

Manual
Software to Estimate Physical Properties (StEPP™)

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I. Getting Started

A. Requirements

To use Software to Estimate Physical Properties (StEPP™), you need:

- A Pentium or more recent processor.
- An English-language version of Windows 95, Windows 98, or Windows NT 4.0. In the case of Windows NT 4.0, Service Pack 3 or more recent is required.
- At least 50 megabytes of hard drive space
- At least 64 megabytes of RAM is recommended
- A graphic VGA or more recent video display
- A CD-ROM drive, which is used to install the software
- A Windows compatible mouse (or any compatible point device) is recommended

B. Installing StEPP®

To install StEPP™ on your computer, you must have the CD-ROM installation disk labeled “ETDOT Programs”. The installation program will copy files from the installation disk to your hard drive. The installation program will cancel the process if you do not have sufficient hard drive space. If anything goes wrong during the installation, you will always be able to quit the install program and run it again. If a previous release of StEPP™ was installed, you should install the new version on top of the old version; this is done by installing to the same directory that the original version was installed to.

1. Log in to Windows normally.
2. Insert the CD-ROM labeled “ETDOT Programs” in the CD-ROM drive.
3. From the Start menu, choose Run.
4. Type **z:\setup** (replace z with the letter of the CD-ROM drive).
5. Press ENTER.
6. Follow the setup instructions on the screen.

Note: Steps 3, 4 and 5 are equivalent to double-clicking on the setup.exe program icon in Explorer or File Manager.

If the software does not work correctly after the installation, you can reach Dr. David W. Hand at (906) 487-2777.

II. Introduction to Software to Estimate Physical Properties

In the process of modeling a treatment system, the most difficult task often involves accurately predicting the physical and chemical properties of the contaminants present in the system. For many treatment and control technologies, such as adsorption and packed tower aeration, models are available that can simulate such processes. However, the effectiveness of such models is severely limited when the properties of the contaminants in the system cannot be accurately determined.

Software to Estimate Physical Properties (StEPP™) was designed to act as a physical property resource tool and seeks to alleviate this problem by providing the capability to easily obtain many of the properties necessary to model chemical and environmental processes. StEPP™ consists of a database of over 600 organic contaminants from which certain properties are available. Table 1 shows a sampling of the classes of compounds for which properties are available in StEPP™. The StEPP™ database consists of critically evaluated property values available in the literature. Because of the lack of quality data in the literature for other properties, StEPP™ provides various parameter estimation methods to supplement the database. Dependence on temperature is included for those properties that vary strongly with temperature. Table 2 shows the properties available from the StEPP™ database and the properties available from parameter estimation methods. Temperature-dependent properties are indicated in Table 2 by an asterisk (*).

Table 1 - Sample Classes of Compounds Available in StEPP™

alkanes	aromatics	nitriles
cycloalkanes	carboxylic acids	dioxins
alkenes	ethers	PCBs
cycloalkenes	esters	ketones
alkynes	thiols	aldehydes
amines	alcohols	epoxides

Table 2 - Properties Available from StEPP™

Property	Available from Database	Available from Parameter Estimation Methods
Vapor Pressure	Yes*	No
Infinite Dilution Activity Coefficient	No	Yes*
Henry's Constant	Yes*	Yes*
Molecular Weight	Yes	Yes
Normal Boiling Point	Yes	No
Liquid Density	Yes*	Yes*
Molar Volume at Operating Temperature	Yes*	Yes*
Molar Volume at Normal Boiling Point	No	Yes
Refractive Index	Yes	No
Aqueous Solubility	Yes	Yes*
Octanol Water Partition Coefficient	Yes	Yes*
Liquid Diffusivity	No	Yes*
Gas Diffusivity	No	Yes*
Water Density	No	Yes*
Water Viscosity	No	Yes*
Water Surface Tension	No	Yes*
Air Density	No	Yes*
Air Viscosity	No	Yes*
* - Denotes temperature-dependent property		

StEPP™ was developed as a physical property resource tool for the Clean Process Advisory System (CPAS™) to aid the conceptual process design engineer in furthering the goal of pollution prevention (Radecki, et al., 1994). StEPP™ is intended for widespread use in air and water treatment. For example, in a packed tower aeration design, the engineer needs to know the following contaminant properties: molecular weight, Henry's constant, normal boiling point, molar volume at the normal boiling point, liquid diffusivity, and gas diffusivity. StEPP™ is designed to provide accurate values for these properties for a wide variety of organic contaminants. StEPP™ is designed both as a stand-alone software package to estimate physical and chemical properties and as a tool that may be directly linked to other CPAS models, such as air stripping and adsorption, in order to provide physical and chemical properties.

StEPP™ is designed for the Microsoft Windows™ environment with a graphical user interface (GUI) in order to maximize user-friendliness. Making use of the Microsoft Windows interface, with its built-in file and hardware control features, frees the programmer from concerns over printer drivers and other "machine" issues and allows more attention to the computation algorithms themselves. The GUI consists of a front-end shell written in Visual Basic™ that calls FORTRAN subroutines in order to perform calculations. The database of over 600 organic contaminants is designed using a relational database engine (Microsoft Access™ 2.0) to allow unprecedented manipulation and display of the results.

This manual is designed to present a description of the properties available in StEPP™, including methods, references, and sample calculations where applicable. The manual also presents a sample program run and description of the windows in the software in order to aid the user.

III. Description of Properties

A. Note on *UNI*versal quasichemical Functional group Activity Coefficient (*UNIFAC*)

Several properties (e.g., activity coefficient, Henry's constant, aqueous solubility, and octanol water partition coefficient) have estimations based on this method. Therefore, the references and detailed information that is common to all properties will be described here rather than in every property that makes use of it.

1. General References for UNIFAC

Arbuckle, W.B., "Estimating Activity Coefficients for Use in Calculating Environmental Parameters," *Environ. Sci. Technol.*, **17**:9, 537-542 (1983).

Arbuckle, W.B., "Using UNIFAC to Calculate Aqueous Solubilities," *Environ. Sci. Technol.*, **20**:10 (1986).

Derr, E.L. and C.H. Deal, "Analytical Solutions of Groups: Correlation of Activity Coefficients through Structural Group Parameters," *I. Chem. E. Symposium Series*, No. 32, 3:40-3:51 (1969).

Fredenslund, Aa., R.L. Jones, and J.M. Prausnitz, "Group-Contribution Estimation of Activity Coefficients in Nonideal Liquid Mixtures," *AIChE Journal*, **31**, 1086-1099 (1975).

Gmehling, J., P. Rasmussen, and Aa. Fredenslund, "Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension. 2," *Ind. Eng. Chem., Process Des. Dev.*, **21**:1:118-127 (1982).

Hansen, H.K. et al., "Vapor-Liquid Equilibria by UNIFAC Group Contribution. 5. Revision and Extension," *Ind. Eng. Chem. Res.*, **30**:10, 2352-2355 (1991).

Kikic, I., P. Alessi, P. Rasmussen, and Aa. Fredenslund, "On the Combinatorial Part of the UNIFAC and UNIQUAC Models," *The Canadian Journal of Chemical Engineering*, **58**, 253-258 (April 1980).

Macedo, E.A., U. Weidlich, J. Gmehling, and P. Rasmussen, "Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension. 3," *Ind. Eng. Chem. Process Des. Dev.*, **22**:4, 676-678 (1983).

- Magnussen, T., et. al., "UNIFAC Parameter Table for Prediction of Liquid-Liquid Equilibria," *Ind. Eng. Chem. Process Des. Dev.*, **20**:2, 331-339 (1981).
- Pierotti, G.J., C.H. Deal, and E.L. Derr, "Activity Coefficients and Molecular Structure," *Industrial and Engineering Chemistry*, **51**:1, 95-102 (1959).
- Rogers, T.N., et al., "Henry's Law Constants for Environmental Applications," Presented at the Second International Conference on Thermodynamics of Aqueous Systems with Industrial Applications, Sponsored by the Design Institute for Physical Property Data (DIPPR[®]) of the American Institute of Chemical Engineers (AIChE), the National Bureau of Standards (NBS), and the National Science Foundation (NSF), Warrenton, VA (May 1987).
- Rogers, T.N., "Predicting Environmental Physical Properties from Chemical Structure Using a Modified UNIFAC Model," Ph.D. Dissertation, Michigan Technological University (1994).
- Skjold-Jorgensen, S., B. Kolbe, J. Gmehling, and P. Rasmussen, "Vapor- Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension," *Ind. Eng. Chem., Process Des. Dev.*, **18**:4, 714-722 (1979).
- Tiegs, D. and J. Gmehling, "Vapor-Liquid Equilibria by UNIFAC Group Contribution. 4. Revision and Extension," *Ind. Eng. Chem. Res.*, **26**:1, 159-161 (1987).
- Wilson, G.M. and C.H. Deal, "Activity Coefficients and Molecular Structure," *Industrial & Engineering Chemistry Fundamentals*, **1**:1, 20-23 (1962).

2. General Information on UNIFAC

The StEPP[™] computer software builds upon the algorithms presented by Arbuckle (1983, 1986) for calculating thermodynamic properties associated with environmental partitioning and phase equilibrium. The infinite dilution activity coefficient, an environmental parameter of key importance in thermodynamics, is related fundamentally to several major properties and also correlates empirically with many others (Arbuckle, 1983; Arbuckle, 1986). Within StEPP[™], the UNIFAC model developed by Fredenslund et al. (1975) is used to predict all properties involving vapor-liquid and liquid-liquid equilibria. UNIFAC

can be used with a few simple thermodynamic relationships to predict environmental quantities such as Henry's constant, aqueous solubility, water solubility in a chemical solvent, and octanol water partition coefficient. Because it is rooted in thermodynamics and accounts for the effect of temperature, this approach has advantages over other purely empirical models. Its group contribution emphasis makes UNIFAC applicable to a large number of chemicals and environmental problems (Pierotti, et al., 1959; Wilson and Deal, 1962; Derr and Deal, 1969).

The original UNIFAC parameter sets for vapor-liquid (e.g. UNIFAC-VLE [Hansen, et al., 1991]) and liquid-liquid (e.g., UNIFAC-LLE [Magnussen, et al., 1981]) equilibria are available to the StEPP™ user in addition to a new UNIFAC parameter set (e.g., UNIFAC-ENV (Rogers, et al., 1987)) developed especially for dilute aqueous mixtures. A set of FORTRAN routines, based on the parameter sets described above, forms the core of StEPP's partitioning and equilibrium property calculations. Listed below are the recommendations within StEPP™, in order of decreasing preference, for selecting the "best" UNIFAC parameter set in a given situation:

- *Infinite Dilution Activity Coefficient*: UNIFAC-ENV, VLE, LLE, user choice
- *Henry's Law Constant*: UNIFAC-ENV, VLE, LLE
- *Aqueous Solubility*: UNIFAC-LLE, ENV, VLE
- *Octanol-Water Partition Coefficient*: UNIFAC-LLE, VLE, (ENV not possible)

Because none of the UNIFAC parameter sets contain interaction values for all possible functional group pairs, the StEPP™ algorithm follows the above order until the options are exhausted, at which time an error message is displayed. At any time, the user can override the automatic choice of the parameter set. The following paragraphs review the application of UNIFAC to specific partitioning and equilibrium calculations within StEPP™ that are used to determine Henry's constant, aqueous solubility, and octanol water partition coefficient.

B. Vapor Pressure

1. Sources Available and Hierarchy

The vapor pressure can be determined in StEPP™ from the following;

1. AIChE/DIPPR® - American Institute of Chemical Engineers/Design Institute for Physical Property Data
2. Carl L. Yaws' book and data compilation (1992)
3. EPA Superfund Public Health Evaluation Manual (1986)

Only one of the three sources will be available for a given chemical. If vapor pressure data was available from (1) then it is in the database. If no data was available from (1), then data from (2) is in the database. If no data was available from (1) or (2) then data from (3) is in the database.

2. References

a) AIChE/DIPPR®

Daubert, T.E., R.P. Danner, H.M. Sibul, and C.C. Stebbins, Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation, Extant 1995, Taylor & Francis, Bristol, Pennsylvania (1995).

b) Carl L. Yaws' book and data compilation (1992)

Yaws, C.L., Thermodynamics and Physical Property Data, Houston: Gulf Publishing Company (1992).

c) EPA Superfund Public Health Evaluation Manual (1986)

EPA Superfund Public Health Evaluation Manual, U.S. Environmental Protection Agency, Office of Emergency and Remedial Response, Washington, D.C., EPA/540/1-86/060 (October 1986).

3. Detailed Information on the Sources Available

a) AIChE/DIPPR®

This source provides a correlation that requires temperature input. The correlation used is:

$$VP = \exp \left[A + \frac{B}{T} + C \ln T + D T^E \right] \text{ in the range } T_{\min} < T < T_{\max}$$

where:

$VP =$ Vapor pressure (Pa)

$A, B, C, D, E =$ Empirical coefficients

$T =$ Temperature (K)

$T_{\min} =$ Minimum temperature for which correlation applies (K)

$T_{\max} =$ Maximum temperature for which correlation applies (K)

From the AIChE/DIPPR[®] data compilation, for Trichloroethylene:

$$A = 59.403$$

$$B = -5471.6$$

$$C = -5.8275$$

$$D = 0.0045098$$

$$E = 1$$

$$T_{\min} = 188.4 \text{ K}$$

$$T_{\max} = 571.15 \text{ K}$$

Sample Calculation for Trichloroethylene at T_{\min} :

$$\begin{aligned} VP &= \exp \left[A + \frac{B}{T} + C \ln T + DT^E \right] \\ &= \exp \left[59.403 + \frac{-5471.6}{188.4} + -5.8275 \ln 188.4 + 0.0045098 (188.4)^1 \right] \\ &= 1.9787 \text{ Pa} \end{aligned}$$

This result agrees with the value reported in Daubert, et al. (1995).

Sample Calculation for Trichloroethylene at 10°C :

$$\begin{aligned} VP &= \exp \left[A + \frac{B}{T} + C \ln T + DT^E \right] \\ &= \exp \left[59.403 + \frac{-5471.6}{283.15} + -5.8275 \ln 283.15 + 0.0045098 (283.15)^1 \right] \\ &= 4690 \text{ Pa} \end{aligned}$$

b) Carl L. Yaws' book and data compilation (1992)

This source provides a correlation that requires temperature input. The correlation used is Antoine's equation:

$$VP = 10^{A - \frac{B}{T+C}} \text{ in the range } T_{\min} < T < T_{\max}$$

where:

$VP =$ Vapor pressure (mm Hg)

$A, B, C =$ Empirical coefficients

$T =$ Temperature (C)

T_{\min} = Minimum temperature for which correlation applies (C)

T_{\max} = Maximum temperature for which correlation applies (C)

From Yaws (1992) for Trichloroethylene:

$$A = 7.0281$$

$$B = 1315.1$$

$$C = 230.01$$

$$T_{\min} = -13\text{ }^{\circ}\text{C}$$

$$T_{\max} = 127\text{ }^{\circ}\text{C}$$

Sample Calculation for Trichloroethylene at T_{\min} :

$$VP = 10^{A - \frac{B}{T+C}} = 10^{7.0281 - \frac{1315.1}{-13 + 230.01}} \\ = 9.3\text{ mm Hg}$$

This result agrees with the value reported in Yaws (1992). Converting to Pa to be consistent with units reported in StEPP™, results in vapor pressure equals 1240 Pa.

c) EPA Superfund Public Health Evaluation Manual (1986)

This source contains discrete vapor pressure data.

C. Infinite Dilution Activity Coefficient

1. Sources Available and Hierarchy

The infinite dilution activity coefficient is available in StEPP™ from:

1. UNIFAC

2. References

See the section titled “Note on UNIFAC”.

3. Detailed Information on the Sources Available

See the section titled “Note on UNIFAC”. A sample application on the method is provided in the following reference:

Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt, Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds, New York: McGraw-Hill Book Company (1982).

