5 Estimating Physical / Chemical and Environmental Fate Properties with EPI Suite™

5.1 How this Chapter is Organized

This chapter discusses Physical / Chemical and Environmental Fate property estimated by EPI Suite™ and explains the significance of the property, how it is estimated, and how it contributes to risk assessment. In addition, the sample chemical that will be the subject of the SF PMN in chapter 14 (isodecyl acrylate CAS 1330-61-6) will be run in EPI Suite™ (version 4.1), and the results for each property will be interpreted and recorded in the Sustainable Futures Summary Assessment Worksheet. The completed Worksheet for isodecyl acrylate is included in chapter 2.

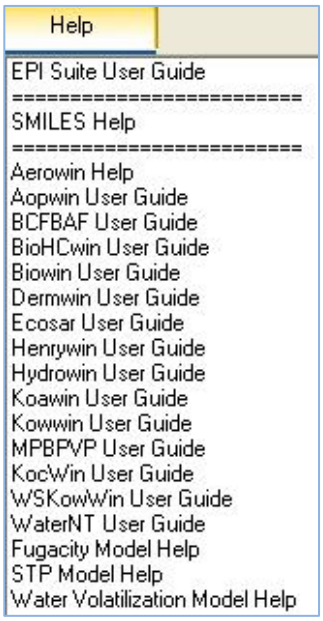
When this manual was written the current version of EPI Suite™ was version 4.1. Please note that a more recent version of EPI Suite™ may be available so check the download page for the current version. EPI Suite™ can be downloaded at no cost from http://www.epa.gov/oppt/exposure/pubs/episuite.htm.

5.2 Introduction to EPI Suite™

5.2.1 What is EPI Suite™?

EPI Suite™ is the EPI (Estimation Programs Interface) Suite™ and is a Windows®-based set of physical / chemical property and environmental fate estimation programs developed by OPPT to screen new chemicals lacking experimental data. The modules within EPI Suite™ version 4.1 are shown in the image below which is the list from the Help screen on the Data Entry (Welcome) Screen. Each module has detailed information on how the predictions are made. A user can enter information once into EPI Suite™ and estimate the following:

- Physical / Chemical properties
  - Melting point
  - Boiling point
  - Vapor Pressure
  - Water Solubility
  - Octanol/water partition coefficient
- Environmental fate properties
  - Henry's Law Constant
  - Soil adsorption coefficient
  - Bioconcentration factor
  - Removal in the Atmosphere
    - Oxidation
    - Photolysis
  - Removal in Soil and Water
    - Hydrolysis
    - Biodegradation
    - Photolysis
    - Chemical decomposition
- Environmental fate models
  - Removal in Wastewater Treatment
  - Multi-media (fugacity) model



It is important to understand that EPI Suite™ is a screening-level tool and should not be used if acceptable measured data are available. Users can enter experimental data into EPI Suite™ to replace conservative default assumptions and improve the estimations of the other properties. All users should use these methods appropriately and interpret results carefully. Click on the Help tab for detailed information on the methods and models contained in EPI Suite™.

An updated version of EPI Suite™ (version 4.1) was released in February of 2011. This new version includes many improvements, including:

- User interface updates
- Integrated structure drawing program
- Structure-searchable data files
- Link to pKa calculation (SPARC)
- Links to additional data sources including environmental fate and aquatic toxicity data
- Enhanced QSARs for many modules, and
- Additional classes for hydrolysis predictions.

5.2.2 How Does EPI Suite™ Work?

The EPI Suite™ interface is linked to the PhysProp Database (maintained by Syracuse Research Corporation) which contains measured data on more than 40,000 chemicals. The chemical structure can be entered using SMILES Notation (see Appendix F), or if the chemical has a CAS Registry Number, the CAS RN may be entered and the structure will be retrieved from the EPI Suite™ built-in database of structures if available. EPI Suite™ also has a name look-up function.

All of the modules can be run using the EPI Suite™ interface, or by running each individual module as a stand-alone program. The advantage of running a module as a stand-alone program is that the user has the ability to change many default parameters that would otherwise not be available through the integrated EPI platform.

The mathematical algorithms and fragment-based formulas in the EPI Suite™ modules will use experimental data if they are available in the PhysProp Database. IMPORTANT: You must click on the PhysProp button to import any measured data that is in that database because available data are not imported automatically. If data are retrieved they are identified as coming from the experimental database, and will be labeled as "(exp. database)" in the results. If the user has any experimental data

for the chemical, that data should be entered into the Data Entry Screen of EPI Suite™. For chemicals that are known liquids with no experimental melting point data, the user should enter 20 deg C as an experimental MP into the input screen for all EPI Suite™ predictions.

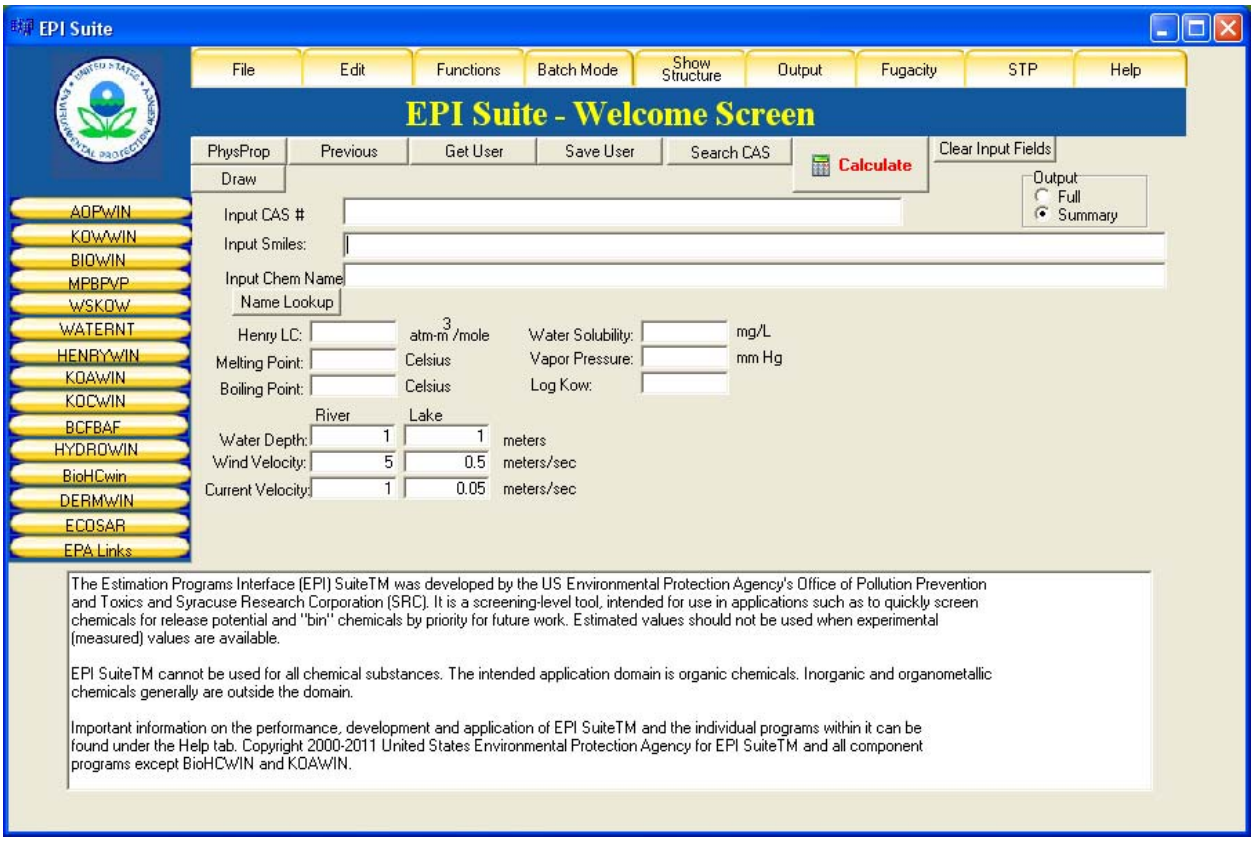
EPI Suite™ can be run in two modes: Summary and Full. The mode can be selected on the Data Entry Screen. When the program is run in "Summary" mode, the user is provided the quantitative or qualitative results for each endpoint with no supplemental information on how the endpoint was predicted. However, in "Full" mode, the user will be given additional information regarding derivation of the prediction including the fragments or equations identified which are relevant to the endpoint, coefficient values, corrections factors, etc. For further explanation on the underlying methods used in EPI Suite™ please refer to the EPI Suite™ web pages at http://www.epa.gov/oppt/exposure/pubs/episuite.htm Interpreting EPI Suite™ Results or Using Available Measured Data to Characterize Chemicals.

