYS; hex
Polychlorinated alkanes	N583																
Polychlorinated biphenyls (PCBs)	1336363	98.93	RREL	62.08	EFDB	0.03	EFDB	37.9	EFDB	47000	EPA/ OPPT, 98; est	0.000415	PHYS	0.0005	NPDWS	291.99	PHYS
Polycyclic aromatic compounds	N590	92.64	EPI; B(a)p	99.16	EPI; B(a)p	0	EPI; B(a)p	0.83	EPI; B(a)p	912	EPA, 99; B(a)p	4.57E-07	PHYS; B(a)p	0.0002	NPDWS; B(a)p	252.32	PHYS; B(a)p
Potassium bromate	7758012	1.85	EPI	94.59	EPI	0	EPI	4.86	EPI	3.2	BCFWIN					167	PHYS
Potassium dimethyldithiocarbamate	128030	76.61	RREL	0.8	EFDB	6.59	EFDB	92.61	EFDB	3.9	BCFWIN	0.000684	HENRY WIN			149.27	AOPWIN

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Potassium N-methyldithiocarbamate	137417	75.91	RREL	0.8	EFDB	3.5	EFDB	95.69	EFDB	3.2	BCFWIN	0.000177	HENRY WIN			107.19	AOPWIN
Profenofos	41198087	99.13	RREL	28.99	EFDB	0	EFDB	71.01	EFDB	2100	Lyman, 5-2	2.21E-08	PHYS			373.64	PHYS
Prometryn	7287196	44.31	RREL	24.49	EFDB	0	EFDB	75.51	EFDB	270	Lyman, 5-2	1.32E-08	PHYS			241.36	PHYS
Pronamide	23950585	70.37	RREL	14.15	EFDB	0.16	EFDB	85.69	EFDB	240	Lyman, 5-2	9.77E-09	PHYS			256.13	PHYS
Propachlor	1918167	76.46	RREL	1.29	EFDB	0.84	EFDB	97.86	EFDB	27	Lyman, 5-2	9.15E-08	PHYS			211.69	PHYS
Propane sultone	1120714	70.61	RREL	0.93	EFDB	0.071	EFDB	99.01	EFDB	3.2	BCFWIN	2.36E-06	PHYS			122.14	PHYS
Propanil	709988	56.46	RREL	7.76	EFDB	0.018	EFDB	92.24	EFDB	1.6	CHMF	1.71E-08	PHYS			218.08	PHYS
Propargite	2312358	99.95	RREL	41.99	EFDB	44.12	EFDB	13.88	EFDB	3700	Lyman, 5-2	4.15E-08	PHYS			350.48	PHYS
Propargyl alcohol	107197	92.06	RREL	0.36	EFDB	0.011	EFDB	99.63	EFDB	3.2	BCFWIN	1.15E-06	PHYS			56.06	PHYS
Propetamphos	31218834	77.51	RREL	1.83	EFDB	0	EFDB	98.17	EFDB	470	Lyman, 5-2	4.81E-08	PHYS			281.31	PHYS
Propiconazole	60207901	68.04	RREL	13.07	EFDB	0	EFDB	86.95	EFDB	400	Lyman, 5-2	4.12E-09	PHYS			342.23	PHYS
beta-Propiolactone	57578	95.91	RREL	0.22	EFDB	0	EFDB	99.77	EFDB	3.2	BCFWIN	0.0000128	PHYS			72.06	PHYS
Propionaldehyde	123386	92.15	RREL	0.37	EFDB	0.66	EFDB	98.97	EFDB	3.2	BCFWIN	0.0000734	PHYS			58.08	PHYS
Propoxur	114261	92.17	RREL	0.43	EFDB	0	EFDB	99.56	EFDB	8.4	CHMF	1.43E-09	PHYS			209.25	PHYS
Propylene (Propene)	115071	98.91	RREL	0.38	EFDB	90.83	EFDB	8.8	EFDB	13	CHMF	0.196	PHYS			42.08	PHYS
2,4-D, propylene glycol butylether ester	1320189	99.55	RREL	14.82	EFDB	0	EFDB	85.18	EFDB	1200	Lyman, 5-2	2.18E-08	HENRY WIN			349.21	AOPWIN
Propylene oxide	75569	92.16	RREL	0.36	EFDB	0.88	EFDB	98.76	EFDB	3.2	BCFWIN	0.0000696	PHYS			58.08	PHYS
Propyleneimine	75558	75.16	RREL	0.82	EFDB	0.35	EFDB	98.83	EFDB	3.2	BCFWIN	8.42E-06	PHYS			57.1	PHYS
Pyridine	110861	92.09	RREL	0.37	EFDB	0.11	EFDB	99.51	EFDB	3.2	BCFWIN	0.000011	PHYS			79.1	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Quinoline	91225	75.94	RREL	1.17	EFDB	0.066	EFDB	98.76	EFDB	8	CHMF	1.67E-06	PHYS			129.16	PHYS
