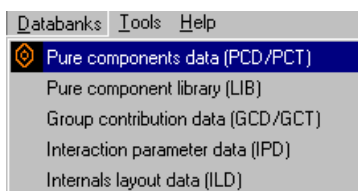# *ChemSep* Tutorial: PCDmanager

Ross Taylor and Harry Kooijman
Updated for version 6.8, August 1, 2011

ChemSep 6.2 saw the introduction of a completely new pure compound data manager that we call *PCDmanager* – **PCD is short for Pure Compound Data**.

To access the databank manager open *ChemSep* and go to the **Databanks** menu. Select **Pure components data (PCD/PCT)** as shown below.

This will start the databank manager looking like this:
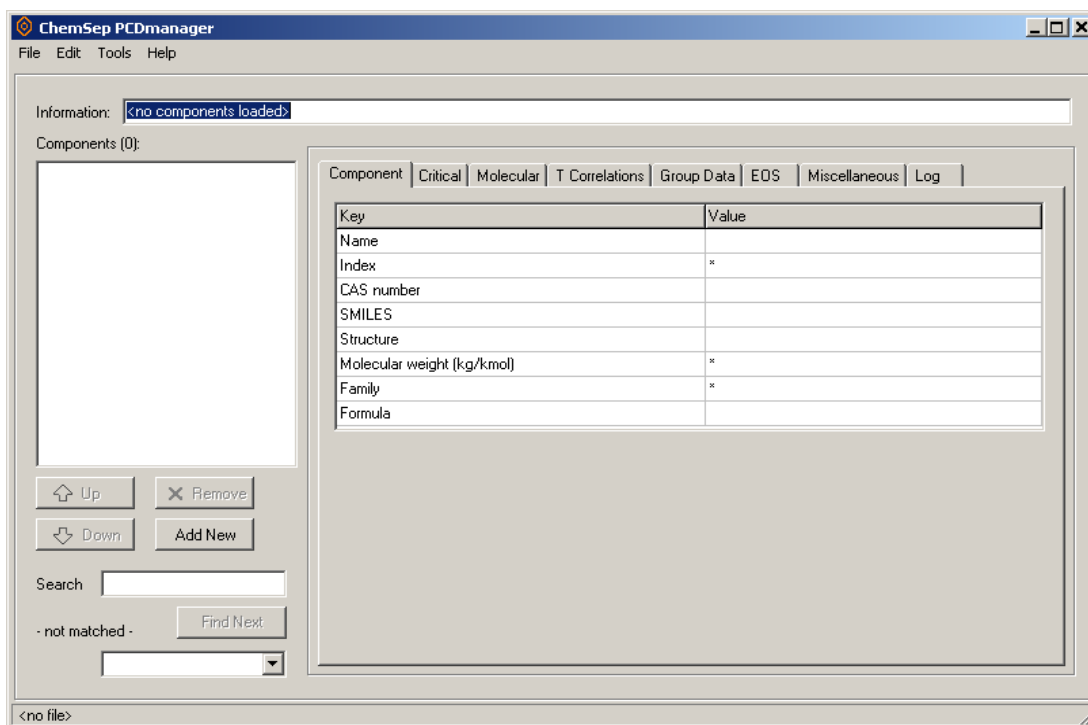
To view and/or edit the physical property data in an existing data file go to the File menu and select Open. Select a pcd file (the default file name that comes with *ChemSep* is chemsep1.pcd and will probably be visible in the file open selection window).

Finding Compounds

Once a file has been loaded the left hand portion will display a list of the compounds included in the databank. You may scroll up and down this list to find compounds of interest. You can also use the keyboard to find components; *PCDmanager* will recognize key strokes and select compounds that match the string of characters that have been typed. In the image below we show this portion of the screen after a successful search for **Benzene**.
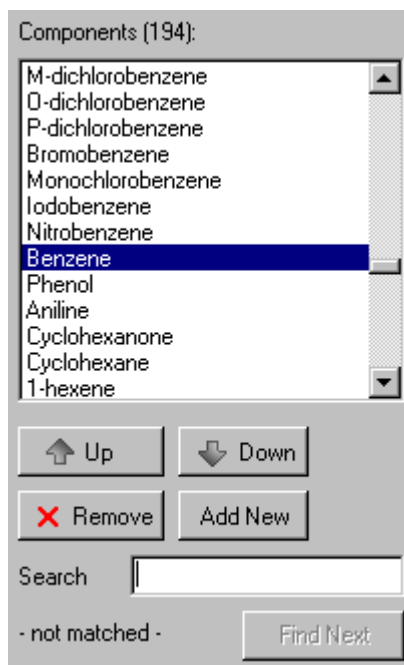
The position in the list of compounds can altered using the up or down arrows. The entire record of all the data available in the pcd file for benzene can be erased using the **Remove** button (with the red X). Note that the *PCDmanager* has a complete **Undo** facility and even completely deleted compound records can be recovered in their entirety.