5.2.3 Evaluations of and Case Studies using EPI Suite™

EPI Suite™ has undergone detailed review by a panel of EPA's independent Science Advisory Board (SAB) (http://yosemite.epa.gov/sab/sabpeople.nsf/WebCommittees/BOARD), and the September 2007 report can be downloaded from http://www.epa.gov/sab/panels/epi_suite_review_panel.htm.The individual estimation modules have been described in numerous journal articles in peer-reviewed technical journals. The full reference citations are given in the Help files for the individual modules.

5.2.4 Running the Sample Chemical, Isodecyl Acrylate, in EPI Suite™

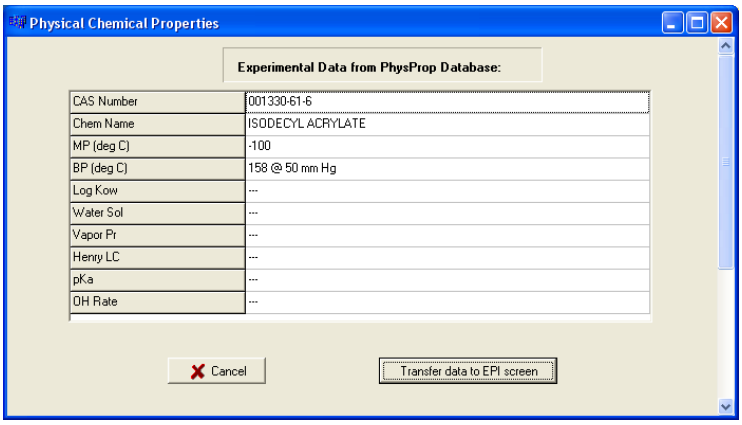
The image below shows the Data Entry Screen (Welcome Screen) for EPI Suite v. 4.1. A chemical can be entered in EPI Suite™ by entering the CAS RN, SMILES, doing a Chemical Name look-up, or clicking on File and importing a ".mol" file (described in chapter 4 of this document). You must click on the PhysProp button to import any measured data that is in that database. The individual modules can be run separately by clicking on the module name on the buttons to the left. The Output mode can be selected by clicking on "Full" or "Summary".



5. Estimating Physical / Chemical and Environmental Fate Properties with EPI Suite™

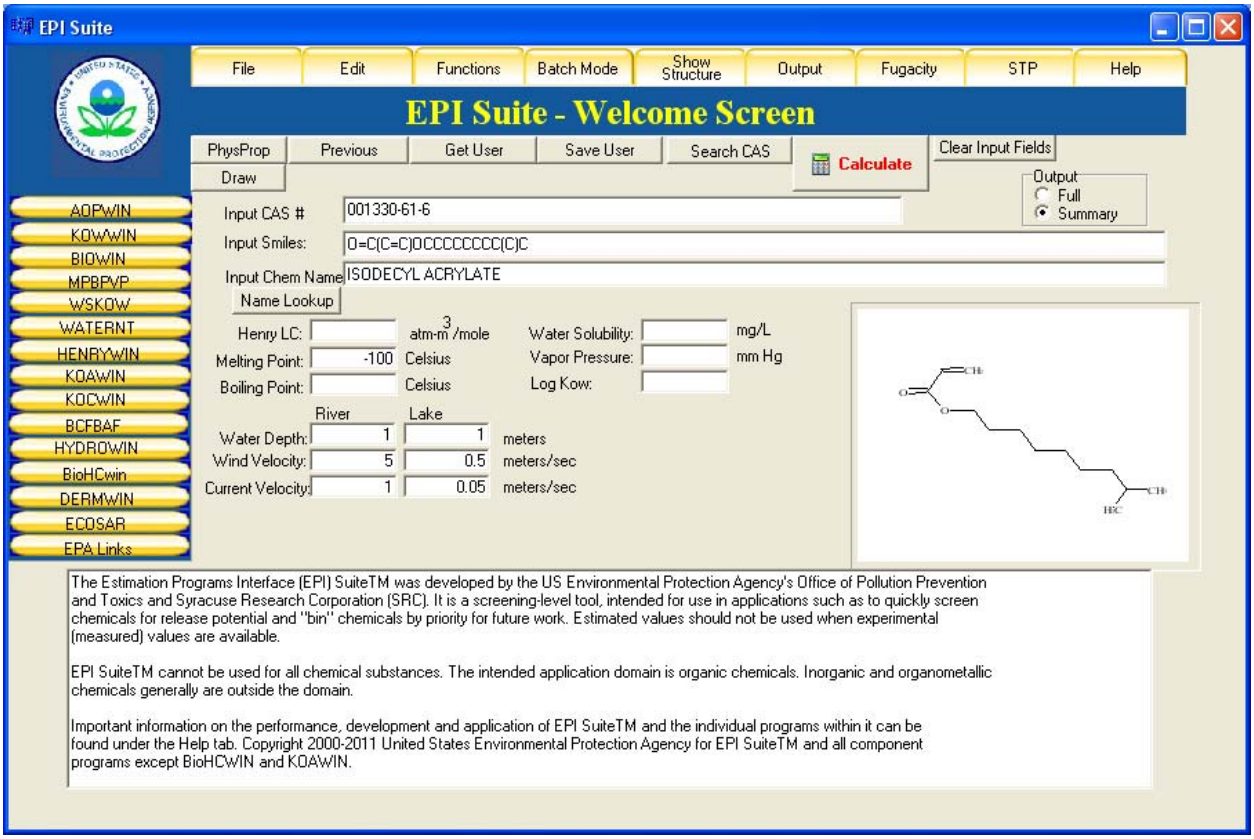
The sample chemical, isodecyl acrylate, is entered into EPI Suite™ by entering the CAS RN 1330-61-6 and clicking on the "Search CAS" button. The structure, SMILES, and name are imported from the accompanying database as shown in the figure at the bottom of this page.