Quinone	106514	51.81	RREL	1.91	EFDB	21.25	EFDB	76.84	EFDB	3.2	Lyman, 5-3	0.000479	PHYS			108.1	PHYS
Quintozene	82688	89.86	RREL	48.35	EFDB	0.52	EFDB	51.14	EFDB	912	CHMF	0.0000442	PHYS			295.34	PHYS
Quizalofop-ethyl	76578148	97.55	RREL	21.59	EFDB	0	EFDB	78.41	EFDB	1100	Lyman, 5-2	1.06E-08	PHYS			372.81	PHYS
Resmethrin	10453868	99.99	RREL	21.82	EFDB	0	EFDB	78.18	EFDB	3900	Lyman, 5-3	1.33E-07	PHYS			338.45	PHYS
Saccharin (manufacturing)	81072	75.13	RREL	0.85	EFDB	0	EFDB	99.15	EFDB	2.9	CHMF	1.23E-09	PHYS			183.19	PHYS
Safrole	94597	66.53	RREL	12.28	EFDB	0.3	EFDB	87.42	EFDB	250	Lyman, 5-2	9.07E-06	PHYS			162.19	PHYS
Selenium and selenium compounds	7782492	43.66	RREL	100	Assump.	0	Assump.	0	Assump.	4.8	EPA, 97	0.00974	PHYS	0.05	NPDWS	78.96	PHYS
Sethoxydim	74051802	83.98	RREL	22.43	EFDB	0	EFDB	77.57	EFDB	1300	Lyman, 5-2	2.16E-11	PHYS			327.49	PHYS
Silver and silver compounds	7440224	66.47	RREL	100	Assump.	0	Assump.	0	Assump.	0.5	EPA, 97					107.87	PHYS
Simazine	122349	23.35	RREL	8.44	EFDB	0	EFDB	91.56	EFDB	27	Lyman, 5-2	9.42E-10	PHYS	0.004	NPDWS	201.66	PHYS
Sodium azide	26628228	1.85	EPI	95.14	EPI	0	EPI	4.86	EPI	1.5	Lyman, 5-3					65.01	AOPWIN
Sodium dicamba	1982690	47.23	RREL	3.35	EFDB	0	EFDB	96.65	EFDB	28	Lyman, 5-2	7.55E-09	HL			243.02	AOPWIN
Sodium dimethyldithiocarbamate	128041	76.61	RREL	0.8	EFDB	6.59	EFDB	92.61	EFDB	3.2	BCFWIN	0.000388	HL			143.21	PHYS
Sodium fluoroacetate	62748	75.08	RREL	0.83	EFDB	0.027	EFDB	99.15	EFDB	3.2	BCFWIN	1.09E-06	HL			100.03	PHYS
Sodium nitrite	7632000	1.85	EPI	94.59	EPI	0	EPI	4.86	EPI	3.2	BCFWIN					69	AOPWIN
Sodium o-phenylphenoxide	132274	95.02	RREL	2.74	EFDB	1.86	EFDB	95.39	EFDB	48	BCFWIN	0.000428	HL			192.19	PHYS
Sodium pentachlorophenate	131522	96.2	RREL	56.27	EFDB	0	EFDB	43.73	EFDB	21	Lyman, 5-2	3.1E-17	PHYS			288.32	PHYS
2,4-D sodium salt	2702729	93.8	RREL	1.71	EFDB	0	EFDB	98.29	EFDB	3.2	BCFWIN	1.96E-10	HL			243.02	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
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Strychnine and salts	N746	2.19	EPI; str	95.43	EPI; str	0	EPI; str	4.11	EPI; str		Ion; str	7.56E-14	PHYS; str			334.42	PHYS; str
Styrene	100425	94.89	RREL	2.12	EFDB	8.27	EFDB	89.61	EFDB	13	CHMF	0.00275	PHYS	0.1	NPDWS	104.15	PHYS
Styrene oxide	96093	75.49	RREL	0.95	EFDB	0.38	EFDB	98.66	EFDB	9.9	CHMF	0.0000158	PHYS			120.15	PHYS
Sulfuric acid	7664939	100	Assump; neu	0	Assump; neu	0	Assump; neu	100	Assump; neu	3.2	BCFWIN	7.65E-12	PHYS			98.08	PHYS
Sulfuryl fluoride (Vikane)	2699798	1.86	EPI	94.62	EPI	0	EPI	4.84	EPI	15	Lyman, 5-3	0.000974	PHYS			102.06	PHYS
Sulprofos	35400432	99.84	RREL	36.37	EFDB	0	EFDB	63.62	EFDB	8600	Lyman, 5-2	1.64E-06	PHYS			322.45	PHYS
Tebuthiuron	34014181	22.53	RREL	7.37	EFDB	0	EFDB	92.63	EFDB	14	Lyman, 5-2	1.2E-10	PHYS			228.32	PHYS