D. Henry's Constant

1. Sources Available and Hierarchy

Henry's constant is available in StEPP™ from the following:

1. Regression of data points
2. UNIFAC fit with a data point
3. UNIFAC at the operating temperature
4. Database
5. UNIFAC at database temperatures

The preferential order of the methods in StEPP™ for determining Henry's law constant is the ordering given above.

2. References

a) Regression of data points

None.

b) UNIFAC fit with a data point

See below for obtaining the UNIFAC values. No references for the fit.

c) UNIFAC at the operating temperature

See the "Note on UNIFAC" section for general references on UNIFAC.

Carroll, J.J., "What Is Henry's Law?," *Chemical Engineering Progress* (September 1991).

d) Database

Ashworth, R.A., G.B. Howe, M.E. Mullins, and T.N. Rogers, "Air-Water Partitioning Coefficients of Organics in Dilute Aqueous Solutions," *Journal of Hazardous Materials*, **18**, 25-36 (1988).

Yaws, C.L., J.W. Miller, P.N. Shah, G.R. Schorr, and P.M. Patel, "Correlation Constants for Chemical Compounds," *Chem. Eng.*, **83**:25, 153-162 (1976).

EPA Superfund Public Health Evaluation Manual, U.S. Environmental Protection Agency, Office of Emergency and Remedial Response, Washington, D.C., EPA/540/1-86/060 (October 1986).

e) UNIFAC at database temperatures

Same as for UNIFAC at operating temperature.

3. Detailed Information on the Sources Available

a) Regression of data points

When more than one discrete data value is available, interpolation and extrapolation to other temperatures are done preferentially from the raw data. For Henry's constant, this extrapolation is performed by assuming a constant enthalpy change of volatilization in the Van't Hoff equation, which implies a linear relationship between $\log H$ and $1/T$ (where H = Henry's constant and T = absolute temperature). Therefore, a linear regression is performed on data points when more than one data point for a given compound is in the database. Note this is only the case with RTI data. The regression performed is of $\ln H$ (atm) vs. $1/T$ (K) data.

A summary of the regression technique is as follows:

Calculate the sums:

$$\begin{aligned}\sum xy &= \sum_{i=1}^{n_{data}} \ln H_i \text{ (atm)} \times \frac{1}{T_i \text{ (K)}} \\ \sum y &= \sum_{i=1}^{n_{data}} \ln H_i \text{ (atm)} \\ \sum x &= \sum_{i=1}^{n_{data}} \frac{1}{T_i \text{ (K)}} \\ \sum x^2 &= \sum_{i=1}^{n_{data}} \left(\frac{1}{T_i \text{ (K)}} \right)^2\end{aligned}$$

Calculate the means, slope, and intercept:

$$\begin{aligned}\sigma_x &= \frac{\sum x}{n_{data}} \\ \sigma_y &= \frac{\sum y}{n_{data}} \\ \text{Slope} &= \frac{[n_{data} \cdot \sum xy] - [\sum x \cdot \sum y]}{[n_{data} \cdot \sum x^2] - [\sum x]^2} \\ \text{Intercept} &= \sigma_y - \text{Slope} \cdot \sigma_x\end{aligned}$$

Calculate $\ln H$ as a function of temperature:

$$\ln H(\text{atm}) = \text{slope} \left(\frac{1}{T(\text{K})} \right) + \text{Intercept}$$

Using this relationship, it is possible to estimate H at any given temperature. Note that the valid temperature range for the correlation encompasses the temperature range of the data.

Sample Calculation for Henry's Constant of Trichloroethylene at 17°C

Henry's Constant

Current Henry's Constant Information

Value (-): 0.308

Source: Regression of Data Points

Accept Selected Henry's Constant

Cancel

Source	Henry's Constant (-)	Temp. (C)	Tmin (C)	Tmax (C)
<input checked="" type="radio"/> Regression of Data Points	0.308	17.0	N/A	N/A
<input type="radio"/> UNIFAC Fit with Data Pt.	0.298	17.0		
<input type="radio"/> UNIFAC at Operating T	0.357	17.0		
<input type="radio"/> Database	0.282	15.0		
RTI	0.282	15.0		
<input type="radio"/> UNIFAC @ Database T's	0.231	9.90		
	0.282	15.0		
	0.349	20.1		
	0.414	25.0		
	0.515	29.9		
<input type="radio"/> User Input				

UNIFAC Group Interaction Database: Environmental VLE

Figure 1 - Henry's Constant Window (TCE, 17°C) Highlighting Data Available

From Figure 1, properties needed to do the regression are Henry's constants at various temperatures from RTI data, which are shown in Table 1.

Table 1 - Henry's Constant Data for TCE Available in StEPP™ (Source: RTI)

Temperature (C)	Henry's Constant (-)	Henry's Constant (atm)
9.9	0.231	297.7610445
15.0	0.282	370.0500544

20.1	0.349	466.0754075
25.0	0.414	562.1185211
29.9	0.515	710.7457273

Note: In Table 1, dimensionless Henry's constants are converted to units of atm by the following relationship: $H[atm] = H[-] \cdot 0.08205[55.5/T[K]]$

Calculate the sums using data from Table 1:

$$\sum xy = \sum_{i=1}^{n_{data}} \left[\ln H_i[atm] \times \frac{1}{T_i[K]} \right] = 0.10450415$$

$$\sum y = \sum_{i=1}^{n_{data}} \ln H_i[atm] = 30.65230448$$

$$\sum x = \sum_{i=1}^{n_{data}} \frac{1}{T_i[K]} = 0.017067221$$

$$\sum x^2 = \sum_{i=1}^{n_{data}} \left[\frac{1}{T_i[K]} \right]^2 = 5.829199E-05$$

Calculate the means, slope, and intercept:

$$\sigma_x = \frac{\sum x}{n_{data}} = \frac{0.017067221}{5} = 0.003413444$$

$$\sigma_y = \frac{\sum y}{n_{data}} = \frac{30.65230448}{5} = 6.130460896$$

$$\begin{aligned} Slope &= \frac{\left[(n_{data} \cdot \sum xy) - \left(\sum x \cdot \sum y \right) \right]}{\left[(n_{data} \cdot \sum x^2) - \left(\sum x \right)^2 \right]} = \frac{\left[(5 \cdot 0.10450415) - (0.017067221 \cdot 30.65230448) \right]}{\left[(5 \cdot 5.8292E-05) - (0.017067221)^2 \right]} \\ &= -3700.150453 \end{aligned}$$

$$\begin{aligned} Intercept &= \sigma_y - Slope \cdot \sigma_x = 6.130460896 - (-3700.150453) \cdot 0.003413444 \\ &= 18.76071726 \end{aligned}$$

Calculate ln H as a function of temperature:

$$\begin{aligned}\ln H_{atm} &= \text{slope} \left(\frac{1}{T(K)} \right) + \text{Intercept} \\ &= -3700.150453 \left(\frac{1}{T(K)} \right) + 18.76071726\end{aligned}$$

Find H at 17° C:

$$\begin{aligned}\ln H_{atm} &= \text{slope} \left(\frac{1}{T(K)} \right) + \text{Intercept} \\ &= -3700.150453 \left(\frac{1}{290.15 K} \right) + 18.76071726 \\ &= 6.008173913 = \ln H_{atm} \Rightarrow \\ H(atm) &= \exp(6.008173913) = 406.7398992 \text{ atm} \Rightarrow \\ H_{atm} &= H_{atm} / 0.082054 / T(K) / 55.5 \\ &= 406.7252601 \text{ atm} / 0.082054 / 290.15 K / 55.5 \\ &= 0.308\end{aligned}$$

This result agrees with the “Regression of Data” result shown in Figure 1.

b) UNIFAC fit with a data point

For the special case in which the user desires a property value for Henry's constant at a temperature different from a single discrete value in the database, UNIFAC is used as an extrapolation tool (see the “Note on UNIFAC” section for a detailed discussion of UNIFAC). A UNIFAC estimate at the database temperature is first used to calculate the "offset" between the UNIFAC prediction and the data point. This offset is then applied at the temperature of interest to correct the UNIFAC estimate to be consistent with the given data value (i.e., the UNIFAC property-versus-temperature curve is forced through the discrete database value). This extrapolation technique takes advantage of the linear relationship between \ln of Henry's constant in atm and $1/\text{Temperature}$. Elsewhere in this paper and in StEPP™, this procedure is referred to as "UNIFAC Fit with Data Point."

Sample Calculation to Estimate Henry's Constant of TCE at 17° C

Figure 2 shows the Henry's constant window from StEPP™ for TCE at 17° C.

Source	Henry's Constant (-)	Temp. (C)	T min (C)	T max (C)
<input checked="" type="radio"/> Regression of Data Points	0.308	17.0	N/A	N/A
<input type="radio"/> UNIFAC Fit with Data Pt.	0.298	17.0		
<input type="radio"/> UNIFAC at Operating T	0.357	17.0		
<input type="radio"/> Database	0.282	15.0		
RTI	0.282	15.0		
<input type="radio"/> UNIFAC @ Database T's	0.338	15.0		
UNIFAC	0.338	15.0		
<input type="radio"/> User Input				

UNIFAC Group Interaction Database: Environmental VLE

Figure 2 - Henry's Constant Window for Trichloroethylene at 17° C

From Figure 2, the nearest temperature at which a data point is available is 15° C. From Figure 2, the database value of Henry's constant at 15° C is 0.282 and the UNIFAC value at 15° C is 0.335. Using these values, the program calculates the offset value at this temperature in the following manner.

Henry's constant values must first be converted to units of atmospheres:

$$\begin{aligned}
 H_{UNIFAC,15C} [atm] &= H_{UNIFAC,15C} \left[\frac{atm}{mol} \right] \frac{1}{RT} C_{H_2O} = 0.335 \left(0.082054 \frac{L \cdot atm}{mol \cdot K} \right) \left(\frac{1}{273.15 + 15} K \right) \left(55.5 \frac{mol}{L} \right) \\
 &= 439.5984689 \text{ atm} \\
 H_{data,15C} [atm] &= H_{data,15C} \left[\frac{atm}{mol} \right] \frac{1}{RT} C_{H_2O} = 0.282 \left(0.082054 \frac{L \cdot atm}{mol \cdot K} \right) \left(\frac{1}{273.15 + 15} K \right) \left(55.5 \frac{mol}{L} \right) \\
 &= 370.0500544 \text{ atm}
 \end{aligned}$$

$$\begin{aligned} \text{Offset} &= \ln(H_{UNIFAC,15C}) - \ln(H_{data,15C}) = \ln(439.5984689 \text{ atm}) - \ln(370.0500544 \text{ atm}) \\ &= 0.17222346 \end{aligned}$$

Then to obtain the UNIFAC fit with a data point at 17° C, this offset is applied to the UNIFAC value obtained at that temperature (0.355) as follows:

$$\begin{aligned} H_{UNIFAC,17C} &= H_{UNIFAC,17C} \exp(-RT C_{H_2O} / C_{H_2O}^{\infty}) = 0.355 \exp\left(\frac{0.082054 \frac{\text{Latm}}{\text{molK}}}{273.15 + 15} \frac{55.5 \frac{\text{mol}}{\text{L}}}{1}\right) \\ &= 465.8431536 \text{ atm} \\ \ln(H_{UNIFAC \text{ Fit with data point, 17 C}}) &= \ln(H_{UNIFAC,17C}) - \text{Offset} = \ln(465.8431536 \text{ atm}) - 0.17222346 \\ &= 5.971625537 = \ln(H_{UNIFAC \text{ Fit with data point, 17 C}}) \Rightarrow \\ H_{UNIFAC \text{ Fit with data point, 17 C}} &= \exp(5.971625537) \\ &= 392.1425952 \text{ atm} \Rightarrow \\ H_{UNIFAC \text{ Fit with data point, 17 C}} &= H_{UNIFAC \text{ Fit with data point, 17 C}} \exp(-RT C_{H_2O} / C_{H_2O}^{\infty}) \\ &= 392.1425952 \text{ atm} / \exp\left(\frac{0.082054 \frac{\text{Latm}}{\text{molK}}}{273.15 + 15} \frac{55.5 \frac{\text{mol}}{\text{L}}}{1}\right) \\ &= 0.299 \end{aligned}$$

This result is in agreement with the “UNIFAC Fit with Data Point” value shown in Figure 2.

c) UNIFAC at the operating temperature

The section entitled “Note on UNIFAC” provides general information on properties that are available from UNIFAC. Information specific to Henry’s constant is given here. By definition, Henry’s constant is equal to the product of the Lewis-Randall infinite dilution activity coefficient and the pure component vapor pressure. In StEPP™, Henry’s constant is estimated by multiplying the infinite dilution activity coefficient estimated by UNIFAC by the solute’s pure component vapor pressure calculated from a temperature-dependent correlation in the StEPP™ database. Equilibrium air-water partitioning of a chemical solute obeys Henry’s Law only when the liquid mixture is very dilute in the solute (Carroll, 1991).

d) Database

The StEPP™ database contains discrete Henry’s constant data available from the following:

1. Research Triangle Institute (RTI)/U.S. Air Force/U.S. EPA experimental measurements (Ashworth, et al., 1988)
2. Yaws (1992)
3. EPA Superfund Public Health Evaluation Manual (1986)

The data from source (1) is available for several compounds at several temperatures (typically from 10° to 30°C). The data for sources (2) and (3) is available at a single discrete temperature. The StEPP™ database contains data from (1) if it is available. If no data is available from source (1) then it will contain data from source (2) if it is available. If no data is available from (1) or (2) then the database contains data from source (3).

e) UNIFAC at database temperatures

For comparison purposes, StEPP™ calculates UNIFAC values for Henry's constant at temperatures corresponding to those for which data is available in the StEPP™ database. Details on the UNIFAC determination of Henry's constants is given in the "UNIFAC at Operating Temperature" section above.

E. Molecular Weight

1. Sources Available and Hierarchy

Molecular weight is available in StEPP™ from the following:

1. AIChE/DIPPR®
2. Group Contribution Method

2. References

a) AIChE/DIPPR®

Daubert, T.E., R.P. Danner, H.M. Sibul, and C.C. Stebbins, Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation, Extant 1995, Taylor & Francis, Bristol, Pennsylvania (1995).

b) Group Contribution Method

Partington, J., "An Advanced Treatise on Physical Chemistry," Vol. I, Fundamental Principles: The Properties of Gases, Longmans, Green, New York (1949).

3. Detailed Information on the Sources Available

a) AICHE/DIPPR®

Molecular weight is available for all chemicals in the AICHE/DIPPR® data compilation.

b) Group Contribution Method

For this method, the molecular weight is determined based on atomic structure via the method of Schroeder. The application of this method is discussed in the following secondary sources:

Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt, Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds, New York: McGraw-Hill Book Company (1982).

Reid, R.C., J.M. Prausnitz, and B.E. Poling, The Properties of Gases and Liquids, 4th Ed., New York: McGraw-Hill Book Company (1987).

F. Normal Boiling Point

1. Sources Available and Hierarchy

1. AICHE/DIPPR®

2. References

a) AICHE/DIPPR®

Daubert, T.E., R.P. Danner, H.M. Sibul, and C.C. Stebbins, Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation, Extant 1995, Taylor & Francis, Bristol, Pennsylvania (1995).

3. Detailed Information on the Source Available

a) AICHE/DIPPR®

Normal boiling point is available as discrete data from this source.

G. *Liquid Density*

1. Sources Available and Hierarchy

1. AIChE/DIPPR[®]
2. Group Contribution Method

The order listed above is the preferential order for selection of the calculation methods.

2. References

a) *AIChE/DIPPR[®]*

Daubert, T.E., R.P. Danner, H.M. Sibul, and C.C. Stebbins, Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation, Extant 1995, Taylor & Francis, Bristol, Pennsylvania (1995).

b) *Group Contribution Method*

Partington, J., "An Advanced Treatise on Physical Chemistry," Vol. I, Fundamental Principles: The Properties of Gases, Longmans, Green, New York (1949).