IMPORTANT: You must click on the PhysProp button to import any measured data that is in that database because available data are not imported automatically.



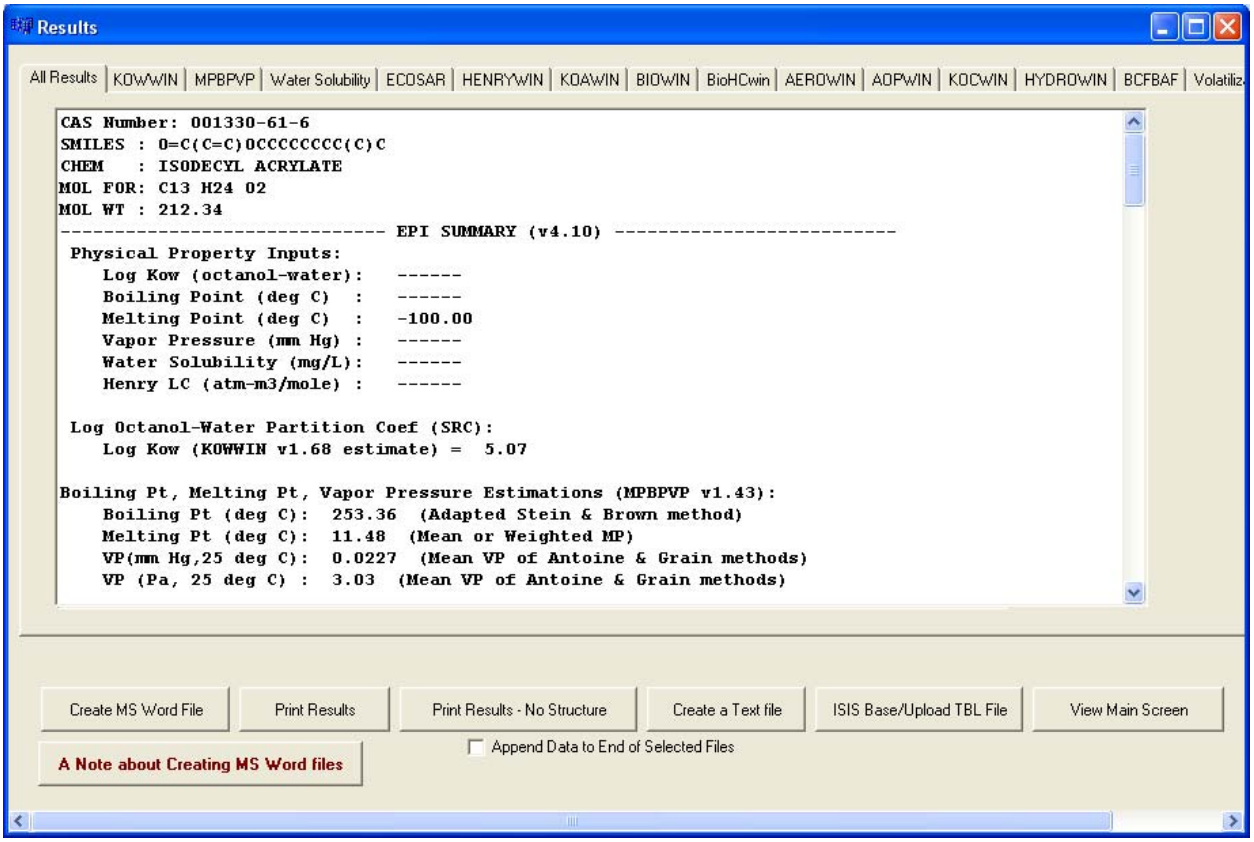
When you click on the PhysProp button you get this screen to the right which shows that a measured MP and BP are available. Click on the Transfer data to EPI screen button to import measured data that will be used in EPI Suite™ modules. In the sample shown here the BP is not imported because the BP is not used in any calculations but will be shown on the results screen.

For this sample we'll run EPI Suite™ in the "Summary" mode, and click on "Calculate" to run all of the modules incorporated into EPI Suite™.



The image below shows the first part of the results. Any experimental data that has been entered by the user or imported from PhysProp is presented under "Physical Property Inputs" at the beginning of the results. The entire results page is more than 2 ½ pages long and is not presented here in its entirety. The results can be printed or saved as an ASCII text file or MS Word file. If you want more information on how each property was estimated click on the tabs with that property and you will be taken to additional information. This "more information" capability is discussed in the Water Solubility section of this chapter.

For this sample chemical exercise we will discuss the relevant properties and include an image of the actual module results for each property, along with an image of the section of the Sustainable Futures Summary Assessment Worksheet where the results should be entered. The reader is encouraged to refer back to the completed full Sustainable Futures Summary Assessment Worksheet for this sample chemical which is included in chapter 2 of this document and in the example SF PMN in chapter 14.



5.3 Physical / Chemical Properties

Physical / Chemical Properties Give Valuable Information
When conducting a risk assessment it is very important to first identify physical / chemical properties of the chemical being evaluated because physical / chemical properties provide information on:

- Physical state,
- Environmental fate,
- Potential routes of exposure for both humans and the environmental, and
- Potential environmental partitioning.

This section presents a discussion on each physical property: what that property is, how it is estimated by EPI Suite™, what it can tell the assessor, and how to properly interpret the results. The reader is walked through running the sample chemical isodecyl acrylate (CAS 1330-61-6) in EPI Suite™, results

will be interpreting using the *Interpretative Assistance Document for Discrete Chemicals*, and then results entered into the Sustainable Futures Summary Assessment.

Not every physical / chemical property estimated by EPI Suite™ is discussed here because not all properties are used in a Sustainable Futures Summary Assessment. The physical / chemical properties discussed here are:

- Melting point (MP)
- Boiling point (BP)
- Vapor Pressure (VP)
- Water Solubility (WSol or WS)
- Octanol/water partition coefficient (Kow or P)

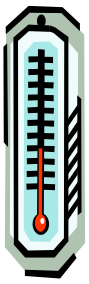
5.3.1 Melting Point (MP), Boiling Point (BP), Vapor Pressure (VP)

MPBPWIN™ is the estimation module in EPI Suite™ that predicts melting point (MP), boiling point (BP) and vapor pressure (VP). These properties can indicate physical state (solid, liquid, gas) and provide information on potential environmental partitioning and fate, as well as potential exposure routes of concern for workers and the general population.

MPBPWIN™ estimates *melting point* by giving a weighted average of the results of two methods: (1) the Joback Method (a group contribution method); and (2) the Gold and Ogle method MP = 0.5839 * BP (in °K). *Boiling point* is estimated using an adaption of the Stein and Brown (1994) method which is also a group contribution method. *Vapor pressure* is estimated use three different methods: (1) Antoine, (2) Modified Grain method, and (3) the Mackay method. For solids the preferred method is the Modified Grain method which will use an experimental MP (if entered) to adjust the vapor pressure from a super-cooled liquid to a solid. For liquids the preferred method is the mean of the Grain method and the Antoine methods. More detailed information on how the estimations are generated is available in the Help screens of the individual modules.