Temephos	3383968	99.9	RREL	37.61	EFDB	0	EFDB	62.39	EFDB	20000	Lyman, 5-2	1.96E-09	PHYS			466.47	PHYS
Terbacil	5902512	46.3	RREL	2.85	EFDB	0	EFDB	97.15	EFDB	16	Lyman, 5-2	1.2E-10	PHYS			216.67	PHYS
Tetrabromobisphenol A (TBBPA)	79947									10580	BCFWIN					543.88	PHYS
1,1,2,2-Tetrachloro-1-fluoroethane (HCFC-121)	354143	61.83	RREL	4.33	EFDB	74.58	EFDB	21.11	EFDB	79	Lyman, 5-2	0.003	HENRY WIN			185.84	PHYS
1,1,1,2-Tetrachloro-2-fluoroethane (HCFC-121a)	354110	61.83	RREL	4.33	EFDB	74.58	EFDB	21.11	EFDB	79	Lyman, 5-2	0.003	HENRY WIN			185.84	PHYS
1,1,1,2-Tetrachloroethane	630206	58.8	RREL	5.77	EFDB	68.76	EFDB	25.48	EFDB	99	Lyman, 5-2	0.00242	PHYS			167.85	PHYS
1,1,2,2-Tetrachloroethane	79345	33.23	RREL	6.38	EFDB	34.85	EFDB	58.8	EFDB	8	CHMF	0.000367	PHYS			167.85	PHYS
Tetrachloroethylene (Perchloroethylene)	127184	88.85	RREL	6.99	EFDB	85.41	EFDB	7.6	EFDB	23	CHMF	0.0177	PHYS	0.005	NPDWS	165.83	PHYS
Tetrachlorvinphos	961115	88.9	RREL	8.29	EFDB	0	EFDB	91.71	EFDB	280	CHMF	1.84E-09	PHYS			365.97	PHYS
Tetracycline hydrochloride	64755	45.42	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	3.2	BCFWIN	1.26E-31	HENRY WIN			444.43	Merck
Tetrafluoroethylene	116143									6.3	Lyman, 5-2	0.828	ACD			100.02	Reaxys
Tetramethrin	7696120	99.49	RREL	21.85	EFDB	0	EFDB	78.15	EFDB	2300	Lyman, 5-2	8.34E-09	PHYS			331.42	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013

		POTW Partition Rates														
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Tetranitromethane	509148									13	Lyman, 5-3	0.00024	ACD			196.03	Reaxys
Thallium and thallium compounds	7440280	53.55	RREL	100	Assump.	0	Assump.	0	Assump.	116	EPA, 97			0.002	NPDWS	205.38	PHYS
Thiabendazole	148798	48.63	RREL	4.05	EFDB	0	EFDB	95.95	EFDB	44	Lyman, 5-2	2.12E-11	PHYS			201.25	PHYS
Thioacetamide	62555	45.56	RREL	2.37	EFDB	0.48	EFDB	97.15	EFDB	3.2	BCFWIN	6.44E-06	PHYS			75.13	PHYS
Thiobencarb	28249776	64.92	RREL	11.6	EFDB	0.015	EFDB	88.4	EFDB	230	Lyman, 5-2	2.67E-07	PHYS			257.78	PHYS
4,4'-Thiodianiline	139651	47.11	RREL	3.27	EFDB	0	EFDB	96.73	EFDB	27	Lyman, 5-2	3.92E-12	PHYS			216.31	PHYS
Thiodicarb	59669260	75.47	RREL	0.98	EFDB	0	EFDB	99.02	EFDB	12	Lyman, 5-2	9.33E-07	PHYS			354.47	PHYS
Thiophanate ethyl	23564069	87.35	RREL	7.12	EFDB	0	EFDB	92.89	EFDB	22	Lyman, 5-2	5.18E-13	HENRY WIN			370.45	PHYS
Thiophanate-methyl	23564058	75.27	RREL	0.9	EFDB	0	EFDB	99.1	EFDB	6.8	Lyman, 5-2	2.94E-13	PHYS			342.4	PHYS
Thiosemicarbazide	79196	45.42	RREL	2.38	EFDB	0	EFDB	97.62	EFDB	3.4	Lyman, 5-3	6.6E-10	PHYS			91.14	PHYS
Thiourea	62566	75.06	RREL	0.83	EFDB	0	EFDB	99.17	EFDB	3.2	BCFWIN	1.98E-09	PHYS			76.12	PHYS
Thiram	137268	75.47	RREL	0.98	EFDB	0.013	EFDB	99.01	EFDB	100	CHMF	1.82E-07	PHYS			240.43	PHYS