The **Search** cell in the image below permits compounds to be found using more sophisticated criteria than their names (or parts thereof).

As an exercise to see what is possible trying typing the following strings into the **Search** cell (click on **Find Next** several times after each string):

C6 (be sure to use capital letters)

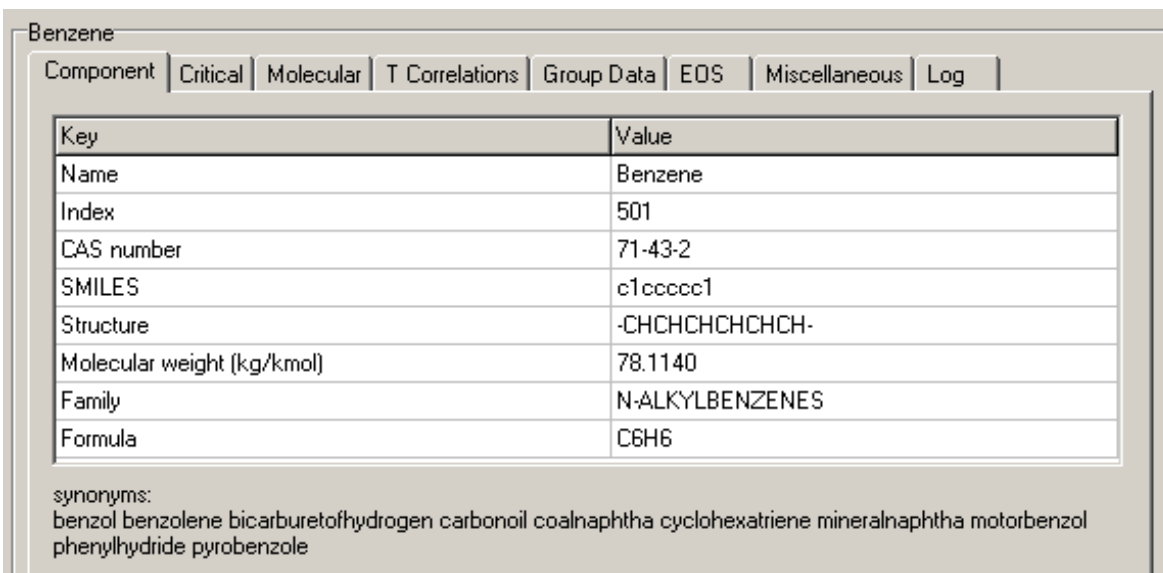Tc=300-400

CH3CH2

403

(C)

56- (don't forget the dash)

Mw=100-200

Pure Compound Constants

The pure compound property constants are recorded for each compound appears on a series of tab sheets in the right hand portion of the *PCDmanager* window. These panels are displayed below for benzene. Please review them to learn what properties are recorded in the *ChemSep* pure component data files.

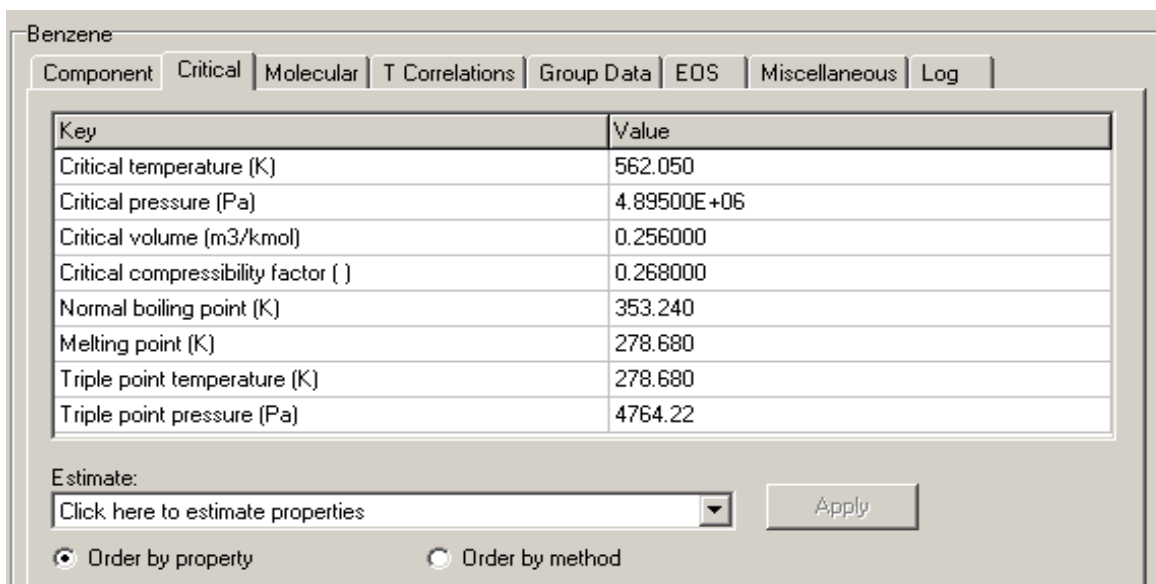A complete list of property constants is provided in Appendix A.