Interpreting Results – Information on Physical State

The estimated MP, BP, and VP indicate the physical state of the chemical to be assessed:



MP < 25 deg C assessed as a liquid
MP > 25 deg C assessed as a solid

BP < 25 deg C assessed as a gas

VP > 10^{-4} exists mostly in the vapor (gas) phase
VP 10^{-5} - 10^{-7} exists in the vapor and particulate phase
VP < 10^{-8} exists mostly in the solid phase

Environmental Partitioning

The chemical's physical state, which can be predicted based melting point, boiling point, and vapor pressure, can give the assessor an indication of to which environmental compartment (s) – air, water / sediment, biota, soil – the chemical will move (partition) once released to the environment. For example:

- Gases are volatilized in the atmosphere.
- Solids may be present in the atmosphere as particulates (dusts).
- Liquids tend to dissolve more rapidly and have higher WS than high melting organic solids.
- High VP means the chemical is more likely to be present in the atmosphere as vapor.

Potential Exposure Information

In a similar manner MP, BP, and VP can indicate potential exposure routes of concern for workers and the general population to the assessor:

- For gases consider the inhalation route.
- For liquids consider dermal contact (a lower MP tends to increase absorption through the skin, digestive tract, and lungs).
- For both liquids and solids consider ingestion as a route.
- For solids potential exposure routes are dermal contact and inhalation of dust.
- For chemicals with a VP < 10^{-6}, there is low concern for inhalation exposure.

MP, BP, VP Results for Sample Chemical

The results for isodecyl acrylate (below) from EPI Suite™ v. 4.10 show that experimental Melting Point and Boiling Point were available in the PhysProp Database. The following values will be entered into the Sustainable Futures Summary Assessment Worksheet We already knew the measured data for isodecyl acrylate (MP and BP) and that it is a liquid (see section 2.G.1) so we expected to get these results. The VP value we will use is 0.0227 mm Hg (indicated above) because this is the more commonly-used unit. The other VP value is in Pascals (Pa) which is used by the International System of Units (SI) and is an older Metric system.

```
Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
    Boiling Pt (deg C):  253.36  (Adapted Stein & Brown method)
    Melting Pt (deg C):  11.48  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  0.0227  (Mean VP of Antoine & Grain methods)
    VP (Pa, 25 deg C) :  3.03  (Mean VP of Antoine & Grain methods)
    MP  (exp database):  -100 deg C
    BP  (exp database):  158 @ 50 mm Hg deg C
```

5.3.2 Water Solubility (WSol or WS)

Water Solubility (abbreviated as WSol or WS) provides information on the degree to which a chemical will dissolve in 1 liter of water. WS indicates to the assessor how the chemical is likely to distribute between environmental compartments (air, soil, or water/sediment). It also indicates the potential for environmental or human exposure through release to aquatic compartment. Chemicals that are not water soluble will not enter the water column and are not likely to be a concern for exposure to humans through ingestion of drinking water.

EPI Suite™ uses two QSAR models to estimate water solubility: WSKOW and WATERNT. WSKOW accepts experimental Log Kow and MP values, and its accuracy greatly improved if an experimental MP is entered. WATERNT is a fragment-based method and like all fragment-based method the accuracy of its estimates is influenced by the relative number of fragments covered by the model – the more fragments covered the more accurate the estimate will be.

Interpreting Results – General Classifications

General classifications based on WS are:

WS (mg/L)	Classification
> 10,000	Very soluble
> 1,000 - 10,000	Soluble
> 100 - 1,000	Moderate solubility
> 0.1 - 100	Slightly soluble
< 0.1	Negligible solubility

Environmental Partitioning

WS gives information on how the chemical will partition between environmental compartments. Chemicals with higher water solubility will partitioning to water, are likely to be removed from soil into ground water by rain run-off, and removed from the atmosphere into ground water by rain washout.

Potential Exposure Information

Generally chemicals with higher WS are more likely to present potential exposure concerns for humans via drinking water ingestion and aquatic biota in surface water. Higher WS means the chemical is more likely to be absorbed through the GI tract and/or lungs. Chemicals with low WS have a higher potential to bioconcentrate in biota.

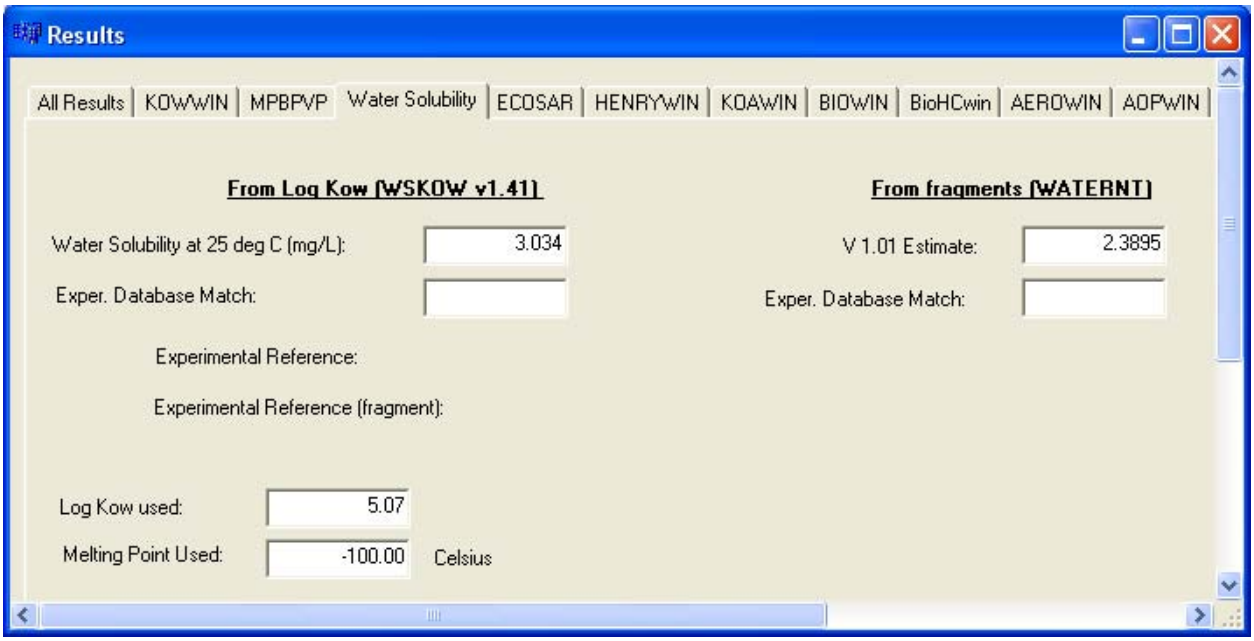
Results for sample chemical

WS results for the sample chemical indicate that both WS QSAR models were run on the chemical and provided slightly different results (see image to the right). We will use the 3.034 mg/L at 25 deg C value which indicates the sample chemical is only slightly soluble in water.

```
Water Solubility Estimate from Log Kow (WSKOW v1.42):
   Water Solubility at 25 deg C (mg/L):  3.034
      log Kow used: 5.07 (estimated)
      melt pt used: -100.00 deg C

Water Sol Estimate from Fragments:
   Wat Sol (v1.01 est) =  2.3895 mg/L
```

If you want more information on how WS was estimated by each of the methods, while you have the results screen open, click on the tab that says Water Solubility and you will get additional information (shown below for the sample chemical).