3. Detailed Information on the Sources Available

a) *AIChE/DIPPR[®]*

This source provides a correlation that requires temperature input. The correlation used is:

$$\rho_l = \frac{A}{B \left(1 + \frac{T - T_{\min}}{C} \right)^D} \quad \text{in the range } T_{\min} < T < T_{\max}$$

where:

ρ_l =	Liquid density (kmol/m ³)
A, B, C, D =	Empirical coefficients
T =	Temperature (K)
T_{\min} =	Minimum temperature for which correlation applies (K)
T_{\max} =	Maximum temperature for which correlation applies (K)

From the AIChE/DIPPR[®] data compilation, for Trichloroethylene:

$$A = 1.0632$$

$$B = 0.27217$$

$$C = 571$$

$$D = 0.2986$$

$$T_{\min} = 188.4 \text{ K}$$

$$T_{\max} = 571 \text{ K}$$

Sample Calculation for Trichloroethylene at T_{\min} :

$$\begin{aligned} \rho_l &= \frac{A}{B \left[1 + \frac{T_{\min}}{C} \right]^D} \\ &= \frac{1.0632}{0.27217 \left[1 + \frac{188.4}{571} \right]^{0.2986}} \\ &= 12.395 \frac{\text{kmol}}{\text{m}^3} \end{aligned}$$

This result agrees with the value reported in Daubert, et al. (1995). The units in StEPP[™] for liquid density are kg/m^3 and this result converted to those units is $1630 \text{ kg}/\text{m}^3$.

Sample Calculation for Trichloroethylene at 10°C :

$$\begin{aligned} \rho_l &= \frac{A}{B \left[1 + \frac{T}{C} \right]^D} \\ &= \frac{1.0632}{0.27217 \left[1 + \frac{283.15}{571} \right]^{0.2986}} \\ &= 11.282 \frac{\text{kmol}}{\text{m}^3} \times 131.388 \frac{\text{kg}}{\text{kmol}} \\ &= 1480 \frac{\text{kg}}{\text{m}^3} \end{aligned}$$

b) Group Contribution Method

This liquid density is calculated from modified Schroeder group contribution method. It is calculated using the molar volume at the normal boiling point and referenced to water to account for the effect of temperature.

The equation used is shown below:

$$\begin{aligned} \left(\frac{\rho_l}{\rho_w} \right)_T &= \left(\frac{\rho_l}{\rho_w} \right)_{NBP} A \Rightarrow \\ \left(\frac{\rho_l}{\rho_w} \right)_T &= \left(\frac{\frac{MW}{V_{b,NBP}}}{\frac{MW_w}{V_{b,NBP,w}}} \right) A \Rightarrow \\ \rho_l &= \rho_w \left(\frac{\frac{MW}{V_{b,NBP}}}{\frac{18.015}{21.0}} \right) 0.95 \end{aligned}$$

where:

ρ_l = Liquid density of compound at the temperature of interest (kg/m^3)

ρ_w = Water density at temperature of interest (g/cm^3)

MW = Molecular weight of compound (g/mol)

MW_w = Molecular weight of water (g/mol)

$V_{b,NBP}$ = Molar volume at the normal boiling point of compound (cm^3/mol)

$V_{b,NBP,w}$ = Molar volume at the normal boiling point of water (cm^3/mol)

A = Empirical factor designed to represent temperature dependency of compound's liquid density referenced to water. It was found to equal 0.95 in limited tests over several classes of compounds.

Sample Calculation for Trichloroethylene at 10° C

From StEPP™:

$$\rho_w = 999.75 \frac{\text{kg}}{\text{m}^3} \cdot \frac{1000 \text{ g}}{\text{kg}} \cdot \frac{1 \text{ m}^3}{100^3 \text{ cm}^3} = 0.99975 \frac{\text{g}}{\text{cm}^3}$$

$$MW = 131.39 \frac{\text{g}}{\text{mol}}$$

$$V_{b,NBP} = 0.102 \frac{\text{m}^3}{\text{kmol}} \cdot \frac{1 \text{ kmol}}{1000 \text{ mol}} \cdot \frac{1000000 \text{ cm}^3}{\text{m}^3} = 102 \frac{\text{cm}^3}{\text{mol}}$$

Solving the equation given above, which has been rearranged slightly:

$$\begin{aligned}\rho_l &= \left[\frac{0.95}{18.015/21.0} \right] \cdot \rho_w \cdot \frac{MW}{V_{b,NBP}} \cdot \frac{1000 \text{ kg/m}^3}{1 \text{ g/cm}^3} \\ &= \left[\frac{0.95}{18.015/21.0} \right] \cdot \left[0.99975 \frac{\text{g}}{\text{cm}^3} \right] \cdot \left[\frac{131.39 \frac{\text{g}}{\text{mol}}}{102 \frac{\text{cm}^3}{\text{mol}}} \right] \cdot \left[\frac{1000 \text{ kg/m}^3}{1 \text{ g/cm}^3} \right] \\ &= 1430 \frac{\text{kg}}{\text{m}^3}\end{aligned}$$

H. Molar Volume at Operating Temperature

1. Sources Available and Hierarchy

The sources available are:

1. AIChE/DIPPR[®]
2. Group Contribution Method

The molar volumes at the operating temperature given above are calculated as the inverse of liquid density multiplied by molecular weight. The order listed above is the preferential order for selection of the calculation methods.

2. References

a) AIChE/DIPPR[®]

Same as for liquid density.

b) Group Contribution Method

Same as for liquid density.

3. Detailed Information on the Sources Available

Molar volumes at the operating temperature for both methods are calculated from the following relationship:

$$V_{b,T} = MW / \rho_l$$

where:

- $V_{b,T}$ = Molar volume at the operating temperature (m^3/kmol)
- MW = Molecular weight (kg/kmol)
- ρ_l = Liquid density (kg/m^3)

a) AICHE/DIPPR®

Sample Calculation for TCE at 10° C

From StEPP™:

$$MW = 131.39 \frac{\text{kg}}{\text{kmol}}$$

$$\rho_l = 1480 \frac{\text{kg}}{\text{m}^3}$$

Calculating molar volume at the operating temperature:

$$\begin{aligned} V_{b,T} &= 131.39 \frac{\text{kg}}{\text{kmol}} / 1480 \frac{\text{kg}}{\text{m}^3} \\ &= 0.0888 \frac{\text{m}^3}{\text{kmol}} \end{aligned}$$

b) Group Contribution Method

Sample Calculation for TCE at 10° C

From StEPP™:

$$MW = 131.39 \frac{\text{kg}}{\text{kmol}}$$

$$\rho_l = 1430 \frac{\text{kg}}{\text{m}^3}$$

Calculating molar volume at the operating temperature:

$$\begin{aligned} V_{b,T} &= 131.39 \frac{\text{kg}}{\text{kmol}} / 1430 \frac{\text{kg}}{\text{m}^3} \\ &= 0.0919 \frac{\text{m}^3}{\text{kmol}} \end{aligned}$$

I. Molar Volume at Normal Boiling Point

1. Sources Available and Hierarchy

Molar volume is available in StEPP™ from:

1. Modified Schroeder group contribution method

2. References

a) Modified Schroeder group contribution method

Partington, J., “An Advanced Treatise on Physical Chemistry,” Vol. I, Fundamental Principles: The Properties of Gases, Longmans, Green, New York (1949).

3. Detailed Information on the Sources Available

a) Modified Schroeder group contribution method

The application of this method is discussed in the following secondary sources:

Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt, Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds, New York: McGraw-Hill Book Company (1982).

Reid, R.C., J.M. Prausnitz, and B.E. Poling, The Properties of Gases and Liquids, 4th Ed., New York: McGraw-Hill Book Company (1987).

J. Refractive Index

1. Sources Available and Hierarchy

The refractive index is available in StEPP™ from:

1. AICHE/DIPPR®

2. References

a) AICHE/DIPPR®

Daubert, T.E., R.P. Danner, H.M. Sibul, and C.C. Stebbins, Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation, Extant 1995, Taylor & Francis, Bristol, Pennsylvania (1995).

3. Detailed Information on the Sources Available

a) AICHE/DIPPR®

Discrete data for refractive index is available from this source.

K. Aqueous Solubility

1. Sources Available and Hierarchy

The available data in StEPP™ is from:

1. UNIFAC fit with a data point
2. UNIFAC at the operating temperature
3. Database
4. UNIFAC at database temperature

The ordering given above is the preferential order for selection of aqueous solubilities in StEPP™.

2. References

a) *UNIFAC fit with a data point*

See below for obtaining the UNIFAC values. No references for the fit.

b) *UNIFAC at the operating temperature*

See the section "Note on UNIFAC" for the general references on UNIFAC. A discussion of this calculation is given in Appendix A.3 of Rogers (1994).

c) *Database*

Yaws, C.L., J.W. Miller, P.N. Shah, G.R. Schorr, and P.M. Patel, "Correlation Constants for Chemical Compounds," *Chem. Eng.*, **83**:25, 153-162 (1976).

EPA Superfund Public Health Evaluation Manual, U.S. Environmental Protection Agency, Office of Emergency and Remedial Response, Washington, D.C., EPA/540/1-86/060 (October 1986).

d) *UNIFAC at database temperature*

See the section "Note on UNIFAC" for the general references on UNIFAC.

3. Detailed Information on the Sources Available

a) *UNIFAC fit with a data point*

For the special case in which the user desires a property value for aqueous solubility at a temperature different from a single discrete value in the database, UNIFAC is used as an extrapolation tool (see the "Note on UNIFAC" section for a detailed discussion of UNIFAC). A UNIFAC estimate at the database temperature is first used to calculate the "offset" between the UNIFAC prediction and the data point. This offset is then applied at the temperature of interest to correct the UNIFAC estimate to be consistent with the given data value (i.e., the UNIFAC property-versus-temperature curve is forced through the discrete database value). This extrapolation technique takes advantage of the linear relationship between aqueous solubility and temperature. Elsewhere in this paper and in StEPP™, this procedure is referred to as "UNIFAC Fit with Data Point."

Sample Calculation to Estimate Aqueous Solubility of TCE at 17° C

Figure 3 shows the aqueous solubility window from StEPP™ for TCE at 17° C.

Source	Aqueous Sol. (PPMw)	Temp. (C)
<input checked="" type="radio"/> UNIFAC Fit with Data Pt.	946	17.0
<input type="radio"/> UNIFAC at Operating T	1.03E+03	17.0
<input type="radio"/> Database	1.10E+03	25.0
<input type="radio"/> UNIFAC at Database T	1.18E+03	25.0
<input type="radio"/> User Input		

UNIFAC Group Interaction Database: Environmental VLE

Figure 3 - Aqueous Solubility Window for TCE at 17° C

From Figure 3, the following values are used in the calculation of the offset:

$$sol_{UNIFAC,25C} = 1180 \text{ PPM}_w$$

$$sol_{data,25C} = 1100 \text{ PPM}_w$$

From these values, an offset to apply at other temperatures is calculated as:

$$\begin{aligned} \text{Offset} &= sol_{UNIFAC,25C} - sol_{data,25C} = 1180 \text{ PPM}_w - 1100 \text{ PPM}_w \\ &= 80 \text{ PPM}_w \end{aligned}$$

Then aqueous solubilities at other temperatures can be estimated from:

$$\begin{aligned} sol_{UNIFAC \text{ Fit with Data Point, } T} &= sol_{UNIFAC, T} - \text{Offset} \Rightarrow \\ sol_{UNIFAC \text{ Fit with Data Point, } 17C} &= sol_{UNIFAC, 17C} - \text{Offset} \\ &= 1030 \text{ PPM}_w - 80 \text{ PPM}_w \\ &= 950 \text{ PPM}_w \end{aligned}$$

This value agrees with that reported in Figure 3 for “UNIFAC Fit with Data Point”.

b) UNIFAC at the operating temperature

The section entitled “Note on UNIFAC” provides general information on properties that are available from UNIFAC. Information specific to aqueous solubility is given here. At the saturation composition, adding an additional differential amount of solute to an aqueous mixture will form a second solute-rich phase containing an equilibrium trace amount of water. The mutual miscibility of a chemical with water can be calculated rigorously from solution thermodynamics and UNIFAC activity coefficient estimates. Phase equilibrium relationships are set up and solved within StEPP™ to predict the organic and water compositions (i.e., solubility limits) of the equilibrium liquid phases. The solubility limit of the organic in the water-rich phase is displayed in StEPP™ as the aqueous solubility.

c) Database

The StEPP™ database contains discrete aqueous solubility data available from the following:

1. Yaws (1992)
2. EPA Superfund Public Health Evaluation Manual (1986)

The data for both sources is available at a single discrete temperature. The StEPP™ database contains data from (1) if it is available. If no data is available from source (1) then the database will contain data from source (2) if it is available.

d) UNIFAC at database temperature

For comparison purposes, StEPP™ calculates a UNIFAC value for aqueous solubility at the temperature corresponding to that for which data is available in the StEPP™ database. Details on the UNIFAC determination of aqueous solubilities is given in the “UNIFAC at Operating Temperature” section above.

L. Octanol Water Partition Coefficient (log K_{ow})

1. Sources Available and Hierarchy

The available data in StEPP™ is from:

1. UNIFAC at the operating temperature
2. Database

3. UNIFAC at database temperature

The ordering given above is the preferential order for selection of octanol water partition coefficients in StEPP™.

2. References

a) UNIFAC at the operating temperature

See the section “Note on UNIFAC” for the general references on UNIFAC. A discussion of this calculation is presented in Appendix A.4 of Rogers (1994).

b) Database

EPA Superfund Public Health Evaluation Manual, U.S. Environmental Protection Agency, Office of Emergency and Remedial Response, Washington, D.C., EPA/540/1-86/060 (October 1986).

c) UNIFAC at database temperature

See the section “Note on UNIFAC” for the general references on UNIFAC.

3. Detailed Information on the Sources Available

a) UNIFAC at the operating temperature

The section entitled “Note on UNIFAC” provides general information on properties that are available from UNIFAC. Information specific to the octanol water partition coefficient is given here. The octanol water partition coefficient is calculated from the UNIFAC activity coefficient model by a series of steps. First, the user selects a temperature of interest and StEPP™ performs a binary octanol-water equilibrium calculation according to the rigorous solution of phase equilibrium relationships. Because the two components are almost immiscible in each other, two phases are predicted: an octanol-rich phase containing dissolved water, and a water-rich phase containing dissolved octanol. Once the composition of each phase has been calculated, infinite dilution activity coefficients for a third component in each phase are then determined. The octanol/water partition coefficient is directly proportional to the ratio of the infinite dilution activity coefficients for a third component distributed between the water-rich and octanol-rich phases.

b) Database

The StEPP™ database contains discrete octanol water partition coefficient data available from the following:

1. EPA Superfund Public Health Evaluation Manual (1986)

The data is available at a single discrete temperature.

c) UNIFAC at database temperature

For comparison purposes, StEPP™ calculates a UNIFAC value for the octanol water partition coefficient at the temperature corresponding to that for which data is available in the StEPP™ database. Details on the UNIFAC determination of octanol water partition coefficients is given in the “UNIFAC at Operating Temperature” section.

M. Liquid Diffusivity

1. Sources Available and Hierarchy

Property estimation methods available in StEPP™ for liquid diffusivity include:

1. Hayduk and Laudie correlation
2. Wilke-Chang correlation
3. Method of Polson

The above ordering is the hierarchy for the case where molecular weight is less than 1000. When molecular weight is greater than 1000, the hierarchy of estimation methods for liquid diffusivity becomes (1) Method of Polson; (2) Hayduk and Laudie correlation, and (3) Wilke-Chang correlation.

2. References

a) Hayduk and Laudie Correlation

Hayduk, W. and H. Laudie, "Prediction of Diffusion Coefficients for Non-electrolytes in Dilute Aqueous Solutions," *Jour. AIChE*, **28**, 611 (1974).

b) Wilke-Chang Correlation

Wilke, C.R. and P.C. Chang, "Correlation of Diffusion Coefficients in Dilute Solutions," *J. AIChE*, **1** (1955).

A discussion of the application of this method is provided in:

Reid, R.C., J.M. Prausnitz, and B.E. Poling, The Properties of Liquids and Gases, 4th ed., New York: McGraw-Hill Book Company (1987).

c) Method of Polson

Polson, A., "Some Aspects of Diffusion in Solution and a Definition of a Colloidal Particle," *Jour. Phys. Coll. Chem.*, **54**, 649 (1950).