Thorium dioxide	1314201	90	Assump.; Th02	100	Assump.; Th02	0	Assump.; Th02	0	Assump.; Th02	10	BCFWIN					264.05	Merck
Titanium tetrachloride	7550450	1.96	EPI	95.41	EPI	0	EPI	4.59	EPI	2.7	BCFWIN					189.73	Merck
Toluene	108883	94.96	RREL	1.43	EFDB	18.26	EFDB	80.32	EFDB	7.4	CHMF	0.00664	PHYS	1	NPDWS	92.14	PHYS
Toluenediisocyanate	26471625	99.48	RREL	2.03	EFDB	0.01	EFDB	97.96	EFDB		Fast Hyd	0.0000111	PHYS			174.16	PHYS
Toluene-2,4-diisocyanate	584849	99.48	RREL	2.03	EFDB	0.01	EFDB	97.96	EFDB		Fast Hyd	0.0000111	PHYS			174.16	PHYS
Toluene-2,6-diisocyanate	91087	99.48	RREL	2.03	EFDB	0.01	EFDB	97.96	EFDB		Fast Hyd	0.0000111	PHYS			174.16	PHYS
o-Toluidine hydrochloride	636215	45.7	RREL	2.52	EFDB	0.15	EFDB	97.35	EFDB	10	Lyman, 5-2	0.0000021	PHYS			143.62	PHYS

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o-Toluidine	95534	99.92	RREL	0.28	EFDB	93.98	EFDB	5.74	EFDB	5.9	CHMF	1.98E-06	PHYS			107.16	PHYS
Toxaphene	8001352	99.01	RREL	62.32	EFDB	0	EFDB	37.68	EFDB	34050	EPA, 99	0.000006	PHYS	0.003	NPDWS	448.26	PHYS
trans-1,3-Dichloropropene	10061026	78.51	RREL	1.07	EFDB	11.91	EFDB	87.02	EFDB	21	Lyman, 5-2	0.000871	PHYS			110.97	PHYS
trans-1,4-Dichloro-2-butene	110576	79.81	RREL	1.94	EFDB	8.72	EFDB	89.34	EFDB	56	Lyman, 5-2	0.000664	PHYS			125	PHYS
Triadimefon	43121433	51.51	RREL	5.46	EFDB	0	EFDB	94.54	EFDB	75	Lyman, 5-2	8.11E-11	PHYS			293.76	PHYS
Triallate	2303175	95.45	RREL	36.61	EFDB	0.13	EFDB	63.28	EFDB	1800	Lyman, 5-2	0.0000193	PHYS			304.67	PHYS
Triaziquone	68768	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	9.25E-16	PHYS			231.26	PHYS
Tribenuron methyl	101200480	77.72	RREL	1.92	EFDB	0	EFDB	98.08	EFDB	68	Lyman, 5-3	1.02E-13	PHYS			395.4	PHYS
Tributyltin fluoride	1983104	50.15	EPI	99.02	EPI	0.04	EPI	0.96	EPI	1200	BCFWIN	0.83	PHYS			309.04	PHYS
Tributyltin methacrylate	2155706	37.65	EPI	96.28	EPI	2.74	EPI	0.98	EPI	770	BCFWIN	0.048	HENRY WIN			375.14	AOPWIN
S,S,S-tributyltrithiophosphate	78488	99.88	RREL	37.22	EFDB	0	EFDB	62.79	EFDB	13000	Lyman, 5-2	2.94E-07	PHYS			314.51	PHYS
Trichlorfon	52686	92.07	RREL	0.37	EFDB	0	EFDB	99.63	EFDB	3.2	BCFWIN	1.7E-11	PHYS			257.44	PHYS
Trichloroacetyl chloride	76028										Fast Hyd	0.0000291	PHYS			181.83	PHYS
1,2,4-Trichlorobenzene	120821	86.46	RREL	22.2	EFDB	9.6	EFDB	68.22	EFDB	720	CHMF	0.00142	PHYS	0.07	NPDWS	181.45	PHYS
1,1,1-Trichloroethane	71556	87.75	RREL	1.38	EFDB	93.82	EFDB	4.8	EFDB	8.9	CHMF	0.0172	PHYS	0.2	NPDWS	133.41	PHYS
1,1,2-Trichloroethane	79005	39.79	RREL	3.59	EFDB	54.49	EFDB	41.92	EFDB	10	CHMF	0.000824	PHYS	0.005	NPDWS	133.41	PHYS
Trichloroethylene	79016	80.97	RREL	1.52	EFDB	90.97	EFDB	7.51	EFDB	17	CHMF	0.00985	PHYS	0.005	NPDWS	131.39	PHYS
2,4,5-Trichlorophenol	95954	75.39	RREL	16.79	EFDB	0.093	EFDB	83.1	EFDB	1910	CHMF	1.62E-06	PHYS			197.45	PHYS