5.3.3 Octanol / Water Partition Coefficient (log Kow or log P)

Octanol / water partition coefficient (Kow or P) provides information on how the chemical will partition between octanol (which represents the lipids or fats in biota) and water. Kow values for various chemicals range widely and for this reason the values are typically reported in log units (i.e., log Kow). Kow or log Kow provides information on how the chemical is likely to partition in biological organisms. Kow is an important parameter that is used to by EPI Suite™ to estimate other properties including water solubility, bioconcentration, soil adsorption, and aquatic toxicity.

The EPI Suite™ method that estimates Kow is KOWWIN and it uses a "fragment constant" method to predict Kow. In the "fragment constant" method, a molecule is divided into fragments (atoms or larger functional groups) and the assigned coefficient values for each fragment are added to give the Kow estimate, which is reported as a log.

Interpreting Results

Log Kow or Log P tells the assessor if the chemical has an affinity for water or fats/lipids. The ranges of Log Kow are:

< 1	Highly soluble in water (hydrophilic)
> 4	Not very soluble in water (hydrophobic)
> 8	Not readily bioavailable
> 10	Not bioavailable - difficult to measure experimentally

Partitioning in Biota

Log Kow indicates how likely a chemical will be absorbed through biological membranes. General trends are given below:

- Liquids with a log Kow of 2-4 tend to absorb well through the skin.
- Chemicals with a log Kow > 4 tend to not absorb well.
- Chemicals with a log Kow of 5-6 tend to bioconcentrate in the lipid portion of the membrane.

Results for Sample Chemical

The Log Kow results for isodecyl acrylate are shown to the right. The Log Kow estimated by KOWWIN is 5.07 and indicates the chemical is not very soluble in water but will tend to bioconcentrate in organisms.

```
Log Octanol-Water Partition Coef (SRC):
   Log Kow (KOWWIN v1.68 estimate) =  5.07
```

5.4 Environmental Fate Properties

Environmental fate properties considered in a Sustainable Futures Summary Assessment are those related to environmental *transport* and *persistence* because these provide information on how a chemical is likely to partition once released to the environment so the potential routes of exposure and populations of concern can be identified.

5.4.1 Properties Relating to Environmental Transport – HLC, Koc, BCF

– Henry's Law Constant (HLC)

Henry's Law Constant (HLC) is the ratio of a chemical concentration in the gas phase to that in the aqueous phase at equilibrium. HLC is expressed as atm-m^3/mole or Pa-m^3/mole. HLC provides an indication of a chemical's volatility from water and gives the assessor an indication of potential environmental partitioning, potential removal in sewage treatment plant, and possible routes of environmental exposure.

HENRYWIN is based on methodology originally described by Hine and Mookerjee but has been updated with additional fragments and correction factors and to allow estimation at different temperatures. HENRYWIN uses three different estimation methods:

1. Vapor pressure / water solubility estimate – This is the most robust and accurate method because it uses measured data, but only works when experimental VP and WS are entered by the user.
2. Group method estimate – This method is preferred over the Bond method because it is more accurate when sufficient fragment coverage is achieved. This method is not always provided since it includes a smaller set of fragments, and as a result there are no estimates for many structure types.
3. Bond contribution method estimate – This method has a larger set of fragments thus can provide estimates for many more structure types.

The ranges of HLC values and the information they provide about the chemical are shown below.

HLC value (atm-m^3/mole)	Classification
> 10^{-1}	Very volatile from water
10^{-1} - 10^{-3}	Volatile from water
10^{-3} - 10^{-5}	Moderately volatile from water
10^{-5} - 10^{-7}	Slightly volatile from water
< 10^{-7}	Nonvolatile

Results for Sample Chemical

The HLC results for our sample chemical are shown below. We did not have experimental VP and WS to enter so the VP-WS estimate is not available. We will use the Group Method so that value, 1.20E-03 is outlined below. Results indicate the sample chemical will be volatile from water.

```
Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
  Bond Method :    1.18E-003  atm-m3/mole  (1.20E+002 Pa-m3/mole)
  Group Method:    1.20E-003  atm-m3/mole  (1.21E+002 Pa-m3/mole)
For Henry LC Comparison Purposes:
  User-Entered Henry LC:  not entered
  Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
     HLC:  2.090E-003 atm-m3/mole  (2.118E+002 Pa-m3/mole)
     VP:   0.0227 mm Hg (source: MPBPVP)
     WS:   3.03 mg/L (source: WSKOWWIN)
```

– Soil Adsorption Coefficient (Koc)

The Soil Adsorption Coefficient (Koc) provides a measure of the ability of a chemical to sorb (adhere) to the organic portion of soil, sediment and sludge. Like Kow, Koc is often expressed as a log due to the wide range of measured Koc values. Koc indicates the potential for the chemical to leach through soil and be introduced into ground water and partition between water and the suspended solids and sediment in the water column. Strong adsorption to soil will impact other fate properties.

KOCWIN estimates Koc using the Molecular Connectivity Index (MCI) and a log Kow-based method. The MCI method is more robust and been in use longer. Fragment corrections are applied in both estimation methods.

Koc is calculated using the following formula: Koc = Kd / %OC X 100 and expressed as Liters per Kilogram of soil. Kd (partitioning between the solid-phase (soil or sediment) and solution-phase (water) at equilibrium) is normalized by multiplying the percent organic carbon content of the soil by 100.

Interpreting Koc Results

Low Koc (not tightly bound to soil)

- Leaches into the soil
- Reduces surface level concentration
- Potential contamination of groundwater
- Contamination of surface water with storm runoff

High Koc (tightly bound to soil)

- Removal from water column via sorption to sediment and particulate matter
- May reduce rate of degradation because the chemical is less available to microorganisms

Interpreting Koc - Other Relevant Factors

- pH – Soil adsorption decrease as ionization increases,
- High clay content – Some chemicals may absorb very strongly to high-clay content soils,
- Bond formation with humic acid in organic matter – Some chemicals, most notably aromatic amines, may form strong chemicals bonds with the humic acid present, decreasing the potential for leaching with ground water.

Log Koc	Adsorption Classifications
> 4.5	Very strong sorption to soil / sediment, negligible migration to ground water
3.5 - 4.4	Strong sorption to soil / sediment, negligible to slow migration to ground water
2.5 - 3.4	Moderate sorption to soil / sediment, slow migration to ground water
1.5 - 2.4	Low sorption to soil / sediment, moderate migration to ground water
< 1.5	Negligible sorption to soil / sediment, rapid migration to ground water

Results for Sample Chemical

Log Koc results for the sample chemical are shown to the right. We will use the more robust MCI method and record the *log* Koc value of 3.037 L/kg because a log value is used by an exposure model, E-FAST (discussed in chapter 12). Results indicate that the chemical is likely to strongly sorb to soil and show slow migration to ground water.

```
Soil Adsorption Coefficient (KOCWIN v2.00):
     Koc    :  1090  L/kg (MCI method)
     Log Koc:  3.037       (MCI method)
     Koc    :  4612  L/kg (Kow method)
     Log Koc:  3.664       (Kow method)
```

– Bioconcentration Factor (BCF)

The Bioconcentration Factor (BCF) provides an indication of the potential for a chemical to bioconcentrate in lipids (fatty tissue) of organisms and is used as a surrogate for bioaccumulation in higher trophic levels of the food web. Most BCF tests are done using aquatic organisms however assessors may extrapolate to terrestrial organisms. BCF, which is unit-less, is the ratio of a chemical's concentration in the tissue of an aquatic organism to its concentration in the ambient water, when exposure of the organism is to waterborne chemicals only (I.e., not to chemical in the organism's diet or sorbed to ingested particles)..