3. Detailed Information on the Sources

a) Hayduk and Laudie Correlation

This correlation is a modification of the Wilke-Chang Correlation and can be used for small molecules in water.

$$D_l = \frac{13.26 \times 10^{-5}}{\mu_w^{1.14} V_b^{0.589}} \frac{\text{cm}^2}{\text{s}} \cdot \frac{1 \text{m}^2}{100^2 \text{cm}^2}$$

Where:

D_l = Liquid diffusivity of compound (m^2/s)

μ_w = Viscosity of water ($\text{cp} = 0.01 \text{ g/cm/s}$)

V_b = Molar volume of solute at normal boiling point (cm^3/gmol)

Sample Calculation for Trichloroethylene at 10° C

Retrieving properties of Trichloroethylene required for the calculation from StEPP™:

$$\begin{aligned} V_b &= 0.102 \frac{\text{m}^3}{\text{kmol}} \cdot \frac{100^3 \text{cm}^3}{\text{m}^3} \cdot \frac{1 \text{kmol}}{1000 \text{gmol}} = 102 \frac{\text{cm}^3}{\text{gmol}} \\ \mu_w &= 0.00131 \frac{\text{kg}}{\text{msec}} \cdot \frac{1000 \text{cp}}{\text{kg/m/s}} = 1.31 \text{cp} \\ D_l &= \frac{13.26 \times 10^{-5}}{\mu_w^{1.14} V_b^{0.589}} \frac{\text{cm}^2}{\text{s}} \cdot \frac{1 \text{m}^2}{100^2 \text{cm}^2} = \frac{13.26 \times 10^{-5}}{(1.31 \text{cp})^{1.14} (102 \frac{\text{cm}^3}{\text{gmol}})^{0.589}} \frac{\text{cm}^2}{\text{s}} \cdot \frac{1 \text{m}^2}{100^2 \text{cm}^2} \\ &= 6.39 \times 10^{-10} \frac{\text{m}^2}{\text{sec}} \end{aligned}$$

b) Wilke-Chang Correlation

This correlation is based on the Stokes-Einstein Equation. For background on the Wilke-Chang correlation, see Treybal (1980). To calculate the liquid diffusivity of a compound in water, the equation takes the following form:

$$D_l = 7.4 \times 10^{-8} \frac{\phi M_w^{1/2} T}{\mu_w V_b^{1/6}} \frac{1 \text{m}^2}{100^2 \text{cm}^2}$$

Where:

D_l = Liquid diffusivity of compound (m^2/s)

M_w = Molecular weight of water

T = Temperature (K)

μ_w = Viscosity of water ($\text{cp} = 0.01 \text{ g/cm/s}$)

V_b = Molar volume of solute at normal boiling point (cm^3/gmol)

ϕ = Association parameter of water (dimensionless) = 2.26

Sample Calculation for Trichloroethylene at 10°C

Retrieving properties of Trichloroethylene required for the calculation from StEPP™:

$$V_b = 0.102 \frac{\text{m}^3}{\text{kmol}} \cdot \frac{100^3 \text{ cm}^3}{\text{m}^3} \cdot \frac{1 \text{ kmol}}{1000 \text{ gmol}} = 102 \frac{\text{cm}^3}{\text{gmol}}$$

$$\mu_w = 0.00131 \frac{\text{kg}}{\text{msec}} \cdot \frac{1000 \text{ cp}}{\text{kg/m/s}} = 1.31 \text{ cp}$$

$$D_l = 7.4 \times 10^{-8} \frac{\phi M_w^{1/2} T}{\mu_w V_b^{1/6}} \frac{1 \text{ m}^2}{100^2 \text{ cm}^2} = 7.4 \times 10^{-8} \frac{2.26 (18.0)^{1/2} 283.15 \text{ K}}{1.31 \text{ cp} (102 \frac{\text{cm}^3}{\text{gmol}})^{1/6}} \frac{\text{cm}^2}{\text{s}} \cdot \frac{1 \text{ m}^2}{100^2 \text{ cm}^2}$$

$$= 6.36 \times 10^{-10} \frac{\text{m}^2}{\text{s}}$$

c) *Method of Polson (1950)*

This method is only applicable for large molecular weight compounds (> 1000). The equation for the calculation of liquid diffusivity is:

$$D_l = 2.74 \times 10^{-5} \text{ MW}^{-1/3} \frac{\text{cm}^2}{\text{s}} \cdot \frac{1 \text{ m}^2}{100^2 \text{ cm}^2}$$

Where:

D_l = Liquid diffusivity of compound (m^2/s)

MW = Molecular weight of compound

Sample Calculation for Trichloroethylene

From StEPP™, MW for Trichloroethylene equals 131.39 (note the correlation would not apply to this compound but the numerical calculation can still be checked).

$$D_l = 0.274 \times 10^{-5} \left(MW \right)^{-\frac{1}{3}} \left(\frac{cm^2}{s} \right) \cdot \frac{1m^2}{100^2 cm^2} = 0.274 \times 10^{-5} \left(131.39 \right)^{-\frac{1}{3}} \left(\frac{cm^2}{s} \right) \cdot \frac{1m^2}{100^2 cm^2}$$

$$= 5.39 \times 10^{-10} \frac{m^2}{s}$$

N. Gas Diffusivity

1. Sources Available and Hierarchy

Property estimation methods available in StEPP™ for gas diffusivity include:

1. Wilke-Lee Modification of Hirschfelder-Bird-Spotz Equation

2. References

a) Wilke-Lee Modification of Hirschfelder-Bird-Spotz Equation

Wilke, C.R. and C.Y. Lee, *Ind. Eng. Chem.*, **47**, 1253 (1955).

Hirschfelder, J.O., R.B. Bird, and E.L. Spotz, *Trans. ASME*, **71**, 921 (1949); *Chem. Rev.*, **44**, 205 (1949).

A discussion of the application of the method is provided in:

Treybal, R.E., Mass-Transfer Operations, 3rd ed., New York: McGraw-Hill Book Company (1980).

3. Detailed Information on the Sources Available

a) Wilke-Lee Modification of Hirschfelder-Bird-Spotz Equation

This correlation can be used to calculate the diffusivity of an organic compound in the gas-phase. Background information on the correlation is provided in Treybal (1980).

$$D_{AB} = \frac{10^{-4} \left[1.084 - 0.249 \sqrt{\frac{1}{M_A} + \frac{1}{M_B}} \right] T^{1.5} \sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{P_t r_{AB}^2 f \left(\frac{KT}{\epsilon_{AB}} \right)} \frac{m^2}{s}$$

Where:

D_{AB} = Gas diffusivity of organic compound A in stagnant gas B (m^2/s)

T = Absolute temperature (K)

M_A = Molecular weight of A

M_B = Molecular weight of B

$P_t =$	Absolute pressure (N/m ²)
$r_{AB} =$	Molecular separation at collision (nm) = $(r_A + r_B) / 2$
$\epsilon_{AB} =$	Energy of molecular attraction = $\sqrt{(\epsilon_A \cdot \epsilon_B)}$
$K =$	Boltzman's constant
$f \left(\frac{K T}{\epsilon_{AB}} \right)$	Collision function

See page 33 of Treybal (1980) for estimating some of the above parameters. Given below are the necessary parameter estimation correlations using air as the stagnant gas, B.

M_A = Molecular weight of organic compound A

$$r_A = 1.18 \left(V_b \right)^{1/3}$$

V_b = Molar volume of A at normal boiling point (m³/kmol)

$$\epsilon_A / K = 1.21 \left(T_{b,A} \right)$$

$T_{b,A}$ = Normal boiling point of A (K)

$$M_B = 28.95$$

$$r_B = 0.3711 \text{ nm}$$

$$\epsilon_B / K = 78.6$$

$$\frac{\epsilon_{AB}}{K} = \sqrt{\frac{\epsilon_A}{K} \cdot \frac{\epsilon_B}{K}}$$

$$EE = \log_{10} \left(\frac{K T}{\epsilon_{AB}} \right)$$

T = Operating Temperature (K)

$$NN = \left[-0.14329 - 0.48343 EE + 0.1939 EE^2 + 0.13612 EE^3 \right] - \left[-0.20578 EE^4 + 0.083899 EE^5 - 0.011491 EE^6 \right]$$

$$f \left(\frac{K T}{\epsilon_{AB}} \right) = 10^{NN}$$

Sample Calculation for Trichloroethylene in Air at 10°C and 101325 Pa
Determination of Required Parameters

A = Trichloroethylene B = Air

M_A = 131.39 kg/kmol (from StEPP™)

V_b = 0.102 m³/kmol (from StEPP™)

$$r_A = 1.18 \left(V_b \right)^{1/3} = 1.18 \left(0.102 \right)^{1/3} = 0.551335 \text{ nm}$$

$$T_{b,A} = 360.15 \text{ K}$$

$$\epsilon_A / K = 1.21 \left(\frac{T_b}{T_A} \right) = 1.21 \left(\frac{360.15}{T} \right) = 435.7815$$

$$M_B = 28.95$$

$$r_B = 0.3711 \text{ nm}$$

$$\epsilon_B / K = 78.6$$

$$r_{AB} = (r_A + r_B) / 2 = (0.551335 \text{ nm} + 0.3711 \text{ nm}) / 2 = 0.4612175 \text{ nm}$$

$$\frac{\epsilon_{AB}}{K} = \sqrt{\frac{\epsilon_A}{K} \cdot \frac{\epsilon_B}{K}} = \sqrt{435.7815 \cdot 78.6} = 185.07411$$

$$T = 283.15 \text{ K}$$

$$EE = \log_{10} (KT / \epsilon_{AB}) = \log_{10} (283.15 / 185.07411) = 0.1846709$$

$$\begin{aligned} NN &= \left[-0.14329 - 0.48343(EE) + 0.1939(EE)^2 + 0.13612(EE)^3 \right. \\ &\quad \left. - 0.20578(EE)^4 + 0.083899(EE)^5 - 0.011491(EE)^6 \right] \\ &= \left[-0.14329 - 0.48343(0.1846709) + 0.1939(0.1846709)^2 \right. \\ &\quad \left. + 0.13612(0.1846709)^3 - 0.20578(0.1846709)^4 \right. \\ &\quad \left. + 0.083899(0.1846709)^5 - 0.011491(0.1846709)^6 \right] \\ &= -0.225317312 \end{aligned}$$

$$f \left(\frac{KT}{\epsilon_{AB}} \right) = 10^{NN} = 10^{-0.225317312} = 0.595227089$$

Calculation of Gas Diffusivity:

$$\begin{aligned} D_{AB} &= \frac{10^{-4} \left[1.084 - 0.249 \sqrt{\frac{1}{M_A} + \frac{1}{M_B}} \right] C T^{1.5} \sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{P_t (r_{AB})^2 f \left(\frac{KT}{\epsilon_{AB}} \right)} \frac{m^2}{s} \\ &= \frac{10^{-4} \left[1.084 - 0.249 \sqrt{\frac{1}{131.39} + \frac{1}{28.95}} \right] C (283.15)^{1.5} \sqrt{\frac{1}{131.39} + \frac{1}{28.95}}}{101325 (0.4612175)^2 0.595227089} \frac{m^2}{s} \\ &= 7.88 \times 10^{-6} \frac{m^2}{s} \end{aligned}$$

O. Water Density

1. Sources Available and Hierarchy

Water density is estimated in StEPP™ from:

1. Correlation developed from polynomial fit of data from McCabe and Smith (1976).

2. Reference

McCabe, W.L. and J.C. Smith, Unit Operations of Chemical Engineering, 3rd ed., New York: McGraw-Hill Book Company (1976).

3. Detailed Information on the Source Available

The correlation used to calculate water density is given below:

$$a_1 = -1.4176800403$$

$$a_2 = 8.9766515240$$

$$a_3 = -12.275501969$$

$$a_4 = 7.4584410413$$

$$a_5 = -1.7384916050$$

$$x_{avg} = 324.65$$

$$F_{avg} = 0.98396$$

$$x_n = T / x_{avg}$$

$$F_n = a_1 + a_2 \cdot \ln x_n + a_3 \cdot (\ln x_n)^2 + a_4 \cdot (\ln x_n)^3 + a_5 \cdot (\ln x_n)^4$$

$$F_x = F_n \cdot F_{avg}$$

$$\rho_w = F_x \cdot 1000$$

where:

$$\rho_w = \text{Water density (kg/m}^3\text{)}$$

$$T = \text{Temperature (K)}$$

Sample Calculation at 10° C

$$a_1 = -1.4176800403$$

$$a_2 = 8.9766515240$$

$$a_3 = -12.275501969$$

$$a_4 = 7.4584410413$$

$$a_5 = -1.7384916050$$

$$x_{avg} = 324.65$$

$$F_{avg} = 0.98396$$

$$x_n = T / x_{avg} = x_n = 283.15 \text{ K} / 324.65$$

$$= 0.872170029$$

$$F_n = a_1 + a_2 \cdot x_n + a_3 \cdot x_n^2 + a_4 \cdot x_n^3 + a_5 \cdot x_n^4$$

$$= \left[1.4176800403 + 8.9766515240 \cdot 0.872170029 + 12.275501969 \cdot 0.872170029^2 + 7.4584410413 \cdot 0.872170029^3 + 1.7384916050 \cdot 0.872170029^4 \right]$$

$$= 1.016047635$$

$$F_x = F_n \cdot F_{avg} = 1.016047635 \cdot 0.983961$$

$$= 0.99975$$

$$\rho_w = F_x \cdot 1000 = 0.99975 \cdot 1000$$

$$= 999.75 \frac{\text{kg}}{\text{m}^3}$$

P. Water Viscosity

1. Sources Available and Hierarchy

Water viscosity is available in StEPP™ from:

1. Correlation presented in Yaws et al. (1976)

2. Reference

Yaws, C.L., J.W. Miller, P.N. Shah, G.R. Schorr, and P.M. Patel, "Correlation Constants for Chemical Compounds," *Chem. Eng.*, **83**:25, 153-162 (1976).

3. Detailed Information on the Source Available

The correlation used to calculate water viscosity is shown below:

$$\mu_w = \exp \left[-24.71 + \frac{4209.0}{T} + 0.04527 \cdot T - (3.376 \times 10^{-5}) T^2 \right]$$

where:

μ_w = Water viscosity (kg/m/s)

T = Temperature (K)

Sample Calculation at 10° C

$$\mu_w = 0.001 \exp \left[-24.71 + \frac{4209.0}{T} + 0.04527 \cdot T - (3.376 \times 10^{-5}) T^2 \right]$$

$$= 0.001 \exp \left[-24.71 + \frac{4209.0}{283.15} + 0.04527 \cdot 283.15 - (3.376 \times 10^{-5}) 283.15^2 \right]$$

$$= 0.00131 \frac{\text{kg}}{\text{m} \cdot \text{s}}$$

Q. Water Surface Tension

1. Sources Available and Hierarchy

The water surface tension is available in StEPP™ from:

1. Correlation developed by Cummins and Westrick (1983)

2. Reference

Cummins, M.D. and J.J. Westrick, "Proceedings ASCE Environmental Engineering Conference," Boulder, Colorado, 442-449 (July 1983).