2,4,6-Trichlorophenol	88062	91.33	RREL	10.51	EFDB	0.077	EFDB	89.41	EFDB	309	CHMF	0.0000026	PHYS			197.45	PHYS

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		POTW Partition Rates														
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1,2,3-Trichloropropane	96184	52.08	RREL	3	EFDB	15.67	EFDB	81.36	EFDB	31	Lyman, 5-2	0.000343	PHYS			147.43	PHYS
Triclopyr triethylammonium salt	57213691	75.32	RREL	0.93	EFDB	0	EFDB	99.07	EFDB	8.1	Lyman, 5-2	7.23E-15	HENRY WIN			355.67	AOPWIN
Triethylamine	121448	48.22	RREL	2.34	EFDB	8.71	EFDB	88.95	EFDB	7.4	Lyman, 5-2	0.000149	PHYS			101.19	PHYS
Trifluralin	1582098	97.4	RREL	58.45	EFDB	0.031	EFDB	41.51	EFDB	5674	EPA, 99	0.000103	PHYS			335.29	PHYS
Triforine	26644462	75.94	RREL	1.17	EFDB	0	EFDB	98.83	EFDB	28	Lyman, 5-2	3.82E-09	PHYS			434.97	PHYS
1,2,4-Trimethylbenzene	95636	94.11	RREL	11.47	EFDB	16.52	EFDB	72	EFDB	340	Lyman, 5-2	0.00616	PHYS			120.2	PHYS
2,3,5-trimethylphenyl methylcarbamate	2655154	77.78	RREL	1.94	EFDB	0.026	EFDB	98.03	EFDB	52	Lyman, 5-2	4.32E-08	HENRY WIN			193.25	AOPWIN
Triphenyltin chloride	639587	39.49	EPI	98.76	EPI	0.23	EPI	0.99	EPI	900	Lyman, 5-2	0.0000623	PHYS			385.46	PHYS
Triphenyltin hydroxide	76879	13.73	EPI	98.62	EPI	0	EPI	1.38	EPI	280	Lyman, 5-2	4.26E-07	PHYS			367.02	PHYS
Tris(2,3-dibromopropyl)-phosphate	126727	99.5	RREL	14.38	EFDB	0.04	EFDB	85.58	EFDB	2.8	CHMF	0.0000218	PHYS			697.62	PHYS
Trypan blue	72571	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	1E-24	HL			960.82	PHYS
Urethane (Ethyl carbamate)	51796	45.43	RREL	2.38	EFDB	0	EFDB	97.6	EFDB	3.2	BCFWIN	6.43E-08	PHYS			89.1	PHYS
Vanadium and vanadium compounds	7440622	31.81	RREL	100	Assump.	0	Assump.	0	Assump.	3.2	BCFWIN; el					50.94	EPI; el
Vinclozolin	50471448	67.65	RREL	5.84	EFDB	0	EFDB	94.16	EFDB	130	Lyman, 5-2	1.74E-08	PHYS			286.12	PHYS
Vinyl acetate	108054	92.4	RREL	0.37	EFDB	3.07	EFDB	96.56	EFDB	2.3	Lyman, 5-3	0.000511	PHYS			86.09	PHYS
Vinyl bromide	593602	94.65	RREL	0.22	EFDB	27.87	EFDB	71.91	EFDB	9.2	CHMF	0.0256	PHYS			106.95	PHYS
Vinyl chloride	75014	92.41	RREL	0.5	EFDB	91	EFDB	8.51	EFDB	10	CHMF	0.0278	PHYS	0.002	NPDWS	62.5	PHYS
Vinyl Fluoride	75025									10	Lyman, 5-2	0.118	ACD			46.044	Reaxys
Vinylidene chloride (1,1-dichloroethylene)	75354	92.02	RREL	0.75	EFDB	90.06	EFDB	9.19	EFDB	24	CHMF	0.0261	PHYS	0.007	NPDWS	96.94	PHYS

Table B-7. Physicochemical Properties for TRI Chemicals and Chemical Categories, in Alphabetical Order DATE: July 2013																	
		POTW Partition Rates															
Chemical Name	CAS Number	Total Removal	Total Removal Ref.	Part. to Sludge	Part. to Sludge Ref.	Part. to Volat.	Part. to Volat. Ref.	Part. to Biodeg.	Part. to Biodeg. Ref.	BCF	BCF Ref.	Henry's Law	Henry's Law Ref.	MCL	MCL Ref.	Mol. Weight	Mol. Weight Ref.