BCF is estimated by BCFBAF, which is a SAR-based method that uses Kow to estimate BCF. BCFBAF, an update of the previous method, BCFWIN, accounts for metabolism and biotransformation under field conditions.

Relationship Between log Kow and Fish BCF
As log Kow increases the solubility in lipids increases. This generally means an increase in the potential to bioconcentrate in aquatic organisms. This relationship begins to change around log KOW of 6. Above this value the situation is more complex because low water solubility limits the rate of uptake by the exposed organism. This means equilibrium may take a very long time to be achieved in bioconcentration studies, possibly too long to be practical. A result is that published data on BCF seem to show that BCF drops with increasing log Kow above log Kow of about 6. Some experts say that "true" bioconcentration potential continues to increase above log Kow approximately 6. Most likely, dietary exposure becomes dominant and exposure to waterborne chemical insignificant (remember–waterborne chemical only is a basic assumption for BCF to be valid!). What this really means is that **no simple "BCF/log KOW" relationship applies** at higher values of log Kow.

Interpreting BCF Results
Chemicals with a high BCF are less water soluble and are expected to bioconcentrate in aquatic organisms. Conversely, low BCF indicates higher water solubility with

BCF	Log BCF	Classifications
> 5000	≥ 3.7	High bioconcentration potential
1000 - 5000	3	Moderate bioconcentration potential
< 1000	< 3	Low bioconcentration potential

Results for Sample Chemical
The log BCF results for the sample chemical (shown below) from the regression-based method is 1.641, indicating the chemical should have a low bioconcentration potential.

```
Bioaccumulation Estimates (BCFBAF v3.01):
  Log BCF from regression-based method = 1.641 (BCF = 43.72 L/kg wet-wt)
  Log Biotransformation Half-life (HL) = -0.5177 days (HL = 0.3036 days)
  Log BCF Arnot-Gobas method (upper trophic) = 2.099 (BCF = 125.7)
  Log BAF Arnot-Gobas method (upper trophic) = 2.100 (BAF = 125.8)
      log Kow used: 5.07 (estimated)
```

5.4.2 Properties Relating to Environmental Persistence

This section discusses properties relating to environmental persistence including:

- Biodegradation,
- Ready Biodegradability,
- Atmospheric Oxidation rates,
- Hydrolysis rates,
- Volatilization rates from Surface Waters (rivers and lakes), and
- Removal in Wastewater or Sewage Treatment Plant.

These properties provide information on how long a chemical could remain in specific environmental compartments. This kind of information allows an assessor to predict potential chemical concentrations in environmental media after release, identify exposed populations, and predict possible exposure.

– Biodegradation

Biodegradation, the degradation of a chemical substance by the action of microorganisms, is estimated by EPI Suite™ using seven models contained in BIOWIN. The potential for a chemical to biodegrade provides useful information on the likely persistence of the chemical in soil, water, and sediment, and potential removal in sewage treatment plants.

Knowing the approximate time required for a chemical to be broken down and potential removal rates in POTWs will help the risk assessor estimate the likely concentration of the chemical at various times and locations downstream after release to surface water. BIOWIN provides this information, which can be used in a variety of ways including serving as the basis for half-lives needed to run other models such as the PBT Profiler.

Chemicals with very long biodegradation times may be highly persistent in the environment IF they are not subject to destruction by other processes such as photolysis, hydrolysis, etc.

Primary biodegradation is a change in molecular structure to form a new compound, and *ultimate* biodegradation is the complete mineralization of the molecule.

Biodegradation can occur in the presence of oxygen or in its absence. Aerobic biodegradation occurs in oxygenated environments like the upper levels of surface water and soils. Anaerobic biodegradation occurs in oxygen-free systems like ground water and sediment and usually occurs much more slowly than when oxygen is present.

BIOWIN contains seven separate models. Version 4.10 designates these models as follows:

Probability of Rapid Biodegradation:
Biowin1: linear regression probability model
Biowin2: nonlinear regression probability model
Expert Survey Biodegradation:
Biowin3: expert survey ultimate biodegradation model
Biowin4: expert survey primary biodegradation model
MITI* Biodegradation Probability:
Biowin5: MITI linear regression model
Biowin6: MITI nonlinear regression model
Anaerobic Biodegradation Probability
Biowin7: anaerobic biodegradation model

* MITI is the Ministry of International Trade and Industry in Japan
Biodegradability estimates made by these models are based on fragment constants that were developed using multiple linear or non-linear regression analyses. For more information on how the methodology

was derived and for a list of the fragment constants used in version 4.10 of BIOWIN see the BIOWIN Help information.

Results for Sample Chemical

The EPI Suite™ results for isodecyl acrylate shown to the right give numeric results that need to be interpreted. Information on how to interpret the values from each of the methods is provided below. This information is also provided in the *Interpretative Assistance Document for Discrete Chemicals* available on the Sustainable Futures web site at http://www.epa.gov/oppt/sf/meetings/train.htm#materials. Results from the BIOWIN evaluation of isodecyl acrylate indicate that the chemical is likely to biodegrade.

```
Probability of Rapid Biodegradation (BIOWIN v4.10):
  Biowin1 (Linear Model)          :   0.8206
  Biowin2 (Non-Linear Model)      :   0.9833
Expert Survey Biodegradation Results:
  Biowin3 (Ultimate Survey Model):   2.8701  (weeks       )
  Biowin4 (Primary Survey Model) :   3.7703  (days        )
MITI Biodegradation Probability:
  Biowin5 (MITI Linear Model)     :   0.7388
  Biowin6 (MITI Non-Linear Model):   0.8668
Anaerobic Biodegradation Probability:
  Biowin7 (Anaerobic Linear Model):  0.6443
Ready Biodegradability Prediction:   YES
```

BIOWIN RESULTS

Probability of Rapid Biodegradation Biowin1 (linear) and Biowin2 (nonlinear)

For both: > 0.50 Likely to biodegrade rapidly
< 0.50 Not likely to biodegrade rapidly

Sample chemical results > 0.50 Likely to biodegrade rapidly

Expert Survey Biodegradation Biowin3 (ultimate) and Biowin4 (primary)

Result	Time Required for Biodegradation
>4.75 - 5	Hours
>4.25 - 4.75	Hours - days
>3.75 - 4.25	Days
>3.25 - 3.75	Days - weeks
>2.75 - 3.25	Weeks
>2.25 - 2.75	Weeks - months
>1.75 - 2.25	Months
<1.75	Longer “recalcitrant”

Sample chemical results Primary 3.7 = Days, Ultimate 2.8 = Weeks

MITI Biodegradation Probability:

Biowin5 (MITI linear) and Biowin6 (MITI nonlinear)

For both: > 0.50 Likely to biodegrade rapidly
< 0.50 Not likely to biodegrade rapidly

Sample chemical results > 0.50 Likely to biodegrade rapidly

Anaerobic Biodegradation Probability

Biowin7 (anaerobic biodegradation)

> 0.50 Likely to biodegrade rapidly
< 0.50 Not likely to biodegrade rapidly

Sample chemical results > 0.50 Likely to biodegrade rapidly

The Ready Biodegradability model in BIOWIN is a fragment-based method that was developed using data on more than 800 chemicals from the Japanese MITI protocol. Results are given as Pass or Not Pass result. It is a very stringent test and a chemical giving a positive response is expected to biodegrade in the environment. A chemical giving a negative result in MITI may still biodegrade under different conditions.