3. Detailed Information on the Source Available

The correlation used to calculate water surface tension is shown below:

$$\sigma = 0.07558301 - 1.3143 \times 10^{-4} T - 4.7616 \times 10^{-7} T^2$$

where:

σ = Water surface tension (N/m)

T = Temperature (°C)

Sample Calculation at 10° C

$$\begin{aligned}\sigma &= 0.07558301 - 1.3143 \times 10^{-4} T - 4.7616 \times 10^{-7} T^2 \\ &= 0.07558301 - 1.3143 \times 10^{-4} (10) - 4.7616 \times 10^{-7} (10)^2 \\ &= 0.0742 \frac{N}{m}\end{aligned}$$

R. Air Density

1. Sources Available and Hierarchy

Air density is estimated in StEPP™ from the following method

1. Ideal gas law

2. Reference

Any general chemistry book

3. Detailed Information on the Sources Available

The ideal gas law is shown below:

$$\rho_{air} = \frac{M_{air} P}{RT}$$

where:

M_{air} = Molecular weight of air = 28.95

P = Pressure (atm)

$R =$ Universal gas constant (L atm/mol K) = 0.08205

$T =$ Temperature (K)

Sample Calculation at 10° C and 101325 Pa (1 atm)

$$\rho_{air} = \frac{M_{air} P}{RT} = \frac{28.95 \frac{g}{mol} |1 atm|}{(0.08205 \frac{L atm}{mol K}) |283.15 K|} = 1.25 \frac{g}{L} \times \frac{1 kg}{1000 g} \times \frac{1000 L}{m^3}$$

$$= 1.25 \frac{kg}{m^3}$$

S. Air Viscosity

1. Sources Available and Hierarchy

The air viscosity is available in StEPP™ from:

1. Correlation developed by Cummins and Westrick (1983)

2. Reference

Cummins, M.D. and J.J. Westrick, "Proceedings ASCE Environmental Engineering Conference," Boulder, Colorado, 442-449 (July 1983).

3. Detailed Information on the Source Available

The correlation used to calculate air viscosity is shown below:

$$\mu_{air} = 1.7E-07 | T^{0.818}$$

where:

$\mu_{air} =$ Air viscosity (kg/m/s)

$T =$ Temperature (K)

Sample Calculation at 10° C

$$\mu_{air} = 1.7E-07 | T^{0.818} = 1.7E-07 | 283.15^{0.818}$$

$$= 1.72 \times 10^{-5} \frac{kg}{m \cdot s}$$

IV. Sample Run of StEPP™

A. Running StEPP[®]

To run StEPP™, load Windows and click twice on the StEPP™ icon in Program Manager. The program will initialize and the window shown in Figure 4 will appear on the screen:

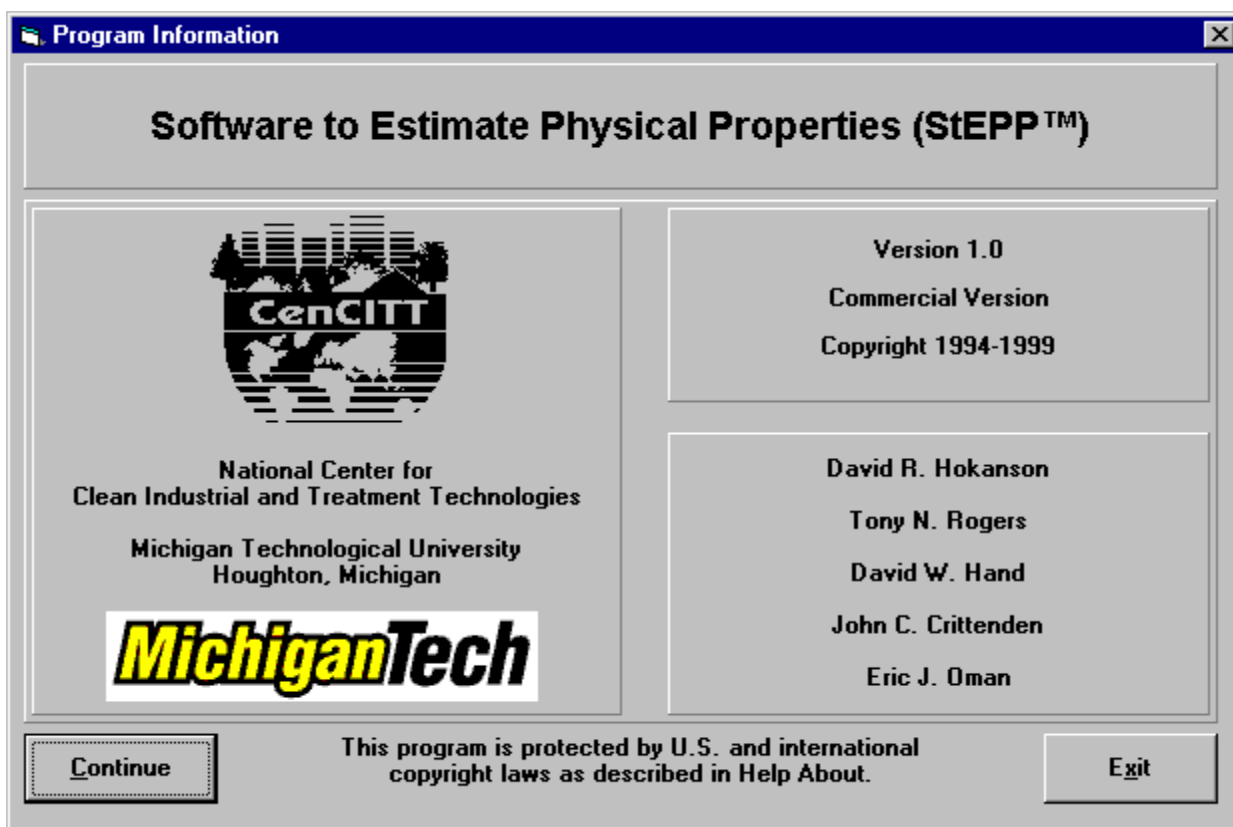


Figure 4 - Title Window in StEPP™

Click on the **Continue** command button shown in Figure 4 and a user agreement will appear. Click on **I Agree** then the StEPP™ main window will appear, as shown in Figure 5:

chemicals, as described in Appendix A). Once this is done, the main window will appear as shown in Figure 6.

StEPP - Software to Estimate Physical Properties

File Units Options Help

Operating Conditions:

Pressure (Pa) 101325

Temperature (C) 10.0

Available Contaminants:

79016 TRICHLOROETHYLENE

79061 ACRYLAMIDE

79094 PROPIONIC ACID

79107 ACRYLIC ACID

79118 CHLOROACETIC ACID

79210 PERACETIC ACID

Find Find Next Occurrence

Synonyms Select Current Contaminant

Selected Contaminants:

Unselect Current Contaminant

Properties of the Contaminant:

Vapor Pressure (Pa)

Infinite Dilution Activity Coeff. (-)

Henry's Constant (-)

Molecular Weight (kg/kmol)

Normal Boiling Point (NBP) (C)

Liquid Density (kg/m3)

Molar Volume at Op. T (m3/kmol)

Molar Volume at NBP (m3/kmol)

Refractive Index @25 C

Aqueous Solubility (PPMw)

log Octanol Water Part. Coeff. (-)

Liquid Diffusivity (m2/s)

Gas Diffusivity (m2/s)

Properties of Air and Water:

Water Density (kg/m3)

Water Viscosity (kg/m/s)

Water Surface Tension (N/m)

Air Density (kg/m3)

Air Viscosity (kg/m/s)

Figure 6 - StEPP™ Main Window for Trichloroethylene at 10° C before Selection

Once trichloroethylene is selected in the **Available Contaminants** list box, it is necessary to have StEPP™ perform calculations of properties for this compound at the desired operating pressure and temperature. The desired operating pressure (101325 *Pa*) and temperature (10° C) have already been entered. The screen now appears as shown in Figure 6. In order to calculate properties, the **Select Current Contaminant** command button shown in Figure 6 is clicked. Once this is done, the StEPP main™ window updates to reflect the property values for trichloroethylene and the properties of air and water at 10° C and 101325 *Pa*. The updated StEPP main™ window is shown in Figure 7.

StEPP - Software to Estimate Physical Properties

File Units Options Help

Operating Conditions:

Pressure (Pa)

Temperature (C)

Available Contaminants:

79016	TRICHLOROETHYLENE
79061	ACRYLAMIDE
79094	PROPIONIC ACID
79107	ACRYLIC ACID
79118	CHLOROACETIC ACID
79210	PERACETIC ACID

Find Find Next Occurrence

Synonyms Select Current Contaminant

Selected Contaminants:

79016	TRICHLOROETHYLENE
79016	TRICHLOROETHYLENE

Unselect Current Contaminant

Properties of the Contaminant:

TRICHLOROETHYLENE

Vapor Pressure (Pa)	4.69E+03
Infinite Dilution Activity Coeff. (-)	8.12E+03
Henry's Constant (-)	0.230
Molecular Weight (kg/kmol)	131.39
Normal Boiling Point (NBP) (C)	87.0
Liquid Density (kg/m3)	1.48E+03
Molar Volume at Op. T (m3/kmol)	0.0886
Molar Volume at NBP (m3/kmol)	0.102
Refractive Index @25 C	1.4750
Aqueous Solubility (PPMw)	821
log Octanol Water Part. Coeff. (-)	2.38
Liquid Diffusivity (m2/s)	6.44E-10
Gas Diffusivity (m2/s)	7.89E-06

Properties of Air and Water:

Water Density (kg/m3)	999.75
Water Viscosity (kg/m/s)	1.31E-03
Water Surface Tension (N/m)	0.0742
Air Density (kg/m3)	1.25
Air Viscosity (kg/m/s)	1.72E-05

Figure 7 - StEPP Main™ Window for Trichloroethylene at 101325 Pa and 10° C

The values that appear in the StEPP main™ window for each property are chosen initially according to a hierarchy. For each individual property available in StEPP™, there may be more than one source of data values, not just the value chosen according to the hierarchy. For this reason, StEPP™ contains an individual property window for each property available in StEPP™ in which the user may choose to select a different value of a particular property to appear in the StEPP main™ window. For example, the property window for Liquid Density for the example given above is shown in Figure 8.

Liquid Density

Current Liquid Density Information		Accept Selected Liquid Density	
Value (kg/m ³)	1.48E+03		
Source	Database	Cancel	

	Source	Liq. Dens (kg/m ³)	Temp (C)	Tmin (C)	Tmax (C)
<input checked="" type="radio"/>	Database	1.48E+03	10.0	-84.8	298
<input type="radio"/>	Group Contribution Method	1.43E+03	10.0		
<input type="radio"/>	User Input				

Note : Result for Liquid Density is at 1 atm below the normal boiling point and at the saturation pressure above the normal boiling point.

Figure 8 - Liquid Density Window (Trichloroethylene, 10° C, 101325 Pa)

In Figure 7, it can be seen that the value for Liquid Density that appears in the StEPP main™ window from the hierarchy is **1.48E+03**. By examining the Liquid Density window in Figure 8, it is seen that the value **1.48E+03** (which has its source highlighted) comes from the source “Database”. Figure 8 also shows that there are two other potential sources of Liquid Density available in StEPP™, namely “Group Contribution Method” and “User Input”. The user may select either of the other choices (if they have values available) in a manner that will be described later.

StEPP™ has the capability to display its results in English units, as opposed to the SI units shown in Figure 7 and in Figure 8. English units can be selected in the **Units** menu on the StEPP main™ window. After doing this, Figure 9 shows the StEPP™ Main Window for the previous example when English units are selected.

StEPP - Software to Estimate Physical Properties

File Units Options Help

Operating Conditions:

Pressure (psi)

Temperature (F)

Available Contaminants:

79016	TRICHLOROETHYLENE
79061	ACRYLAMIDE
79094	PROPIONIC ACID
79107	ACRYLIC ACID
79118	CHLOROACETIC ACID
79210	PERACETIC ACID

Find Find Next Occurrence

Synonyms Select Current Contaminant

Selected Contaminants:

79016	TRICHLOROETHYLENE
79016	TRICHLOROETHYLENE

Unselect Current Contaminant

Properties of the Contaminant:

TRICHLOROETHYLENE

Vapor Pressure (psi)	0.681
Infinite Dilution Activity Coeff. (-)	8.12E+03
Henry's Constant (-)	0.230
Molecular Weight (lb/lb-mol)	131.39
Normal Boiling Point (NBP) (F)	189
Liquid Density (lb/ft3)	92.5
Molar Volume at Op. T (ft3/lb-mol)	1.42
Molar Volume at NBP (ft3/lb-mol)	1.63
Refractive Index @77 F	1.4750
Aqueous Solubility (PPMw)	821
log Octanol Water Part. Coeff. (-)	2.38
Liquid Diffusivity (ft2/s)	6.93E-09
Gas Diffusivity (ft2/s)	8.49E-05

Properties of Air and Water:

Water Density (lb/ft3)	62.41
Water Viscosity (lb/ft/s)	8.77E-04
Water Surface Tension (lbf/ft)	5.09E-03
Air Density (lb/ft3)	0.0778
Air Viscosity (lb/ft/s)	1.16E-05

Figure 9 -StEPP main™ Window (Trichloroethylene, 14.696 psi, 50° F)

Figure 10 shows the liquid density window for the previous example when English units are selected.

Liquid Density

Current Liquid Density Information		Accept Selected Liquid Density		
Value (lb/ft ³)	92.5	Cancel		
Source	Database			

	Source	Liq. Dens (lb/ft ³)	Temp (F)	Tmin (F)	Tmax (F)
<input checked="" type="radio"/>	Database	92.5	50.0	-121	568
<input type="radio"/>	Group Contribution Method	89.5	50.0		
<input type="radio"/>	User Input				

Note : Result for Liquid Density is at 1 atm below the normal boiling point and at the saturation pressure above the normal boiling point.

Figure 10 - Liquid Density Window (Trichloroethylene, 14.696 psi, 50° F)

C. Windows in StEPP[®]

StEPP[™] is designed for the Microsoft Windows interface. As such, there are several windows contained in StEPP[™]. The major windows will be described in detail here. The major windows in StEPP[™] that will be described are:

- StEPP main[™] Window
- Vapor Pressure Window
- Infinite Dilution Activity Coefficient Window
- Henry's Constant Window
- Molecular Weight Window
- Normal Boiling Point Window
- Liquid Density Window
- Molar Volume at the Operating Temperature Window
- Molar Volume at the Normal Boiling Point Window
- Refractive Index Window
- Aqueous Solubility Window
- Octanol Water Partition Coefficient Window
- Liquid Diffusivity Window
- Gas Diffusivity Window
- Water Density Window
- Water Viscosity Window
- Water Surface Tension Window
- Air Density Window
- Air Viscosity Window

1. Main StEPP™

The user has the option of viewing the StEPP main™ window either in the SI system of units or in the English system of units. To toggle between English and SI units, click on the appropriate choice in the **Units** menu on the StEPP main™ window. Figure 11 shows the StEPP main™ window in SI units for TCE as the selected contaminant at 10° C and 101325 Pa.

StEPP - Software to Estimate Physical Properties

File Units Options Help

Operating Conditions:

Pressure (Pa) 101325

Temperature (C) 10.0

Available Contaminants:

79016	TRICHLOROETHYLENE
79061	ACRYLAMIDE
79094	PROPIONIC ACID
79107	ACRYLIC ACID
79118	CHLOROACETIC ACID
79210	PERACETIC ACID

Find Find Next Occurrence

Synonyms Select Current Contaminant

Selected Contaminants:

79016	TRICHLOROETHYLENE
79016	TRICHLOROETHYLENE

Unselect Current Contaminant

Properties of the Contaminant:

TRICHLOROETHYLENE	
Vapor Pressure (Pa)	4.69E+03
Infinite Dilution Activity Coeff. (-)	8.12E+03
Henry's Constant (-)	0.230
Molecular Weight (kg/kmol)	131.39
Normal Boiling Point (NBP) (C)	87.0
Liquid Density (kg/m3)	1.48E+03
Molar Volume at Op. T (m3/kmol)	0.0886
Molar Volume at NBP (m3/kmol)	0.102
Refractive Index @25 C	1.4750
Aqueous Solubility (PPMw)	821
log Octanol Water Part. Coeff. (-)	2.38
Liquid Diffusivity (m2/s)	6.44E-10
Gas Diffusivity (m2/s)	7.89E-06

Properties of Air and Water:

Water Density (kg/m3)	999.75
Water Viscosity (kg/m/s)	1.31E-03
Water Surface Tension (N/m)	0.0742
Air Density (kg/m3)	1.25
Air Viscosity (kg/m/s)	1.72E-05

Figure 11 - StEPP™ Main Window (Trichloroethylene Selected, 10° C, 101325 Pa)

Figure 12 shows the StEPP™ main window in English units for TCE as the selected contaminant at an operating pressure of 14.696 *psi* and an operating temperature of 50° F.