Component Panel

The *Component* panel displays the most basic information about the compound, its name, index number (usually this is the index number assigned by DIPPR), its CAS number, SMILES string, structural formula, molecular weight, family (from the DIPPR list) and formula. The formula is constructed from the structural formula and cannot be entered from the keyboard. With that sole exception all of the other entries can be altered simply to clicking in a cell to the right and typing a new entry. To accept a new entry press *Enter* or click in another cell.

At the foot of this tab page is a list of synonyms for the compound on display. These synonyms are from the file chemsep.syn that is located in the pcd subdirectory. This is a plain text file that can be edited using a text editor (such as Notepad, but not Word).

Critical Properties

This panel displays some of the most important properties, namely the critical constants, normal boiling point, melting point, and the triple point temperature and pressure. The critical constants are needed in any application of an equation of state to estimate thermodynamic properties.

Note the white line near the foot of this panel that says *Click here to estimate properties*. As this line suggests, you can click here to obtain estimates of the various properties that are listed on this panel (the same opportunity to estimate properties is available on several other panels). This ability to estimate missing properties is one of the most valuable aspects of *PCDmanager*.

Molecular Properties

Benzene	
Component	**Critical**	**Molecular**	**T Correlations**	**Group Data**	**EOS**	**Miscellaneous**	**Log**

Key	Value
Liquid molar volume at normal boiling point (m3/kmol)	0.0894100
Acentric factor ( )	0.209000
Radius of gyration (m)	3.00400E-10
Solubility parameter (sqrt(J/m3))	18700.0
Dipole moment (Coulomb.m)	0.000000
Van der Waals volume (m3/kmol)	0.0484000
Van der Waals area (m2/kmol)	6.00000E+08
IG heat of formation (J/kmol)	8.28800E+07
IG Gibbs energy of formation (J/kmol)	1.29600E+08
IG absolute entropy (J/kmol/K)	269300
Heat of fusion at melting point (J/kmol)	9.86600E+06
Heat of vaporization at normal boiling point (J/kmol)	×
Standard net heat of combustion (J/kmol)	-3.13600E+09

Estimate:

[▼]   Apply

◉ Order by property   ○ Order by method

Perhaps the most important property on this panel is the acentric factor. This property is widely used in the estimation of other physical properties. If the parameter is not available, it is set equal to zero.

Equation of State Parameters

Some models make use of a special value for the acentric factor sometimes referred to as the SRK acentric factor. If available that value is displayed on this panel. If it is not available then *ChemSep* will automatically assume that the SRK acentric factor is equal to the acentric factor displayed on line 2 of the ***Molecular Properties Panel***. This panel also displays the parameters for the API version of the SRK Equation of State (if available).

Finally, this panel also shows the special values of the acentric factor, solubility parameter, and liquid molar volume that are used in the Chao-Seader models for thermodynamic properties. In the event that the cells for the Chao-Seader parameter contain a * then these parameters are set equal to the values listed on lines 1, 2 and 4 of the ***Molecular Properties Panel***.

Miscellaneous Properties

This panel displays a number of other properties that did not fit on the other panels.

The UNIQUAC parameters are needed if the UNIQUAC model is to be used to estimate activity coefficients.

The parachor is a property used in the prediction of surface tension. If not available in the databank it can sometimes be estimated from the surface tension correlation that is available for many compounds (see **Temperature Dependant Properties**).

The Lennard-Jones parameters are available for few compounds. They are used in the estimation of transport properties. If unavailable, they can be estimated from critical properties.