– Atmospheric Oxidation Half-life

Atmospheric oxidation (the rates at which a chemical will be broken down in the atmosphere) gives the assessor information on the likely persistence of a chemical in the atmosphere and the potential of the chemical to travel long distances from the original point of release. EPI Suite™ uses AOPWIN to

estimate the rate at which certain organic compounds will be destroyed by reactions with compounds in the atmosphere.

The two atmospheric oxidation processes evaluated by AOPWIN are chemical reactions with:

1. *Hydroxyl radicals* – Reaction with hydroxyl radicals (OH• radicals) is the dominant atmospheric oxidation process for most chemicals that are released to the atmosphere. OH• radicals are produced in sunlight and exist in a steady state in the atmosphere.
2. *Ozone* – Ozone (O3) reacts with a chemical when one or more functional groups are attached to any olefinic or acetylenic unit. Reaction with ozone is also important for a limited number of chemical classes including hydrazines, phenols, alkyl lead compounds, and furans.

Interpreting Results

Half-life	Classification
< 2 hours	Rapid
2 hrs – < 1 day	Moderate
1 – 10 days	Slow
>10 days	Negligible
> 2 days	Potential for long range transport in air

Chemicals with a half-life > 2 days will meet the Persistence criteria for New Chemicals Category for Persistent, Bioaccumulative, and Toxic Chemicals (see http://www.epa.gov/oppt/newchems/pubs/pbtpolcy.htm).

Results for Sample Chemical

The AOPWIN results for isodecyl acrylate (below) indicate that it will react at a moderate rate (5.8 hrs) with hydroxyl radicals and at a slower rate (6.5 days) with ozone. The fraction of the chemical that is sorbed to organic particles in the air may be resistant to atmospheric oxidation.

```
Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant =  22.2422 E-12 cm3/molecule-sec
     Half-Life =     0.481 Days (12-hr day; 1.5E6 OH/cm3)
     Half-Life =     5.771 Hrs
  Ozone Reaction:
     OVERALL Ozone Rate Constant =     0.175000 E-17 cm3/molecule-sec
     Half-Life =     6.549 Days (at 7E11 mol/cm3)
  Fraction sorbed to airborne particulates (phi):
     5.83E-005 (Junge-Pankow, Mackay avg)
     4.79E-005 (Koa method)
   Note: the sorbed fraction may be resistant to atmospheric oxidation
```

– Hydrolysis Half-life

HYDROWIN™ estimates the rate at which a chemical will react with water. Being able to predict hydrolysis rates helps the assessor estimate both how long the chemical and/or its hydrolysis products will remain in water bodies after being released to the environment. During hydrolysis the chemical is catalyzed (broken down) by acids (hydronium) or bases (hydroxide ions). Hydrolysis processes are pH sensitive and are an important degradation process at typical environmental pH ranges from the more acidic 5 to the more basic 9 with 7 being neutral.

HYDROWIN™ estimates acid- and base-catalyzed rate constants for esters, carbamates, epoxides, halomethanes, and certain alkyl halides. Neutral hydrolysis rates are currently not estimated. HYDROWIN™ provides estimations by converting acid, neutral, and base rate constants to half-lives at pH 7 and 8.

Important Notes on Hydrolysis

- Some classes of chemicals hydrolyze extremely rapidly (i.e., in hours), such as acid chlorides, epoxides, and siloxanes.
- Changes in temperature can dramatically change the rate of the reaction, with a 10 degree change resulting in a 250% change in rate
- Besides natural bodies of water, hydrolysis may also occur in clouds, fog, or moist soil, and effluent.
- Knowing the Hydrolysis Half-Life tells the assessor what species to assess:
    - For chemicals with a rapid (<1hr) Hydrolysis Half-Life it is important to assess the hydrolysis product,
    - Chemicals with Hydrolysis Half-Life between 1 hour and 14 days, assess BOTH the parent compound and the hydrolysis product, and
    - Chemicals with Hydrolysis Half-Life >14 days assess the parent compound.

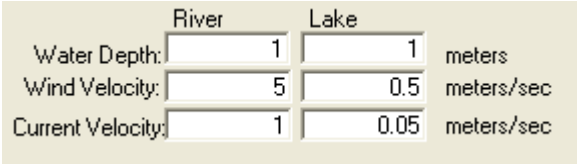
Results for Sample Chemical

The HYDROWIN results for isodecyl acrylate (below) predict that the chemical will have a half-life of more than 10 years at pH 7 (neutral) and more than 1 year at pH 8 (more basic).

```
Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
 Total Kb for pH > 8 at 25 deg C :  2.071E-002  L/mol-sec
 Kb Half-Life at pH 8:       1.061  years
 Kb Half-Life at pH 7:      10.607  years
   (Total Kb applies only to esters, carbmates, alkyl halides)
```

– Volatilization Half-life from Surface Waters

The Water Volatilization Program in EPI Suite™ estimates volatilization half-lives from a model river and lake by using molecular weight, Henry's Law Constant, water solubility and the various volatilization parameters for Model Lakes (still water) and Model Rivers (moving water). Volatilization from surface water provides information on the potential environmental partitioning of a chemical. Default parameters for water depth, wind velocity and current velocity of the river or lake provided on the EPI Welcome Screen (right). The default values can be changed if more precise information is available.



Unlike many of the modules in EPI Suite™ this Water Volatilization Program is not a "stand-alone" program and cannot be run independently of the other modules without the EPI interface and other supported EPI modules.

The model does not take into account potential adsorption to sediment and organic matter suspended in the water column. For chemicals with a high Koc the volatilization half-lives for a model river and model lake are expected to be significantly lower than predicted in the Water Volatilization Program.

Results for Sample Chemical

The Water Volatilization Program predicts that the sample chemical will have a half-life of more than 2 hours from a model river and more than 6 days from a model river.

```
Volatilization from Water:
    Henry LC:  0.0012 atm-m3/mole  (estimated by Group SAR Method)
    Half-Life from Model River:      2.198  hours
    Half-Life from Model Lake :      146.2  hours   (6.09 days)
```