StEPP - Software to Estimate Physical Properties

File Units Options Help

Operating Conditions:

Pressure (psi) **14.696**

Temperature (F) **50**

Available Contaminants:

79016 **TRICHLOROETHYLENE**

79061 ACRYLAMIDE

79094 PROPIONIC ACID

79107 ACRYLIC ACID

79118 CHLOROACETIC ACID

79210 PERACETIC ACID

Find Find Next Occurrence

Synonyms Select Current Contaminant

Selected Contaminants:

79016 TRICHLOROETHYLENE

79016 **TRICHLOROETHYLENE**

Unselect Current Contaminant

Properties of the Contaminant:

TRICHLOROETHYLENE

Vapor Pressure (psi)	0.681
Infinite Dilution Activity Coeff. (-)	8.12E+03
Henry's Constant (-)	0.230
Molecular Weight (lb/lb-mol)	131.39
Normal Boiling Point (NBP) (F)	189
Liquid Density (lb/ft ³)	92.5
Molar Volume at Op. T (ft ³ /lb-mol)	1.42
Molar Volume at NBP (ft ³ /lb-mol)	1.63
Refractive Index @77 F	1.4750
Aqueous Solubility (PPMw)	821
log Octanol Water Part. Coeff. (-)	2.38
Liquid Diffusivity (ft ² /s)	6.93E-09
Gas Diffusivity (ft ² /s)	8.49E-05

Properties of Air and Water:

Water Density (lb/ft ³)	62.41
Water Viscosity (lb/ft/s)	8.77E-04
Water Surface Tension (lbf/ft)	5.09E-03
Air Density (lb/ft ³)	0.0778
Air Viscosity (lb/ft/s)	1.16E-05

Figure 12 - StEPP™ Main Window (Trichloroethylene Selected, 14.696 psi, 50° F)

2. Vapor Pressure

StEPP™ has the capability to predict vapor pressure at the temperature of interest. To activate the Vapor Pressure window, click the left mouse button on the vapor pressure label or the vapor pressure value in the StEPP main™ window. The Vapor Pressure window for trichloroethylene at 101325 Pa and 10 C is shown in Figure 13.

Vapor Pressure

Current Vapor Pressure Information		Accept Selected Vapor Pressure	
Value (Pa)	4.69E+03		
Source	DIPPR801	Cancel	

Source	Vapor Pressure (Pa)	Temp. (C)	Tmin (C)	Tmax (C)
<input checked="" type="radio"/> DIPPR801	4.69E+03	10.0	-84.8	298
<input type="radio"/> Antoine's Equation	Not Available			
<input type="radio"/> Superfund	Not Available			
<input type="radio"/> User Input				

Figure 13 - Vapor Pressure Window (Trichloroethylene, 101325 Pa, 10° C)

Figure 14 shows the vapor pressure window for English units (Trichloroethylene, 14.696 *psi*, 50° F).

Vapor Pressure

Current Vapor Pressure Information		Accept Selected Vapor Pressure	
Value (psi)	0.681		
Source	DIPPR801	Cancel	

Source	Vapor Pressure (psi)	Temp. (F)	Tmin (F)	Tmax (F)
<input checked="" type="radio"/> DIPPR801	0.681	50.0	-121	568
<input type="radio"/> Antoine's Equation	Not Available			
<input type="radio"/> Superfund	Not Available			
<input type="radio"/> User Input				

Figure 14 - Vapor Pressure Window (Trichloroethylene, 14.696 *psi*, 50° F)

3. Infinite Dilution Activity Coefficient

StEPP™ has the capability to predict infinite dilution activity coefficient at the temperature of interest. To activate the Activity Coefficient window, click the left mouse button on the activity coefficient label or the activity coefficient value in the StEPP main™ window. The Activity Coefficient window for trichloroethylene at 101325 *Pa* and 10° C is shown in Figure 15.

Infinite Dilution Activity Coefficient

Current Activity Coefficient Information		
Value (-)	8.12E+03	
Source	UNIFAC	

Accept Selected Activity Coefficient

Cancel

Source	Activity Coefficient (-)	Temp. (C)
<input checked="" type="radio"/> UNIFAC	8.12E+03	10.0

UNIFAC Group Interaction Database: Environmental VLE

Figure 15 - Activity Coefficient Window (Trichloroethylene, 101325 Pa, 10° C)

Figure 16 shows the activity coefficient window for English units (Trichloroethylene, 14.696 *psi*, 50° F).

Infinite Dilution Activity Coefficient

Current Activity Coefficient Information		
Value (-)	8.12E+03	
Source	UNIFAC	

Accept Selected Activity Coefficient

Cancel

Source	Activity Coefficient (-)	Temp. (F)
<input checked="" type="radio"/> UNIFAC	8.12E+03	50.0

UNIFAC Group Interaction Database: Environmental VLE

Figure 16 - Activity Coefficient Window (Trichloroethylene, 14.696 *psi*, 50° F)

4. Henry's Constant

StEPP™ has the capability to predict Henry's constant at the temperature of interest. To activate the Henry's Constant window, click the left mouse button on the Henry's constant label or the Henry's constant value in the StEPP main™ window. The Henry's constant window for trichloroethylene at 101325 Pa and 10° C is shown in Figure 17.

Current Henry's Constant Information		Accept Selected Henry's Constant			
Value (-)	0.230	Cancel			
Source	Regression of Data Points				

Source	Henry's Constant (-)	Temp. (C)	Tmin (C)	Tmax (C)
<input checked="" type="radio"/> Regression of Data Points	0.230	10.0	N/A	N/A
<input type="radio"/> UNIFAC Fit with Data Pt.	0.232	10.0		
<input type="radio"/> UNIFAC at Operating T	0.292	10.0		
<input type="radio"/> Database	0.231	9.90		
RTI	0.231	9.90		
<input type="radio"/> UNIFAC @ Database T's	0.291	9.90		
UNIFAC	0.291	9.90		
<input type="radio"/> User Input				

UNIFAC Group Interaction Database: Environmental VLE

Figure 17 - Henry's Constant Window (Trichloroethylene, 101325 Pa, 10° C)

Figure 18 shows the Henry's constant window for English units (Trichloroethylene, 14.696 psi, 50° F).

Henry's Constant

Current Henry's Constant Information		Accept Selected Henry's Constant		
Value (-)	0.230	Cancel		
Source	Regression of Data Points			

Source	Henry's Constant (-)	Temp. (F)	Tmin (F)	Tmax (F)
<input checked="" type="radio"/> Regression of Data Points	0.230	50.0	N/A	N/A
<input type="radio"/> UNIFAC Fit with Data Pt.	0.232	50.0		
<input type="radio"/> UNIFAC at Operating T	0.292	50.0		
<input type="radio"/> Database	0.231	49.8		
RTI	0.231	49.8		
<input type="radio"/> UNIFAC @ Database T's	0.291	49.8		
UNIFAC	0.291	49.8		
<input type="radio"/> User Input				

UNIFAC Group Interaction Database: Environmental VLE

Figure 18 - Henry's Constant Window (Trichloroethylene, 14.696 *psi*, 50° F)

5. Molecular Weight

StEPP™ has the capability to determine a contaminant's molecular weight. To activate the Molecular Weight window, click the left mouse button on the molecular weight label or the molecular weight value in the StEPP main™ window. The molecular weight window for trichloroethylene for SI units is shown in Figure 19.

Molecular Weight

Current Molecular Weight Information	
Value (kg/kmol)	131.39
Source	Database

Accept Selected Molecular Weight

Cancel

Source	Molecular Weight (kg/kmol)
<input checked="" type="radio"/> Database	131.39
<input type="radio"/> Group Contribution Method	131.38
<input type="radio"/> User Input	

Figure 19 - Molecular Weight Window (Trichloroethylene, SI Units)

Figure 20 shows the molecular weight window for English units (Trichloroethylene).

Molecular Weight

Current Molecular Weight Information	
Value (lb/lb-mol)	131.39
Source	Database

Accept Selected Molecular Weight

Cancel

Source	Molecular Weight (lb/lb-mol)
<input checked="" type="radio"/> Database	131.39
<input type="radio"/> Group Contribution Method	131.38
<input type="radio"/> User Input	

Figure 20 - Molecular Weight Window (Trichloroethylene, English Units)

6. Normal Boiling Point

StEPP™ has the capability to determine a contaminant's normal boiling point. To activate the Normal Boiling Point window, click the left mouse button on the normal boiling point label or the normal boiling point value in the StEPP main™ window. The normal boiling point window for trichloroethylene is shown in Figure 21 for SI units.

The figure shows a software window titled "Normal Boiling Point". It contains a section for "Current Normal Boiling Point Information" with two input fields: "Value (C)" set to 87.0 and "Source" set to Database. To the right are two buttons: "Accept Selected Normal Boiling Point" and "Cancel". Below this is a table with two columns: "Source" and "Normal Boiling Point (C)". The table has two rows: "Database" (selected with a radio button) with a value of 87.0, and "User Input" (unselected) with an empty field.

Source	Normal Boiling Point (C)
<input checked="" type="radio"/> Database	87.0
<input type="radio"/> User Input	

Figure 21 - Normal Boiling Point Window (Trichloroethylene, SI Units)

Figure 22 shows the normal boiling point window for English units (Trichloroethylene).

The figure shows a software window titled "Normal Boiling Point". It contains a section for "Current Normal Boiling Point Information" with two input fields: "Value (F)" set to 189 and "Source" set to Database. To the right are two buttons: "Accept Selected Normal Boiling Point" and "Cancel". Below this is a table with two columns: "Source" and "Normal Boiling Point (F)". The table has two rows: "Database" (selected with a radio button) with a value of 189, and "User Input" (unselected) with an empty field.

Source	Normal Boiling Point (F)
<input checked="" type="radio"/> Database	189
<input type="radio"/> User Input	

Figure 22 - Normal Boiling Point Window (Trichloroethylene, English Units)

7. Liquid Density

StEPP™ has the capability to predict a contaminant's liquid density. To activate the Liquid Density window, click the left mouse button on the liquid density label or the liquid density value in the StEPP main™ window. The liquid density window for trichloroethylene at 101325 *Pa* and 10° C is shown in Figure 23.

Current Liquid Density Information		Accept Selected Liquid Density	
Value (kg/m3)	1.48E+03	Cancel	
Source	Database		

Source	Liq. Dens (kg/m3)	Temp (C)	Tmin (C)	Tmax (C)
<input checked="" type="radio"/> Database	1.48E+03	10.0	-84.8	298
<input type="radio"/> Group Contribution Method	1.43E+03	10.0		
<input type="radio"/> User Input				

Note : Result for Liquid Density is at 1 atm below the normal boiling point and at the saturation pressure above the normal boiling point.

Figure 23 - Liquid Density Window (Trichloroethylene, 101325 Pa, 10° C)

Figure 24 shows the liquid density window for English units (Trichloroethylene, 14.696 *psi*, 50° F).

Liquid Density					
Current Liquid Density Information				Accept Selected Liquid Density	
Value (lb/ft ³)	92.5				
Source	Database				
Cancel					
Source	Liq. Dens (lb/ft ³)	Temp (F)	Tmin (F)	Tmax (F)	
<input checked="" type="radio"/> Database	92.5	50.0	-121	568	
<input type="radio"/> Group Contribution Method	89.5	50.0			
<input type="radio"/> User Input					
Note : Result for Liquid Density is at 1 atm below the normal boiling point and at the saturation pressure above the normal boiling point.					

Figure 24 - Liquid Density Window (Trichloroethylene, 14.696 *psi*, 50° F)

8. Molar Volume at the Operating Temperature

StEPP™ has the capability to predict a contaminant's molar volume at the operating temperature. To activate the Molar Volume at the Operating Temperature window, click the left mouse button on the molar volume at the operating temperature label or the molar volume at the operating temperature value in the StEPP main™ window. The molar volume at the operating temperature window for trichloroethylene at 101325 *Pa* and 10° C is shown in Figure 25.

Molar Volume at Operating Temperature					
Current Molar Volume (Operating T) Information				Accept Selected Molar Volume	
Value (m ³ /kmol)	0.0886				
Source	Database				
Cancel					
Source	Molar Vol. (m ³ /kmol)	Temp. (C)	Tmin (C)	Tmax (C)	
<input checked="" type="radio"/> Database	0.0886	10.0	-84.8	298	
<input type="radio"/> Group Contribution Method	0.0917	10.0			
<input type="radio"/> User Input					

Figure 25 - Molar Volume at Operating Temperature Window (Trichloroethylene, 101325 *Pa*, 10° C)

Figure 26 shows the molar volume at the operating temperature window for English units (Trichloroethylene, 14.696 *psi*, 50° F).

Molar Volume at Operating Temperature

Current Molar Volume (Operating T) Information

Value (ft3/lb-mol)

Source

	Source	Molar Vol. (ft3/lb-mol)	Temp. (F)	Tmin (F)	Tmax (F)
<input checked="" type="radio"/>	Database	<input type="text" value="1.42"/>	<input type="text" value="50.0"/>	<input type="text" value="-121"/>	<input type="text" value="568"/>
<input type="radio"/>	Group Contribution Method	<input type="text" value="1.47"/>	<input type="text" value="50.0"/>		
<input type="radio"/>	User Input	<input type="text"/>	<input type="text"/>		

Figure 26 - Molar Volume at Operating Temperature Window (Trichloroethylene, 14.696 *psi*, 50° F)

9. Molar Volume at the Normal Boiling Point

StEPP™ has the capability to predict a contaminant's molar volume at the operating temperature. To activate the Molar Volume at the Normal Boiling Point window, click the left mouse button on the molar volume at the normal boiling point label or the molar volume at the normal boiling point value in the StEPP main™ window. The molar volume at the normal boiling point window for trichloroethylene is shown in Figure 27 for SI units. Note that the temperature is 76.6° C, which is the normal boiling point for trichloroethylene in SI units (see Figure 21).

Molar Volume at Normal Boiling Point											
Current Molar Volume (NBP) Information		<input type="button" value="Accept Selected Molar Volume"/>									
Value (m ³ /kmol)	0.102										
Source	Schroeder's Method	<input type="button" value="Cancel"/>									
<table border="1"> <thead> <tr> <th>Source</th> <th>Molar Vol. (m³/kmol)</th> <th>Temp. (C)</th> </tr> </thead> <tbody> <tr> <td><input checked="" type="radio"/> Schroeder's Method</td> <td>0.102</td> <td>87.0</td> </tr> <tr> <td><input type="radio"/> User Input</td> <td></td> <td></td> </tr> </tbody> </table>			Source	Molar Vol. (m ³ /kmol)	Temp. (C)	<input checked="" type="radio"/> Schroeder's Method	0.102	87.0	<input type="radio"/> User Input		
Source	Molar Vol. (m ³ /kmol)	Temp. (C)									
<input checked="" type="radio"/> Schroeder's Method	0.102	87.0									
<input type="radio"/> User Input											

Figure 27 - Molar Volume at Normal Boiling Point Window (Trichloroethylene, 101325 Pa, 76.6° C)

Figure 28 shows the molar volume at the normal boiling point window for English units (Trichloroethylene, 14.696 *psi*, 170° *F*). Note that the temperature is 170° *F*, which is the normal boiling point for trichloroethylene in English units (see Figure 22).