The Rackett parameter is used in the Rackett model for liquid density. If not available, it is set equal to the critical compressibility.

The COSTLD volume is used in the estimation of liquid density. If not available, it is set equal to the critical volume.

Log Panel

The log tab panel records changes that you make to the pcd file. The log can be saved on exit so that you can retain a permanent record of your changes. As an exercise click on one of the panels that display property constants, change one of them (any of them) and then click on the log panel to see what it displays. To return the data record to its original value click *Ctrl-Z*. Click again in the log panel to see what has changed.

As a second exercise, use the *Remove* button in the left-hand quarter to erase the record of a compound. Check to see what appears in the Log panel. Restore the compound record using *Ctrl-Z*.

Temperature Dependent Properties

Many pure compound properties depend on the temperature. *PCDmanager* has a special tab page for these properties.

Select one of these properties to show the property constants and a table of (calculated) values of the selected property. The value on the **Table** tab that is highlighted by the blue background is at the normal boiling point. Select the **Plot** tab to display a plot instead of the table. Right click on the plot to display an overlaid menu of options to format the plot to your taste (as shown below). These plots can be copied into other applications such as word processors and spreadsheets.
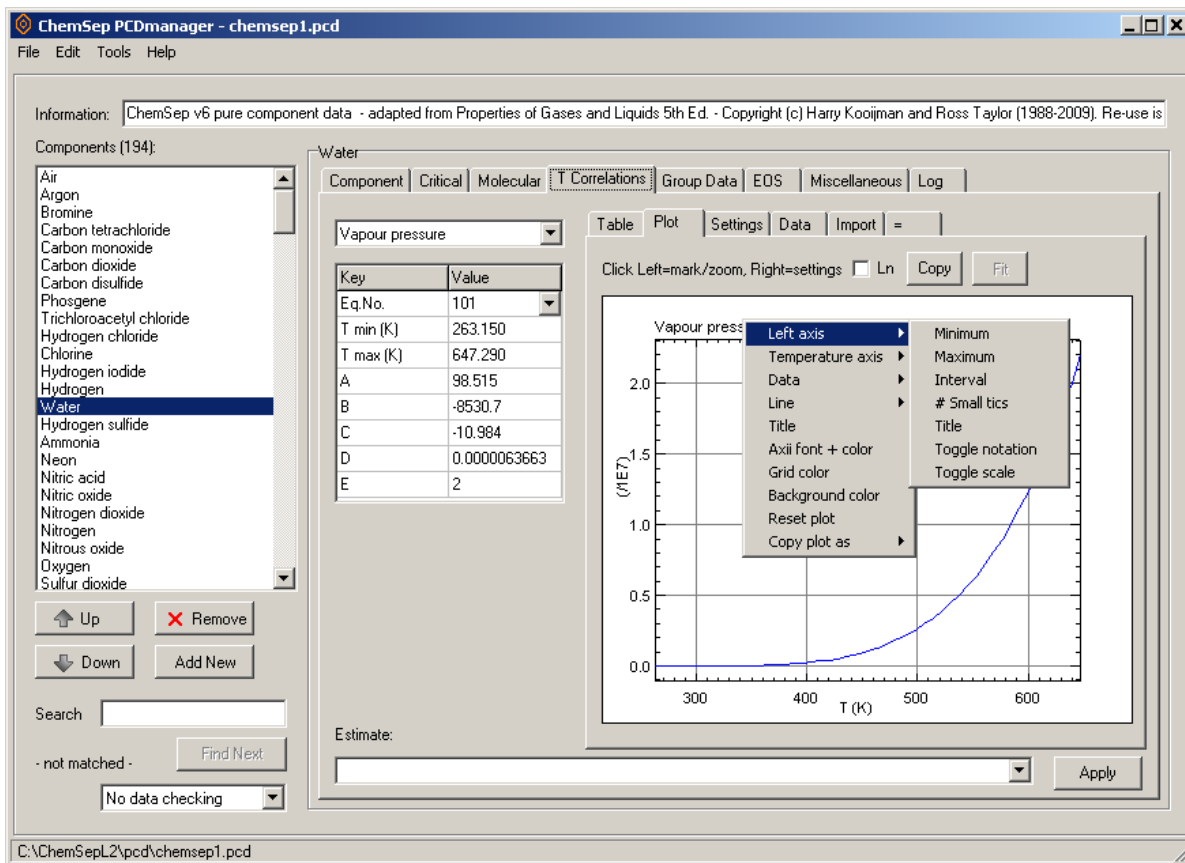
The *Plot* tab selected in the above illustration displays the selected property function graphically. The *Table* tab shows the same information in table format:

T (K)	Pa
263.150	205.905
270.990	391.291
278.829	712.465
286.669	1247.71
294.508	2108.78
302.348	3450.07
310.188	5478.79
318.027	8465.67
325.867	12755.9
333.706	18780.0
341.546	27063.9
349.386	38238.7
357.225	53048.9

Mass densities

Copy Table Data

#Points 51

The *Settings* tab shown below left displays the plot title information and the axis characteristics.