Warfarin and salts	N874	3.41	EPI; wrf	97.07	EPI; wrf	0	EPI; wrf	3.23	EPI; wrf	56	Lyman, 5-2; wrf	2.77E-09	PHYS; wrf			308.34	PHYS; wrf
Xylene (mixed isomers)	1330207	96.07	RREL	3.03	EFDB	14.03	EFDB	82.94	EFDB	150	Lyman, 5-2	0.00663	PHYS	10	NPDWS	106.17	PHYS
m-Xylene	108383	96.25	RREL	3.25	EFDB	14.38	EFDB	82.38	EFDB	13	CHMF	0.00718	PHYS			106.17	PHYS
o-Xylene	95476	95.78	RREL	2.84	EFDB	12.01	EFDB	85.16	EFDB	11	CHMF	0.00518	PHYS			106.17	PHYS
p-Xylene	106423	96.12	RREL	2.98	EFDB	15.57	EFDB	81.45	EFDB	19	CHMF	0.0069	PHYS			106.17	PHYS
2,6-Xylidine	87627	47.12	RREL	3.25	EFDB	0.17	EFDB	96.58	EFDB	15	Lyman, 5-2	2.52E-06	PHYS			121.18	PHYS
Zinc and zinc compounds	7440666	66.15	RREL	100	Assump.	0	Assump.	0	Assump.	47	EPA, 97	0.0245	PHYS			65.37	PHYS
Zineb	12122677	97.61	RREL	0.13	EFDB	0	EFDB	99.87	EFDB	5.7	Lyman, 5-2	2.72E-09	PHYS			275.73	PHYS

* When chlorine dioxide dissolves in water, it rapidly reacts to form chlorate, chlorite, and chloride ions. The IRIS oral toxicity data for chlorine dioxide is largely based on the toxicity of sodium chlorite. The water decay term for chlorine dioxide used in the RSEI model reflects rapid hydrolysis to sodium chlorite, which is toxic and does not decay rapidly in water.

Table B-8. Physicochemical Property Reference Notes For Tables B-6 and B-7 DATE: July 2013	
Reference Code	Source Description
ACD	ACD Labs, as listed in ChemSpider online database, www.chemspider.com, accessed December 2013.
AOPWIN	Atmospheric Oxidation Program, Syracuse Research Corp., v. 1.88. 1994-1998. Syracuse, NY.
AOPWIN; ave	AOPWIN provided calculations for two isomers; an arithmetic average of the two was used.
AOPWIN; exp	Experimental data (instead of estimated data) in AOPWIN used.
AOPWIN; isom.	Molecular weight of an isomer from AOPWIN used.
Assump.	For Incinerator DRE value, assumed the typical municipal waste combustor destruction/removal efficiency for organics is 99 percent. For the POTW Partition (Sludge) value, assumed that all metals and metal compounds partition 100 percent to sludge.
Assump.; hydr	Assumed that all hydrazine biodegrades.
Assump.; neu	Assumed strong acids are completely neutralized by POTW. Neutralization assigned to biodegradation category rather than sorption to sludge or volatilization categories because neutralization and biodegradation are both chemical transformation processes.
Assump.; Th02	Based on physical properties and standard EPA assumptions regarding inorganic chemicals, assumed that POTW removal rate for thorium dioxide is 90%, and that it partitions completely to sludge.
Assump.; TiCl4	Titanium tetrachloride reacts rapidly with water, including moisture in the air, to form hydrochloric acid and other titanium compounds (ATSDR FAQs). To estimate a decay constant for both water and air, it was assumed that 99% of titanium tetrachloride reacted within 1 minute, according to first-order kinetics.
B(a)p	Benzo(a)pyrene used as surrogate for polycyclic aromatic compounds for physicochemical properties.
BCFWIN	Bioconcentration Factor Estimation Program, Syracuse Research Corp., v. 3.02. 1994-1998. Syracuse, NY.
BCFWIN eq.	Used Kow from PhysProp with BCFWIN equation to estimate BCF.
Bodek	Bodek, I., W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt. 1988. Environmental Inorganic Chemistry. Pergamon Press. New York. The Kd value for aluminum is based on Langmuir isotherm data.
by law	PCBs and dioxins are assumed to have an Incinerator DRE of 99.9999 percent, as required by TSCA regulation.