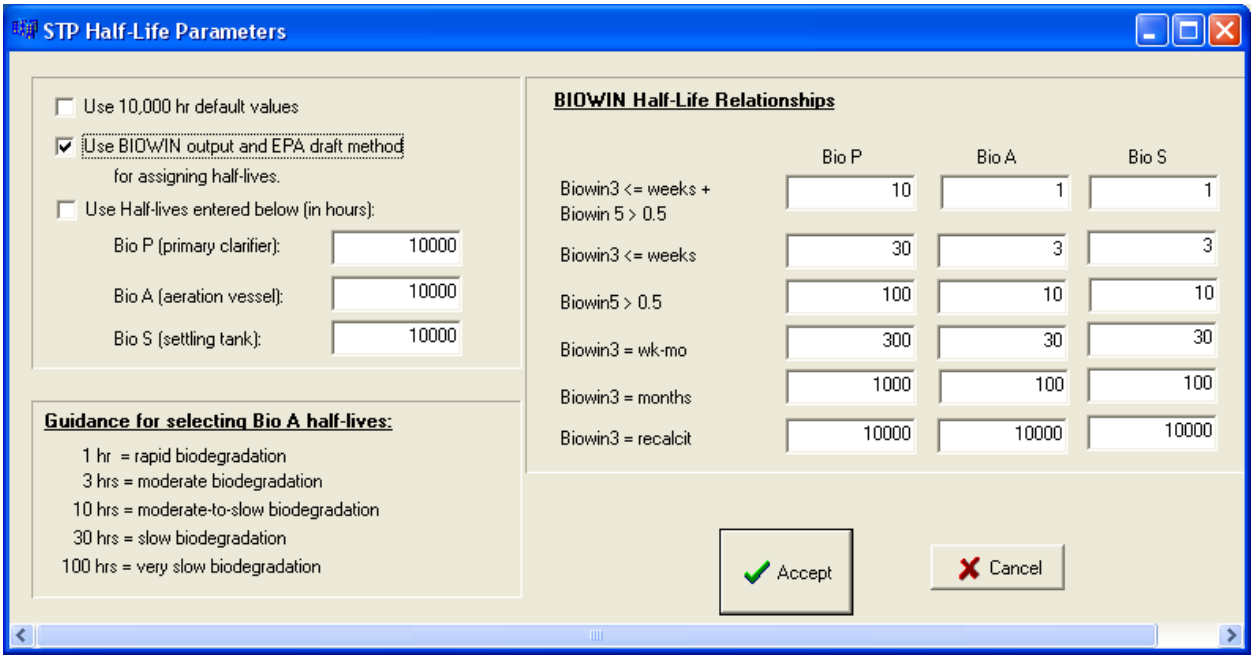
– Removal in Sewage Treatment Plant

STPWIN is the method used by EPI Suite™ to estimate Percent Removal in Sewage Treatment Plants, also expressed as POTW removal. Knowing the removal in STP or POTW tells the assessor how much of the chemical could remain after treatment in the POTW and be discharged to surface water and effect aquatic life or humans through ingestion of fish or drinking water.

The three processes in a sewage treatment plant that act to remove a chemical from the waste stream are:

- Biodegradation in the primary clarifier (Bio P),
- Removal in the aeration vessel (Bio A), and
- Removal by sludge adsorption in the settling tank (Bio S).

The default method used by STPWIN assumes negligible biodegradation, (half-life = 10,000 hours) is the default value for the primary clarifier (Bio P), aeration vessel (Bio A), and final settling tank (Bio S). The default parameters used by STPWIN can be seen by clicking on the STP tab at the top of the EPI Suite™ Welcome Screen. The two other options for running STP that can be selected (shown to the left of the image below) are using BIOWIN output and EPA Draft method for assigning half-lives or entering half-life values. It is suggested that the EPA Draft method be used (shown selected below) because it accounts for biodegradation.



Results for Sample Chemical

EPA Draft Method
Running STPWIN using the EPA Draft method which accounts for biodegradation gives a removal rate of Nearly 100%, however unless experimental data indicate otherwise, the EPA will not use a value greater than 90% when determining rate of removal from STP.

```
Removal In Wastewater Treatment (recommended maximum 95%):
   Total removal:              99.94  percent
   Total biodegradation:       79.78  percent
   Total sludge adsorption:    20.05  percent
   Total to Air:                0.10  percent
     (using Biowin/EPA draft method)
```

Byproducts
The last property listed in the Sustainable Futures Summary Assessment Worksheet under Environmental Transport and Fate is "Byproducts" and includes Degradation Products and Metabolites. There are no EPI Suite™ methods to predict byproducts so the assessor must rely on professional judgment or the use of other predictive methods to identify degradation pathways.

It is important for an assessor to understand what possible chemical compounds could form, and at what rates, when a chemical degrades in the environment or metabolizes in the body. These byproducts may or may not present toxicity concerns separate from the parent compound. Professional judgment tells us that the sample chemical will form acrylic acid and isodecyl alcohol by enzymatic degradation in soils.

5.5 Entering Predictions into SF Worksheet

The section of the Sustainable Futures Summary Assessment Worksheet shown below shows that the Physical / Chemical and Environmental Fate Property estimation results have been entered. The reader is encouraged to refer back to the completed full Sustainable Futures Summary Assessment Worksheet for this sample chemical which is included in chapter 2 of this document. A blank worksheet is included in Appendix H.

PHYSICAL/CHEMICAL PROPERTIES:	
Melting Point (deg C)	–100 (Experimental data from PhysProp database)
Boiling Point (deg C)	158 (Experimental data from PhysProp database)
Boiling Point Pressure (mm Hg)	50 (Experimental data from PhysProp database)
Vapor Pressure (mm Hg)	2.27E-02 (EPI v4.10, MPBPVP v1.43)
Water Solubility at 25 deg C (g/L)	3.034 (EPI v4.10, WSKOW v1.42)
Log K_{ow}	5.07 (EPI v4.10, KOWWIN v1.68)

ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC (atm-m^3/mol)	1.20E-03 (EPI v4.10, HENRYWIN v3.20 Group Method)
Soil Adsorption Coefficient – log K_{OC}	3.037 (EPI v4.10, KOCWIN v2.00)
Log Bioconcentration Factor – BCF	1.641 (EPI v4.10, BCFBAF v3.01)
Persistence	
Probability of Rapid Biodegradation	Likely to biodegrade rapidly (EPI v4.10, BIOWIN v4.10)
Ultimate Biodeg Model	Weeks (EPI v4.10, BIOWIN v4.10)
Primary Biodeg Model	Days (EPI v4.10, BIOWIN v4.10)
Ready Biodegradability (MITI Model)	Likely to biodegrade rapidly (EPI v4.10, BIOWIN v4.10)
Atmospheric Half-life	Reacts at moderate rate (5.8 hrs) w. OH radicals, slower rate (6.5 days) w. ozone, does not react with nitrate radicals (EPI v4.10, AopWin v1.92)
Hydrolysis Half-life	> 10 yrs at pH 7, > 1 year at pH 8 (EPI v4.10, HYDROWIN v2.00)
Volatilization Half-life for Model River	> 2 hours (EPI v4.10, WVOLNT)
Volatilization Half-life for Model Lake	> 6 days (EPI v4.10, WVOLNT)
Removal in STP (EPA Draft Method)	99% predicted, Recommended Max is 95% (EPI v4.10, STPWIN)
Experimental Data	Not available
Byproducts	
Degradation Products	Acrylic acid, isodecyl alcohol (Professional Judgment)
Metabolites	Not available

5.6 Obtaining Additional Training Materials on EPI Suite™

The training materials covering EPI Suite™ that were developed by EPA for use in the 3 day Sustainable Futures hands-on training sessions may provide you with additional information.

Check the Sustainable Futures web site at http://www.epa.gov/oppt/sf/meetings/train.htm#materials for information on how to get copies of the training materials. These materials are frequently updated and it was decided that the most effective way to provide up-to-date copies is provide a contact name so that visitors can request the materials they need. For PDF copies of the presentations contact Kelly Mayo-Bean, U.S. EPA (mayo.kelly@epa.gov).

Intentionally Left Blank