The Data tab shown below right displays the information on the *Plot* tab. This is the same set of numbers that appears on the *Table* tab, but we can also see that the line settings for the plot also are displayed. We will return to this tab below.

Title | Vapour pressure (Pa)

Font | Arial   Colors | Grid | Back

Axes line thickness 1   ☑ Grid   Reset

X
Name	T (K)
Start	263.15
End	647.29
Interval	100
Tics	9
Notation	Fixed
Scale	Linear

Y
Name	
Start	-1099294
End	2.314467E+0
Interval	5000000
Tics	4
Notation	Scientific
Scale	Linear

Name	
Color	16711680
Line thicknes	1
Symbol	0
X-axis	1
Y-axis	1
263.150	205.905
270.990	391.291
278.829	712.465
286.669	1247.71
294.508	2108.78
302.348	3450.07
310.188	5478.79
318.027	8465.67

The *Import* tab allows PCDmanager to import data from a properly formatted text file. Click on the *Open folder* symbol on the *Import* tab to find the appropriate file and read the data. We see in the illustration below that PCDmanager can read plain text files, plot files created by *ChemSep*, and DIPPR text files.
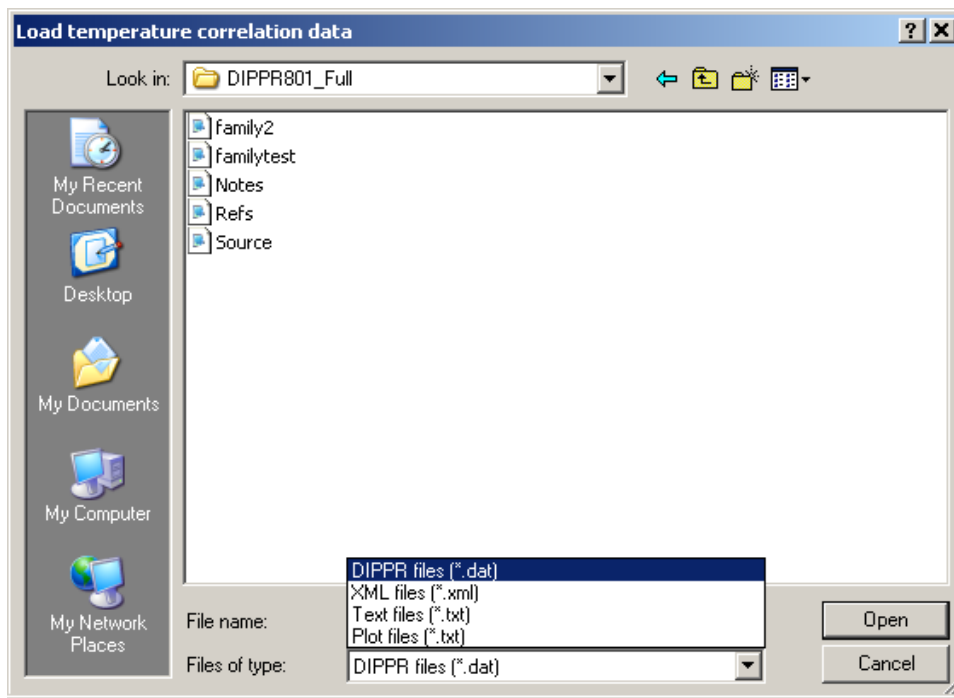
If (and only if) you have the full DIPPR source file available you may open it with this feature and import the actual data points contained therein. The *Import* tab will then display a list of the data points found (in this case we show the vapor pressure data for water).
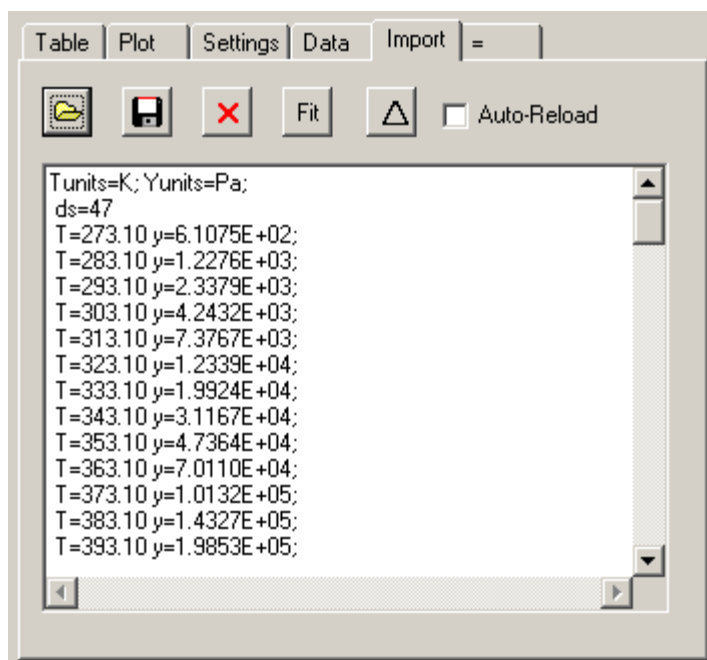
We now return to the *Data* tab and see this (the window has been stretched to accommodate the additional data).