Chem Spider	ChemSpider online database. www.chemspider.com. Accessed December 2013.
CHMF	CHEMFATE database, a data source within the Environmental Fate Data Base (EFDB), Syracuse Research Corporation. Downloaded from http://syrres.com/efdb.htm, 2000.
CHMF*	According to CHEMFATE, the compound "Hydrolyzes rapidly in water." Assumed a half-life of 10 minutes to estimate a first-order decay rate.
CHMF; hexa	A BCF value was estimated in CHEMFATE using log Kow, even though the value of log Kow was above the range for Lyman, 5-2. A solubility value was available, but the BCF estimated using that value in Lyman, 5-3 seemed too low, given the log Kow value and the Koc value in ChemFate.
CHMF; octa	A Koc value was estimated in CHEMFATE using a solubility value in Lyman, 4-5. The solubility value was slightly below the range for Lyman, 4-5. This estimated Koc value was then used to estimate a BCF value using Lyman, 5-4. The Koc estimate was accepted, and a BCF value was estimated, because the very high Kow and the very low solubility suggest that soil sorption and bioconcentration are significant processes to capture in the model.
CHMF; photo	Water decay rate estimated based on information on photodegradation in CHEMFATE.

Table B-8. Physicochemical Property Reference Notes For Tables B-6 and B-7 DATE: July 2013	
Reference Code	Source Description
C.I.	Koc and BCF values were estimated based on Lyman, 4-8 and 5-2, even though the log Kow value was above the upper ends of the ranges for these two equations. Given the high log Kow, soil sorption and bioconcentration are significant processes to capture in the model.
CRC	Handbook of Chemistry and Physics. 70th Edition. CRC Press, Inc. Boca Raton, FL.
CRC; est	Handbook of Chemistry and Physics. 70th Edition. CRC Press, Inc. Boca Raton, FL. Estimated from periodic table for C2F4ClH.
CRC; 0 degrees C	Handbook of Chemistry and Physics. 70th Edition. CRC Press, Inc. Boca Raton, FL. Calculated at 0 degrees Celsius.
Cu(CN)2	Copper cyanide used as surrogate for cyanide compounds for all physicochemical properties except those used in air modeling.
EFDB	Environmental Fate Data Base, Syracuse Research Corporation. 1995. Syracuse, NY.
el	Metal compounds are assumed to behave like the elemental metal.
EPA, 88a	U.S. EPA, 1988. Ambient Water Quality Criteria for Aluminum. 1988. EPA 440/5-86-008. August.
EPA, 92	U.S. EPA. 1992. Human Health Risk Assessment for the Use and Disposal of Sewage Sludge: Benefits of Regulation. Ppd by Abt Associates for the U.S. EPA Office of Water.
EPA, 97	U.S. EPA, 1997. Water Quality Benefits Analysis for Proposed Pretreatment Standards for Existing and New Sources for the Industrial Laundries Point Source Category. EPA 821-R-97-009. November.
EPA/OPPT, 98; est	U.S. EPA/OPPT. 1998. Technical Support Document for Determination of Bioaccumulation (BAF) and Bioconcentration (BCF) Values for Persistent Bioaccumulative Toxic (PBT) Chemicals and for Identification of PBT Chemicals. Jerry Smrchek, PhD., Biologist, Existing Chemicals Assessment Branch, Risk Assessment Division. September. Estimated using equation 1 from page 2 of document and logKow from SRC PhysProp.
EPA/OPPT, 98; high	U.S. EPA/OPPT. 1998. Technical Support Document for Determination of Bioaccumulation (BAF) and Bioconcentration (BCF) Values for Persistent Bioaccumulative Toxic (PBT) Chemicals and for Identification of PBT Chemicals. Jerry Smrchek, PhD., Biologist, Existing Chemicals Assessment Branch, Risk Assessment Division. September. High end of the range taken.
EPA/OPPT, 99	U.S. EPA/OPPT. 1999. Memorandum from Jerry Smrchek, PhD., Biologist, Existing Chemicals Assessment Branch, Risk Assessment Division to Dan Bushman, Toxics Release Inventory Branch, Environmental Assistance Division. May 26. Subject: Bioaccumulation/Bioconcentration Assessment for Lead and Lead Compounds.
EPA, 99	U.S. EPA. 1999. Persistent Bioaccumulative Toxic (PBT) Chemicals; Final Rule. Federal Register, Part VII, 40 CFR Part 372, Vol. 64, No. 209, pp.58666-58753, October 29.
EPI	STP Estimation Program, Syracuse Research Corp., v. 1.66. 1994-1998. Syracuse, NY.
Fast Hyd	Hydrolysis is so rapid that Koc and BCF values were not estimated.