Molar Volume at Normal Boiling Point											
Current Molar Volume (NBP) Information		<input type="button" value="Accept Selected Molar Volume"/>									
Value (ft ³ /lb-mol)	1.63										
Source	Schroeder's Method	<input type="button" value="Cancel"/>									
<table border="1"> <thead> <tr> <th>Source</th> <th>Molar Vol. (ft³/lb-mol)</th> <th>Temp. (F)</th> </tr> </thead> <tbody> <tr> <td><input checked="" type="radio"/> Schroeder's Method</td> <td>1.63</td> <td>189</td> </tr> <tr> <td><input type="radio"/> User Input</td> <td></td> <td></td> </tr> </tbody> </table>			Source	Molar Vol. (ft ³ /lb-mol)	Temp. (F)	<input checked="" type="radio"/> Schroeder's Method	1.63	189	<input type="radio"/> User Input		
Source	Molar Vol. (ft ³ /lb-mol)	Temp. (F)									
<input checked="" type="radio"/> Schroeder's Method	1.63	189									
<input type="radio"/> User Input											

Figure 28 - Molar Volume at Normal Boiling Point Window (Trichloroethylene, 14.696 *psi*, 170° *F*)

10. Refractive Index

StEPP™ has the capability to estimate a contaminant's refractive index. To activate the Refractive Index window, click the left mouse button on the refractive index label or the refractive index value in the StEPP main™ window. The refractive index window for trichloroethylene in SI units is shown in Figure 29.

Refractive Index							
<div>Current Refractive Index Information</div> <div>Value (-) <input type="text" value="1.4750"/></div> <div>Source <input type="text" value="Database"/></div>		<div>Accept Selected Refractive Index</div> <div>Cancel</div>					
<table border="1"> <thead> <tr> <th>Source</th> <th>Refractive Index @25 C</th> </tr> </thead> <tbody> <tr> <td><input checked="" type="radio"/> Database</td> <td><input type="text" value="1.4750"/></td> </tr> <tr> <td><input type="radio"/> User Input</td> <td><input type="text"/></td> </tr> </tbody> </table>		Source	Refractive Index @25 C	<input checked="" type="radio"/> Database	<input type="text" value="1.4750"/>	<input type="radio"/> User Input	<input type="text"/>
Source	Refractive Index @25 C						
<input checked="" type="radio"/> Database	<input type="text" value="1.4750"/>						
<input type="radio"/> User Input	<input type="text"/>						

Figure 29 - Refractive Index Window for Trichloroethylene

The refractive index window for trichloroethylene in English units is shown in Figure 30.

Refractive Index							
<div>Current Refractive Index Information</div> <div>Value (-) <input type="text" value="1.4750"/></div> <div>Source <input type="text" value="Database"/></div>		<div>Accept Selected Refractive Index</div> <div>Cancel</div>					
<table border="1"> <thead> <tr> <th>Source</th> <th>Refractive Index @77 F</th> </tr> </thead> <tbody> <tr> <td><input checked="" type="radio"/> Database</td> <td><input type="text" value="1.4750"/></td> </tr> <tr> <td><input type="radio"/> User Input</td> <td><input type="text"/></td> </tr> </tbody> </table>		Source	Refractive Index @77 F	<input checked="" type="radio"/> Database	<input type="text" value="1.4750"/>	<input type="radio"/> User Input	<input type="text"/>
Source	Refractive Index @77 F						
<input checked="" type="radio"/> Database	<input type="text" value="1.4750"/>						
<input type="radio"/> User Input	<input type="text"/>						

Figure 30 - Refractive Index Window for Trichloroethylene

11. Aqueous Solubility

StEPP™ has the capability to predict a contaminant's aqueous solubility. To activate the Aqueous Solubility window, click the left mouse button on the aqueous solubility label or the aqueous solubility value in the StEPP main™ window. The aqueous solubility window for trichloroethylene at 101325 Pa and 10° C is shown in Figure 31.

Aqueous Solubility

Current Aqueous Solubility Information		
Value (PPMw)	821	
Source	UNIFAC Fit with Data Pt.	

Accept Selected Aqueous Solubility

Cancel

Source	Aqueous Sol. (PPMw)	Temp. (C)
<input checked="" type="radio"/> UNIFAC Fit with Data Pt.	821	10.0
<input type="radio"/> UNIFAC at Operating T	906	10.0
<input type="radio"/> Database	1.10E+03	25.0
<input type="radio"/> UNIFAC at Database T	1.18E+03	25.0
<input type="radio"/> User Input		

UNIFAC Group Interaction Database: Environmental VLE

Figure 31 - Aqueous Solubility Window (Trichloroethylene, 101325 Pa, 10° C)

Figure 32 shows the aqueous solubility window for English units (Trichloroethylene, 14.696 *psi*, 50° F).

Aqueous Solubility

Current Aqueous Solubility Information		
Value (PPMw)	821	
Source	UNIFAC Fit with Data Pt.	

Accept Selected Aqueous Solubility

Cancel

Source	Aqueous Sol. (PPMw)	Temp. (F)
<input checked="" type="radio"/> UNIFAC Fit with Data Pt.	821	50.0
<input type="radio"/> UNIFAC at Operating T	906	50.0
<input type="radio"/> Database	1.10E+03	77.0
<input type="radio"/> UNIFAC at Database T	1.18E+03	77.0
<input type="radio"/> User Input		

UNIFAC Group Interaction Database: Environmental VLE

Figure 32 - Aqueous Solubility Window (Trichloroethylene, 14.696 *psi*, 50° F)

12. Octanol Water Partition Coefficient

StEPP™ has the capability to predict a contaminant's octanol water partition coefficient. To activate the Octanol Water Partition Coefficient window, click the left mouse button on the octanol water partition coefficient label or the octanol water partition coefficient value in the StEPP main™ window. The octanol water partition coefficient window for trichloroethylene at 101325 *Pa* and 10° C is shown in Figure 33.

Octanol Water Partition Coefficient (Kow)

Current Oct. Water Part. Coeff. Information		
Value of log Kow (-)	2.38	
Source	Database	

Accept Selected Partition Coefficient

Cancel

Source	log Kow (-)	Temp. (C)
<input type="radio"/> UNIFAC @ Operating T	Not Available	
<input checked="" type="radio"/> Database	2.38	25.0
<input type="radio"/> UNIFAC @ Database T	Not Available	
<input type="radio"/> User Input		

UNIFAC Group Interaction Database: UNIFAC Kow Calculation Not Possible

Figure 33 - Octanol Water Partition Coefficient Window (Trichloroethylene, 101325 Pa, 10° C)

Figure 34 shows the octanol water partition coefficient window for English units (Trichloroethylene, 14.696 *psi*, 50° F).

Octanol Water Partition Coefficient (Kow)

Current Oct. Water Part. Coeff. Information		
Value of log Kow (-)	2.38	
Source	Database	

Accept Selected Partition Coefficient

Cancel

Source	log Kow (-)	Temp. (F)
<input type="radio"/> UNIFAC @ Operating T	Not Available	
<input checked="" type="radio"/> Database	2.38	77.0
<input type="radio"/> UNIFAC @ Database T	Not Available	
<input type="radio"/> User Input		

UNIFAC Group Interaction Database: UNIFAC Kow Calculation Not Possible

Figure 34 - Octanol Water Partition Coefficient Window (Trichloroethylene, 14.696 *psi*, 50° F)

13. Liquid Diffusivity

StEPP™ has the capability to predict a contaminant's liquid diffusivity. To activate the Liquid Diffusivity window, click the left mouse button on the liquid diffusivity label or the liquid diffusivity value in the StEPP main™ window. The liquid diffusivity window for trichloroethylene at 101325 *Pa* and 10° C is shown in Figure 35.

The screenshot shows a software window titled "Liquid Diffusivity". It contains a section for "Current Liquid Diffusivity Information" with a value of 6.44E-10 m²/s from the Hayduk and Laudie source. To the right are buttons for "Accept Selected Liquid Diffusivity" and "Cancel". Below this is a table with four rows of source data.

	Source	Liquid Diff. (m²/s)	Temp. (C)
<input checked="" type="radio"/>	Hayduk and Laudie	6.44E-10	10.0
<input type="radio"/>	Polson, 1950	5.39E-10	10.0
<input type="radio"/>	Wilke-Chang	6.41E-10	10.0
<input type="radio"/>	User Input		

Figure 35 - Liquid Diffusivity Window (Trichloroethylene, 101325 Pa, 10° C)

Figure 36 shows the liquid diffusivity window for English units (Trichloroethylene, 14.696 *psi*, 50° F).

Liquid Diffusivity

Current Liquid Diffusivity Information		Accept Selected Liquid Diffusivity	
Value (ft ² /s)	6.93E-09	Cancel	
Source	Hayduk and Laudie		

	Source	Liquid Diff. (ft ² /s)	Temp. (F)
<input checked="" type="radio"/>	Hayduk and Laudie	6.93E-09	50.0
<input type="radio"/>	Polson, 1950	5.80E-09	50.0
<input type="radio"/>	Wilke-Chang	6.90E-09	50.0
<input type="radio"/>	User Input		

Figure 36 - Liquid Diffusivity Window (Trichloroethylene, 14.696 psi, 50° F)

14. Gas Diffusivity

StEPP™ has the capability to predict a contaminant's gas diffusivity. To activate the Gas Diffusivity window, click the left mouse button on the gas diffusivity label or the gas diffusivity value in the StEPP main™ window. The gas diffusivity window for trichloroethylene at 101325 Pa and 10° C is shown in Figure 37.

Gas Diffusivity

Current Gas Diffusivity Information		Accept Selected Gas Diffusivity	
Value (m ² /s)	7.89E-06	Cancel	
Source	Wilke-Lee		

	Source	Gas Diffusivity (m ² /s)	Temp. (C)
<input checked="" type="radio"/>	Wilke-Lee	7.89E-06	10.0
<input type="radio"/>	User Input		

Figure 37 - Gas Diffusivity Window (Trichloroethylene, 101325 Pa, 10° C)

Figure 38 shows the gas diffusivity window for English units (Trichloroethylene, 14.696 *psi*, 50° F).

Gas Diffusivity

Current Gas Diffusivity Information		
Value (ft ² /s)	8.49E-05	
Source	Wilke-Lee	

Accept Selected Gas Diffusivity

Cancel

	Source	Gas Diffusivity (ft ² /s)	Temp. (F)
<input checked="" type="radio"/>	Wilke-Lee	8.49E-05	50.0
<input type="radio"/>	User Input		

Figure 38 - Gas Diffusivity Window (Trichloroethylene, 14.696 *psi*, 50° F)

15. Water Density

StEPP™ has the capability to predict water density. To activate the water density window, click the left mouse button on the water density label or the water density value in the StEPP main™ window. The water density window at 101325 *Pa* and 10° C is shown in Figure 39.

Water Density

Current Water Density Information		
Value (kg/m ³)	999.75	
Source	Correlation of Data	

Accept Selected Water Density

Cancel

	Source	H2O Dens. (kg/m ³)	Temp. (C)	Tmin (C)	Tmax (C)
<input checked="" type="radio"/>	Correlation of Data	999.75	10.0	0.0	100.0
<input type="radio"/>	User Input				

Figure 39 - Water Density Window (101325 *Pa*, 10° C)

Figure 40 shows the water density window for English units (14.696 *psi*, 50° F).

Water Density				
Current Water Density Information			Accept Selected Water Density	
Value (lb/ft ³)	62.41			
Source	Correlation of Data		Cancel	
Source	H2O Dens. (lb/ft ³)	Temp. (F)	Tmin (F)	Tmax (F)
<input checked="" type="radio"/> Correlation of Data	62.41	50.0	32.0	212.0
<input type="radio"/> User Input				

Figure 40 - Water Density Window (14.696 *psi*, 50° F)

16. Water Viscosity

StEPP™ has the capability to predict water viscosity. To activate the water viscosity window, click the left mouse button on the water viscosity label or the water viscosity value in the StEPP main™ window. The water viscosity window at 101325 *Pa* and 10° C is shown in Figure 41.

Water Viscosity				
Current Water Viscosity Information			Accept Current Selected Viscosity	
Value (kg/m/s)	1.31E-03			
Source	Yaws, et. al. (1976)		Cancel	
Source	H2O Visc. (kg/m/s)	Temp. (C)	Tmin (C)	Tmax (C)
<input checked="" type="radio"/> Yaws, et. al. (1976)	1.31E-03	10.0	0.0	370.0
<input type="radio"/> User Input				

Figure 41 - Water Viscosity Window (101325 *Pa*, 10° C)

Figure 42 shows the water viscosity window for English units (14.696 *psi*, 50° F).

Water Viscosity				
Current Water Viscosity Information			Accept Current Selected Viscosity	
Value (lb/ft/s)	8.77E-04			
Source	Yaws, et. al. (1976)		Cancel	
Source	H2O Visc. (lb/ft/s)	Temp. (F)	Tmin (F)	Tmax (F)
<input checked="" type="radio"/> Yaws, et. al. (1976)	8.77E-04	50.0	32.0	698.0
<input type="radio"/> User Input				

Figure 42 - Water Viscosity Window (14.696 *psi*, 50° F)

17. Water Surface Tension

StEPP™ has the capability to predict water surface tension. To activate the water surface tension window, click the left mouse button on the water surface tension label or the water surface tension value in the StEPP main™ window. The water surface tension window at 101325 *Pa* and 10° C is shown in Figure 43.

Water Surface Tension				
Current Water Surface Tension Information			Accept Selected H2O Surface Tension	
Value (N/m)	0.0742			
Source	Cummins, et. al. (1983)		Cancel	
Source	Surf. Tens. (N/m)	Temp. (C)	Tmin (C)	Tmax (C)
<input checked="" type="radio"/> Cummins, et. al. (1983)	0.0742	10.0	N/A	N/A
<input type="radio"/> User Input				

Figure 43 - Water Surface Tension Window (101325 *Pa*, 10° C)

Figure 44 shows the water surface tension window for English units (14.696 *psi*, 50° F).

Water Surface Tension					
Current Water Surface Tension Information			Accept Selected H2O Surface Tension		
Value (lbf/ft)	5.09E-03				
Source	Cummins, et. al. (1983)		Cancel		
Source	Surf. Tens. (lbf/ft)	Temp. (F)	Tmin (F)	Tmax (F)	
<input checked="" type="radio"/> Cummins, et. al. (1983)	5.09E-03	50.0	N/A	N/A	
<input type="radio"/> User Input					

Figure 44 - Water Surface Tension Window (14.696 *psi*, 50° F)

18. Air Density

StEPP™ has the capability to predict air density. To activate the air density window, click the left mouse button on the air density label or the air density value in the StEPP main™ window. The air density window at 101325 *Pa* and 10° C is shown in Figure 45.

Air Density					
Current Air Density Information			Accept Selected Air Density		
Value (kg/m3)	1.25				
Source	Ideal Gas Law		Cancel		
Source	Air Dens. (kg/m3)	Temp. (C)	Tmin (C)	Tmax (C)	
<input checked="" type="radio"/> Ideal Gas Law	1.25	10.0	N/A	N/A	
<input type="radio"/> User Input					

Figure 45 - Air Density Window (101325 *Pa*, 10° C)

Figure 46 shows the air density window for English units (14.696 *psi*, 50° F).

Air Density					
Current Air Density Information				Accept Selected Air Density	
Value (lb/ft ³)		0.0778			
Source		Ideal Gas Law		Cancel	
Source	Air Dens. (lb/ft ³)	Temp. (F)	Tmin (F)	Tmax (F)	
<input checked="" type="radio"/> Ideal Gas Law	0.0778	50.0	N/A	N/A	
<input type="radio"/> User Input					

Figure 46 - Air Density Window (14.696 *psi*, 50° F)

19. Air Viscosity

StEPP™ has the capability to predict air viscosity. To activate the air viscosity window, click the left mouse button on the air viscosity label or the air viscosity value in the StEPP main™ window. The air viscosity window at 101325 *Pa* and 10° C is shown in Figure 47.

Air Viscosity					
Current Air Viscosity Information				Accept Selected Air Viscosity	
Value (kg/m/s)		1.72E-05			
Source		Cummins, et. al. (1983)		Cancel	
Source	Air Visc. (kg/m/s)	Temp. (C)	Tmin (C)	Tmax (C)	
<input checked="" type="radio"/> Cummins, et. al. (1983)	1.72E-05	10.0	N/A	N/A	
<input type="radio"/> User Input					

Figure 47 - Air Viscosity Window (101325 *Pa*, 10° C)

Figure 48 shows the air viscosity window for English units (14.696 *psi*, 50° F).