Name		Name	47	Name	175	Name	2909
Color	16711680	Color	255	Color	255	Color	255
Line thickness	1	Line thickness	0	Line thickness	0	Line thickness	0
Symbol	0	Symbol	1	Symbol	2	Symbol	3
X-axis	1	X-axis	1	X-axis	1	X-axis	1
Y-axis	1	Y-axis	1	Y-axis	1	Y-axis	1
263.150	205.905	273.1	610.75	273.15	610.9	273.16	611.73
270.990	391.291	283.1	1227.6	283.15	1227.6	274.15	657.16
278.829	712.465	293.1	2337.9	293.15	2339	278.15	872.6
286.669	1247.71	303.1	4243.2	303.15	4246	283.15	1228.1
294.508	2108.78	313.1	7376.7	313.15	7384	288.15	1705.6
302.348	3450.07	323.1	12339	323.15	12349	293.15	2338.8
310.188	5478.79	333.1	19924	333.15	19940	298.15	3169.1
318.027	8465.67	343.1	31167	343.15	31190	303.15	4245.5
325.867	12755.9	353.1	47364	353.15	47390	308.15	5626.7
333.706	18780.0	363.1	70110	363.15	70140	313.15	7381.4
341.546	27063.9	373.1	101320	373.15	101350	318.15	9589.8
349.386	38238.7	383.1	143270	383.15	143270	323.15	12344

The first two columns show the same information we saw before, the numbers having been computed from the correlation used to estimate, in this example, the vapor pressure of water. The additional columns (taken two at a time) show the experimental data that was imported from the DIPPR source file.

Returning to the *Plot* tab we now see the data superimpose on the correlation.
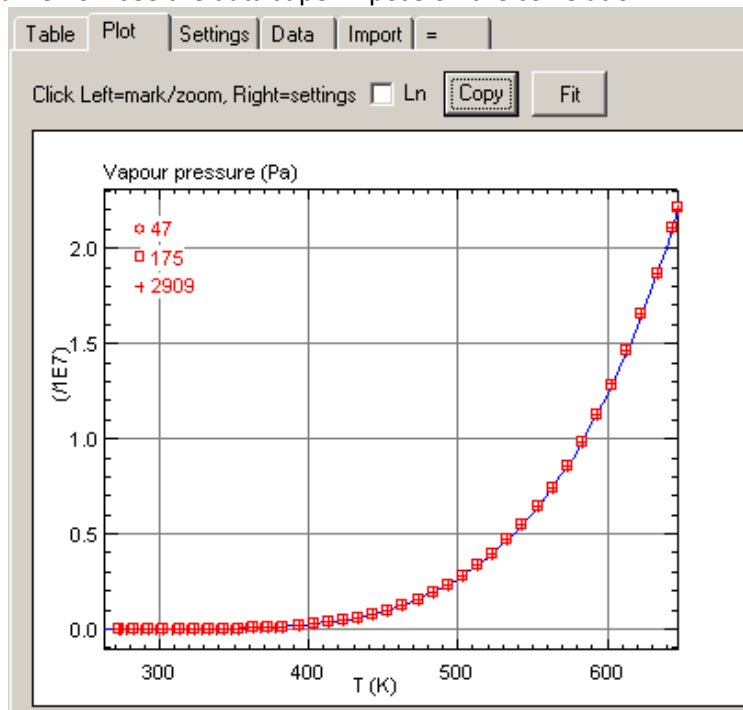
A word of caution about temperature dependent parameters is in order. You can select the equation used to calculate the property as well as enter the limits. The equations available are listed below. **All temperature dependent properties require the temperature in Kelvin.** Note that some equations use a dimensionless temperature.