Gas	Koc and BCF values were not estimated due to chemical being in gas phase at ambient environmental temperatures.
Gerritse	Gerritse, R.G., R. Vriesema, J.W. Dalenberg, and H.P. De Roos. 1982. Effect of Sewage Sludge on Trace Element Mobility in Soils. J. Environ. Qual. 11(3):359-364. Kd values measured in column studies using sand with an foc of 0.0355, a CEC of 0.22 meq/g, zero clay content, and a solution pH of 5.
HCN	Hydrogen cyanide used as surrogate for cyanide compounds for physicochemical properties used in air modeling.
hex	Hexabromobiphenyl used as surrogate for polybrominated biphenyls for physicochemical properties.
HENRYWIN	Henry's Law Estimation Program, Syracuse Research Corp., v. 3.02. 1994-1998. Syracuse, NY.
HL	EPA estimates based on SRC data. File 'hl.xls.'

Table B-8. Physicochemical Property Reference Notes For Tables B-6 and B-7 DATE: July 2013	
Reference Code	Source Description
Howard	Used mean of values reported in Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan and E.M. Michalenko. 1991. Handbook of Environmental Degradation Rates.Lewis Publishers, Inc. Chelsea, MI.
HYDRO	HYDROWIN, Syracuse Research Corp., 1991-97. Syracuse, NY.
Ion	Koc and/or BCF values were not estimated due to ionization.
Jorg	Jorgensen, S.E. and I. Johnsen. 1981. Principles of Environmental Science and Technology. Elsevier, NY.
KOWWIN	Log Kow Estimation Program, Syracuse Research Corp., v. 3.02. 1994-1998. Syracuse, NY.
KOWWIN; exp	Experimental value for Kow provided in KOWWIN program.
Lyman, 4-5	Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society. Washington, D.C. Eq'n 4-5 used to estimate Koc.
Lyman, 4-8	See above reference; Equation 4-8 used to estimate Koc.
Lyman, 5-2	See above reference; Equation 5-2 used to estimate BCF.
Lyman, 5-3	See above reference; Equation 5-3 used to estimate BCF.
Lyman, 5-4	See above reference; Equation 5-4 used to estimate BCF.
Merck	Budavari, S. (ed.). 1989. The Merck Index. Merck & Co., Inc. Rahway, NJ.
Merck, est.	Molecular weight for asbestos calculated from molecular formula for chrysotile in Merck Index.
Merck; calc	Molecular weight calculated based on information presented in Merck Index.
methyl	Methylmercury used as a surrogate for mercury and mercury compounds for physicochemical properties.
methoxy	2-Methoxyethanol (Ethylene glycol monomethyl ether) used as surrogate for glycol ethers for physicochemical properties.
met	Metiram used as surrogate for EBDCs for physicochemical properties.
NAB	RREL Treatability Database reported greater than 95.9% removal in a bench scale study; EPA conservatively assumed 90% removal and 10% pass-through.
nic	Nicotine used as surrogate for nicotine and salts category for physicochemical properties.
NPDWS	MCLs taken from the National Primary Drinking Water Standards (U.S. EPA, 1994).
NPDWS; fpl	MCL for asbestos is expressed in million fibers/liter; does not affect model results because MCL is not modeled.
NPDWS; TTreq.	No MCL in place; instead, a treatment technique is required.
PCKOC	KOC Estimation Program, Syracuse Research Corp., v. 1.66. 1994-1998. Syracuse, NY.
penta	Pentachlorophenol used as surrogate for chlorophenols for physicochemical properties.
PHYS	PhysProp database, Syracuse Research Corporation. Downloaded from http://esc.syrres.com/interkow/physdemo.htm, 2000.

Table B-8. Physicochemical Property Reference Notes For Tables B-6 and B-7 DATE: July 2013	
Reference Code	Source Description
PRNA	PIRANHA, Pesticide and Industrial Chemical Risk Analysis and Hazard Assessment, Version 2.0. Environmental Research Laboratory, Office of Research and Development, U.S. EPA, 1991.
Reaxys	Reaxys chemical database. Www.reaxys.com. Accessed December 2013.
RREL	RREL Treatability Database, Version 5.0. Risk Reduction Engineering Laboratory. U.S. EPA. Cincinnati, OH.
str	Strychnine used as surrogate for strychnine and salts category for physicochemical properties.
SUM	POTW removal efficiency was obtained by summing the three POTW partition values before scaling them to represent 100 percent of chemical removal by POTW.
wrf	Warfarin used as surrogate for warfarin and salts category for physicochemical properties.
WSKOW	Water Solubility and KOW Estimation Program, Syracuse Research Corp., v. 1.33. 1994-1998. Syracuse, NY.