Air Viscosity

Current Air Viscosity Information	
Value (lb/ft/s)	1.16E-05
Source	Cummins, et. al. (1983)

Accept Selected Air Viscosity

Cancel

Source	Air Visc. (lb/ft/s)	Temp. (F)	Tmin (F)	Tmax (F)
<input checked="" type="radio"/> Cummins, et. al. (1983)	1.16E-05	50.0	N/A	N/A
<input type="radio"/> User Input				

Figure 48 - Air Viscosity Window (14.696 *psi*, 50° F)

V. Exporting StEPP™ Data to Other ETDOT Applications

It is possible to export chemical properties from StEPP™ into other ETDOT applications, such as Adsorption Design Software (AdDesignS™) and Aeration System Analysis Program (ASAP™). There are two methods for performing the export, both of which are available in the **Options** menu (see Figure 49): (1) *Create Export File for AdDesignS/ASAP* and (2) *Copy to Clipboard for AdDesignS/ASAP*.

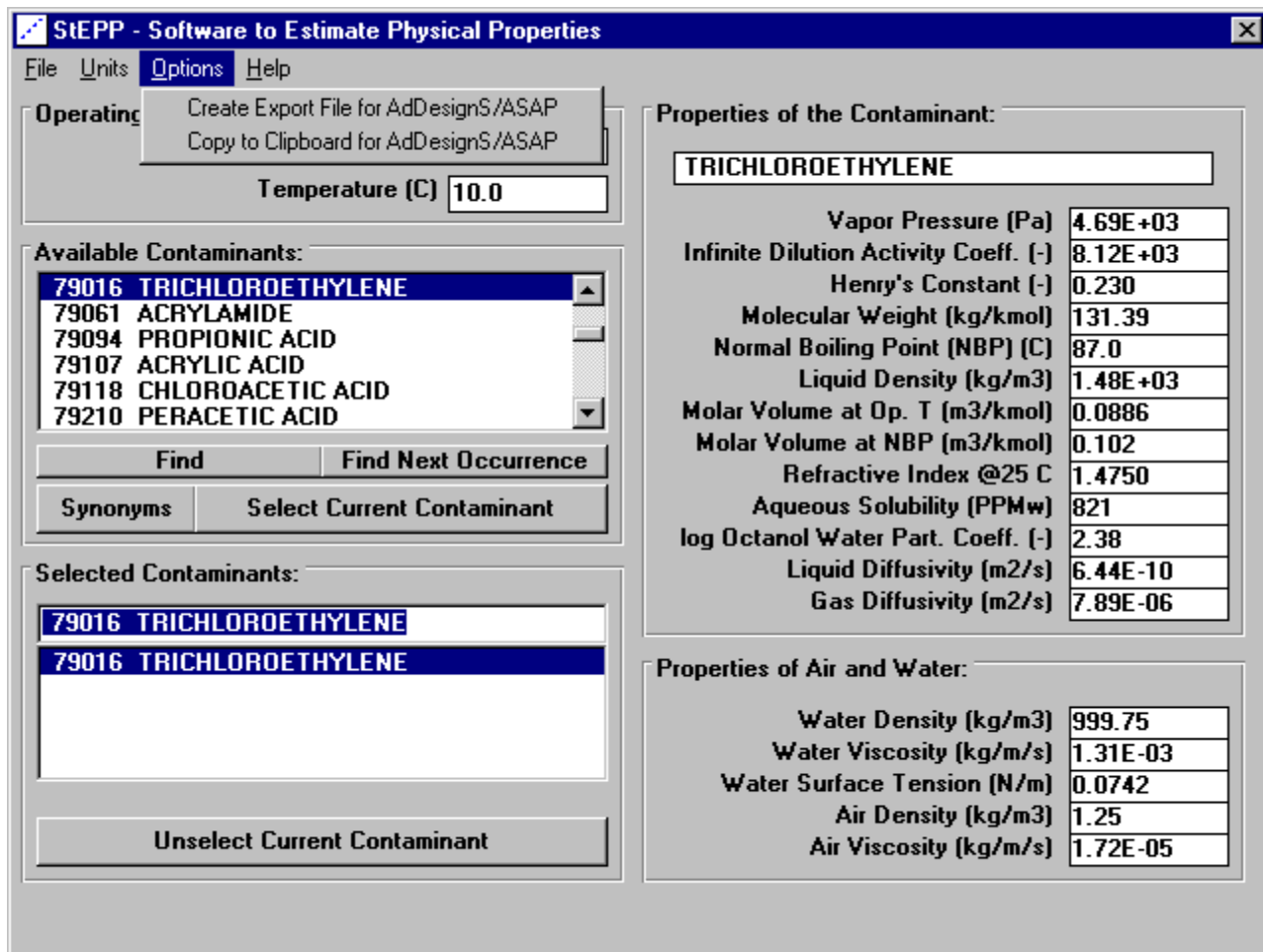


Figure 49 –StEPP™ Main Window Showing Options Menu
(TCE; 10 °C; 101,325 Pa)

A. Export Method 1: Create Export File for AdDesignS/ASAP

In this method, data is passed from StEPP™ to another ETDOT application by writing the appropriate data to a file in StEPP™ and then reading the data from the file into another ETDOT application. To generate the export file in StEPP™, click on the *Create Export*

File for AdDesignSM/ASAPSM choice in the **Options** menu. The **Save StEPPSM Export File** window shown in Figure 49 will appear.

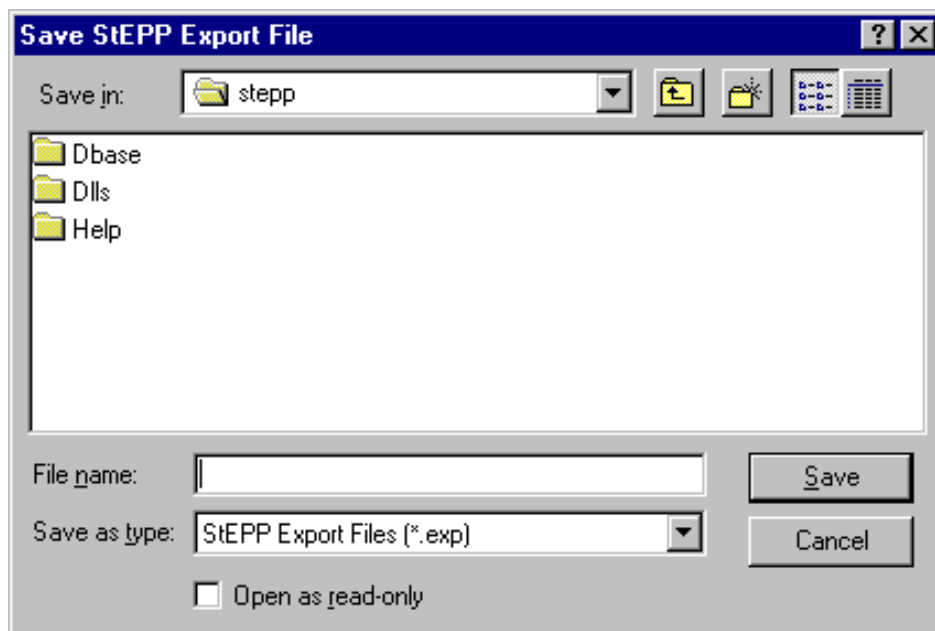


Figure 50 – Save StEPPSM Export File Window

In the *File Name* field shown in Figure 50, give the export file a name (the default file extension for StEPPSM export files is **.exp**). For this sample case of exporting the properties of TCE, which is the only chemical selected for this example (see Figure 49), the export file will be given the name: **tce.exp**. Figure 51 shows the **Save StEPPSM Export File Window** for this sample file name. Note that the user may also select a folder in which to save the file in the *Save In* field shown in Figure 51.

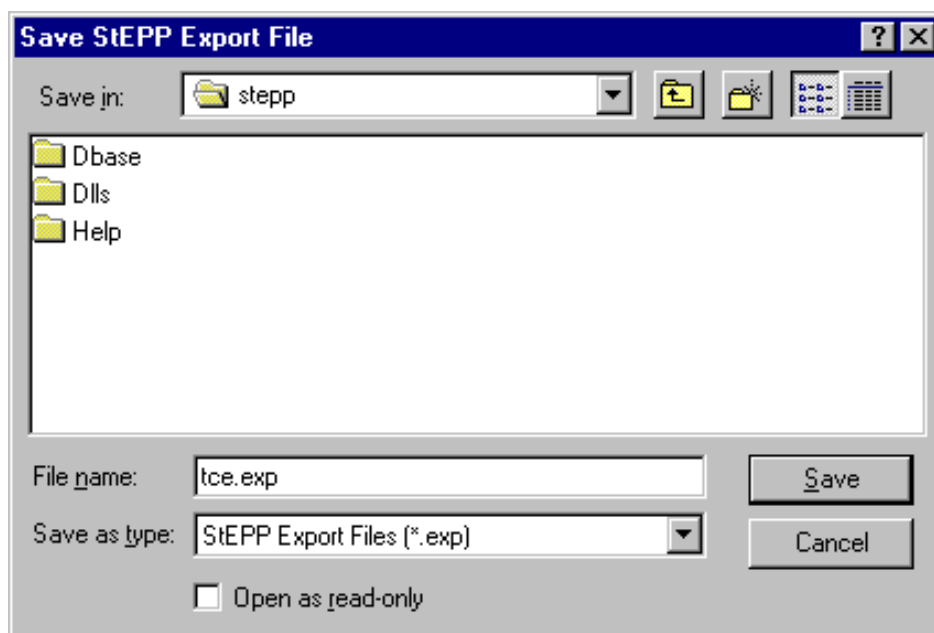


Figure 51 – Save StEPP™ Export File Window Showing Sample File Name

To save the export file, click on the **Save** button shown in Figure 51. The message box shown in Figure 52 appears indicating that the StEPP™ export file has been generated successfully.

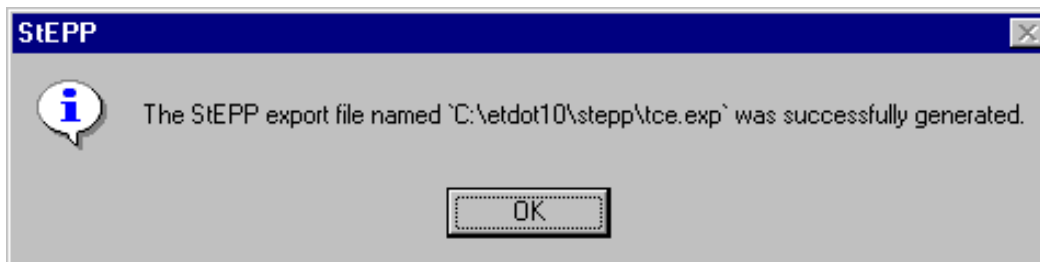


Figure 52 – Message Box Indicating Status of the Save StEPP™ Export File Process

Within other ETDOT applications (e.g. ASAP™, AdDesignS™), it is possible to import the StEPP™ export file created here. The process of importing StEPP™ properties in this fashion is described in the other ETDOT manuals.

B. Export Method 2: Copy to Clipboard for AdDesignS/ASAP

In this method, data is passed from StEPP™ to another ETDOT application by copying the appropriate data from StEPP™ into the Windows clipboard and then pasting the data from the Windows clipboard into another ETDOT application. To copy the data from StEPP™ into the Windows clipboard, click on the *Copy to Clipboard for AdDesignS™/ASAP™* choice in the **Options** menu. The message box shown in Figure 53

will appear, indicating the StEPP™ properties have been successfully copied to the clipboard.

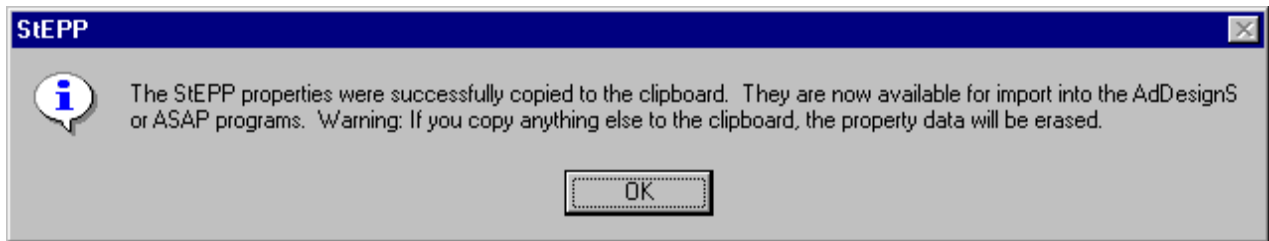


Figure 53 - Message Box Indicating Status of the Copy to Clipboard Process

Within other ETDOT applications (e.g. ASAP™, AdDesignS™), it is possible to import the StEPP™ properties from the clipboard. The process of copying StEPP™ properties from the clipboard in this fashion is described in the other ETDOT manuals.

Appendix A – Description of Chemical Name Synonyms Feature in StEPP™

StEPP™ contains a feature allowing the user to have access to common synonyms for chemical names contained in the StEPP™ database. The reference for the synonyms contained in StEPP™ is:

Howard, P.H. and M. Neal. *Dictionary of Chemical Names and Synonyms*, Lewis Publishers: New York, 2544 pp. (1992).

An example of how to make use of the synonyms feature in StEPP™ is provided. Load StEPP™ and click on the **Continue** button on the StEPP™ title window. The StEPP™ main window appears as shown in Figure A.1 below.

StEPP - Software to Estimate Physical Properties

File Units Options Help

Operating Conditions:

Pressure (Pa) 101325

Temperature (C) 25.0

Available Contaminants:

56235 CARBON TETRACHLORIDE

56495 METHYL CHOLANTHRENE

56531 DIETHYLSTILBESTROL

56553 BENZ(A)ANTHRACENE

57147 1,1-DIMETHYLHYDRAZINE

57578 BETA-PROIOLACTONE

Find Find Next Occurrence

Synonyms Select Current Contaminant

Selected Contaminants:

Unselect Current Contaminant

Properties of the Contaminant:

Vapor Pressure (Pa)

Infinite Dilution Activity Coeff. (-)

Henry's Constant (-)

Molecular Weight (kg/kmol)

Normal Boiling Point (NBP) (C)

Liquid Density (kg/m3)

Molar Volume at Op. T (m3/kmol)

Molar Volume at NBP (m3/kmol)

Refractive Index @25 C

Aqueous Solubility (PPMw)

log Octanol Water Part. Coeff. (-)

Liquid Diffusivity (m2/s)

Gas Diffusivity (m2/s)

Properties of Air and Water:

Water Density (kg/m3)

Water Viscosity (kg/m/s)

Water Surface Tension (N/m)

Air Density (kg/m3)

Air Viscosity (kg/m/s)

Figure A.1 –StEPP™ Main Window

Click on the **Synonyms** button in the **Available Contaminants** frame shown in Figure A.1. Once this is done, the **Synonyms** window will appear, as shown in Figure A.2.

List of Synonyms

Please enter the string you want to search for in the synonyms database:

Search

No. of Hits:

CAS #:

Name:

IUPAC Name:

OK **Cancel**

Figure A.2 – Synonyms Window

As an example, type in **Trichloroethene**, a synonym for the IUPAC chemical name Trichloroethylene, on the **Synonyms** window (see Figure A.2) as the string to search for in the synonyms database. Then click the **Search** button on the **Synonyms** window to execute the search for Trichloroethene in the synonyms database. Once this is done, the **Synonyms** window appears as shown in Figure A.3, presenting the results for this synonym search.

List of Synonyms

Please enter the string you want to search for in the synonyms database:

Search

No. of Hits: 1

CAS #: 79016

Synonym: trichloroethene

IUPAC Name: ethylene, trichloro

79016	trichloroethene
-------	-----------------

OK **Cancel**

Figure A.3 – Synonyms Window Showing Result of Search for Trichloroethene

The search found **Trichloroethene** to be a synonym for a chemical with CAS number 79016 and IUPAC name **ethylene, trichloro**. This is the expected result. For the user to select this chemical in StEPP™, simply click on the **OK** button at the bottom of the **Synonyms** window. To exit the **Synonyms** window without selecting the chemical found by the search, click the **Cancel** button.