Number	Equation
Temperature Dependent Property Correlations	
1	$Y = A$
2	$Y = A + BT$
3	$Y = A + BT + CT^2$
4	$Y = A + BT + CT^2 + DT^3$
5	$Y = A + BT + CT^2 + DT^3 + ET^4$
10	$Y = \exp(A - B/(T + C))$
11	$Y = \exp(A)$
12	$Y = \exp(A + BT)$
13	$Y = \exp(A + BT + CT^2)$
14	$Y = \exp(A + BT + CT^2 + DT^3)$
15	$Y = \exp(A + BT + CT^2 + DT^3 + ET^4)$
16	$Y = A + \exp(B/T + C + DT + ET^2)$
17	$Y = A + \exp(B + CT + DT^2 + ET^3)$
45	$Y = AT + \dfrac{1}{2}BT^2 + \dfrac{1}{3}CT^3 + \dfrac{1}{4}DT^4 + \dfrac{1}{5}ET^5$
75	$Y = B + 2CT + 3DT^2 + 4ET^3$
100	$Y = A + BT + CT^2 + DT^3 + ET^4$
101	$Y = \exp(A + B/T + C \ln T + DT^E)$
102	$Y = AT^B/(1 + C/T + D/T^2)$
103	$Y = A + B\exp(-C/T^D)$
104	$Y = A + B/T + C/T^3 + D/T^8 + E/T^9$
105	$Y = A/B^{1 + (1 - T/C)^D}$
106	$Y = A(1 - T_r)^{B + CT_r + DT_r^2 + ET_r^3} \qquad T_r = T/T_c$

107	$Y = A + B\left(\dfrac{C/T}{\sinh(C/T)}\right)^2 + D\left(\dfrac{E/T}{\sinh(E/T)}\right)^2$
114	$Y = A^2/\tau + B - 2AC\tau - AD\tau^2 - C^2\tau^3/3 - CD\tau^4/2 - D^2\tau^5/5 \qquad \tau = 1 - T/T_c$
115	$Y = \exp(A + B/T + C\ln T + DT^2 + E/T^2)$
116	$Y = A + B\tau^{0.35} + C\tau^{2/3} + D\tau + E\tau^{4/3} \qquad \tau = 1 - T/T_c$
117	$Y = AT + BC/\tanh(C/T) + DE/\tanh(E/T)$
120	$Y = A - B/(T + C)$
121	$Y = A + B/T + C\ln T + DT^E$
122	$Y = A + B/T + C\ln T + DT^2 + E/T^2$
207	$Y = \exp(A - B/(T + C))$
208	$Y = 10^{(A - B/(T + C))}$
209	$Y = 10^{A(1/T - 1/B)}$
210	$Y = 10^{A + B/T + CT + DT^2}$
211	$Y = A\left(\dfrac{B - T}{B - C}\right)^D$

A special note about the Antoine equation which has the following form:

$$\ln P_{sat} = A - \frac{B}{T + C}$$

P_{sat} is the vapor pressure. *ChemSep* requires the temperature to be specified in Kelvin and returns the vapor pressure in Pascals. Parameters from other sources may need to be converted to this form of the equation before being entered in the databank.

Interface Settings can be found on the *Tools* menu:
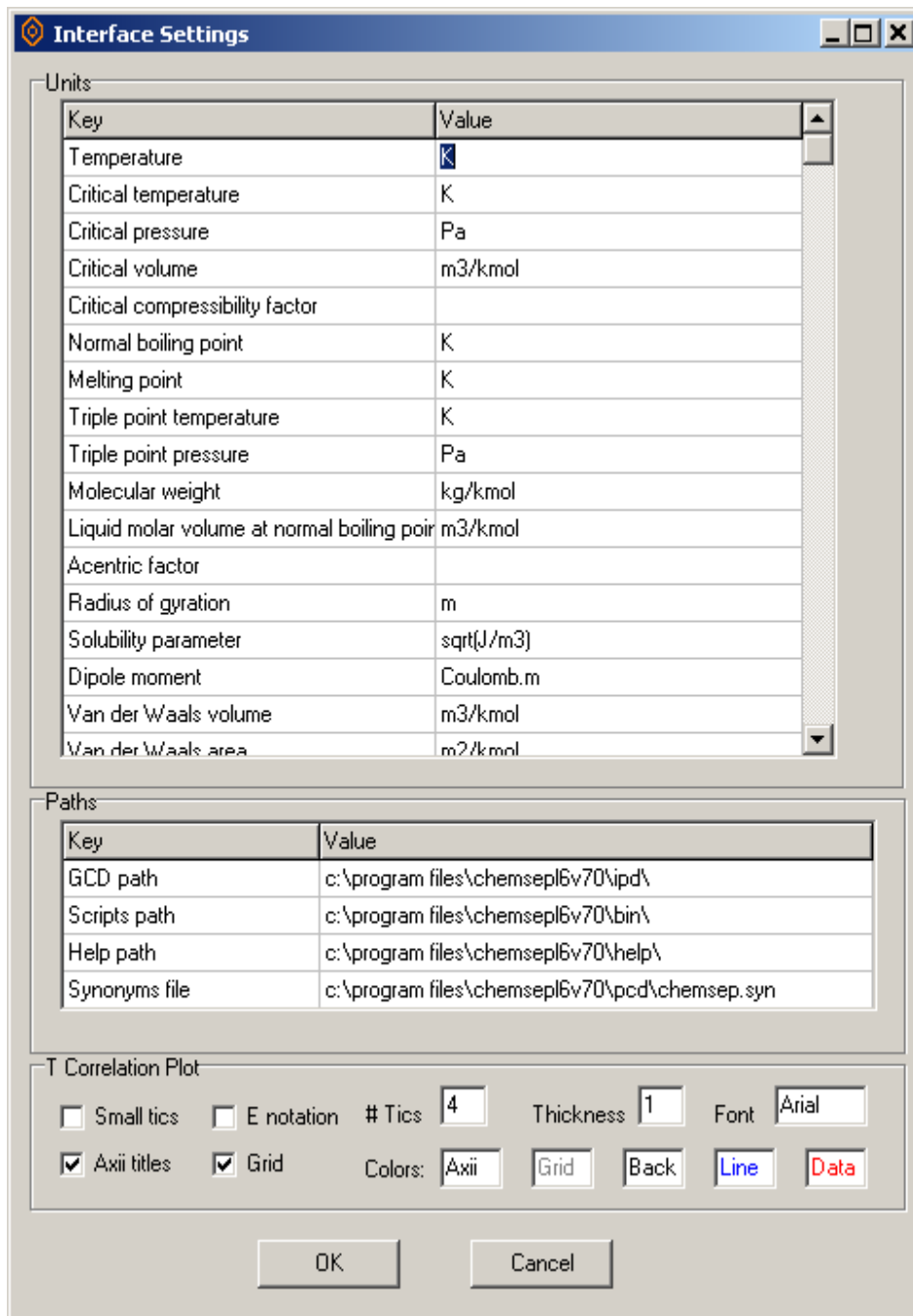
The paths section at the bottom simply tells *PCDmanager* where to find certain files. Normally you will not need to change the settings in this panel.

The data in the pcd file is recorded in SI units (with the sole exception that we use kmol rather than the more correct mol for molar amounts). However, data can be displayed (and entered using any convenient units. The units panel summarizes the set of units used for displaying each of the properties shown on the other panels. You can change the units simply be replacing the existing unit string with your preferred alternative. For example, to see the critical temperature in degrees Fahrenheit rather than the default Kelvin simply replace the K with an F.

Adding Compounds Not in the Databank

There will be many occasions when the available databanks do not contain all of the compounds needed for a simulation. There are several ways to add a new compound to an existing (or new) databank:

1. Direct entry of data from the keyboard

2. Importing data from the Web

3. Importing data from a PCT (Pure Compound Text) file. See, also, Appendix B.

4. Importing data from the DIPPR databank.

Creating a New Compound Record

Click on the **Add New** button (near the bottom of the central vertical row of buttons) and you will be asked if you wish to create a new component:

Type the name of the compound into the window that appears:
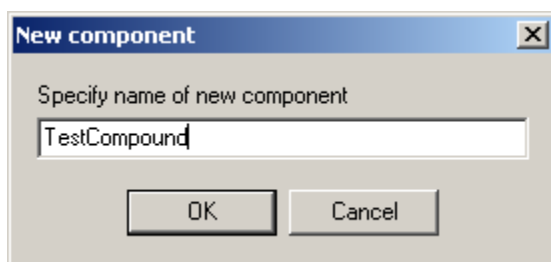
Click OK and a new record will be created for this compound:
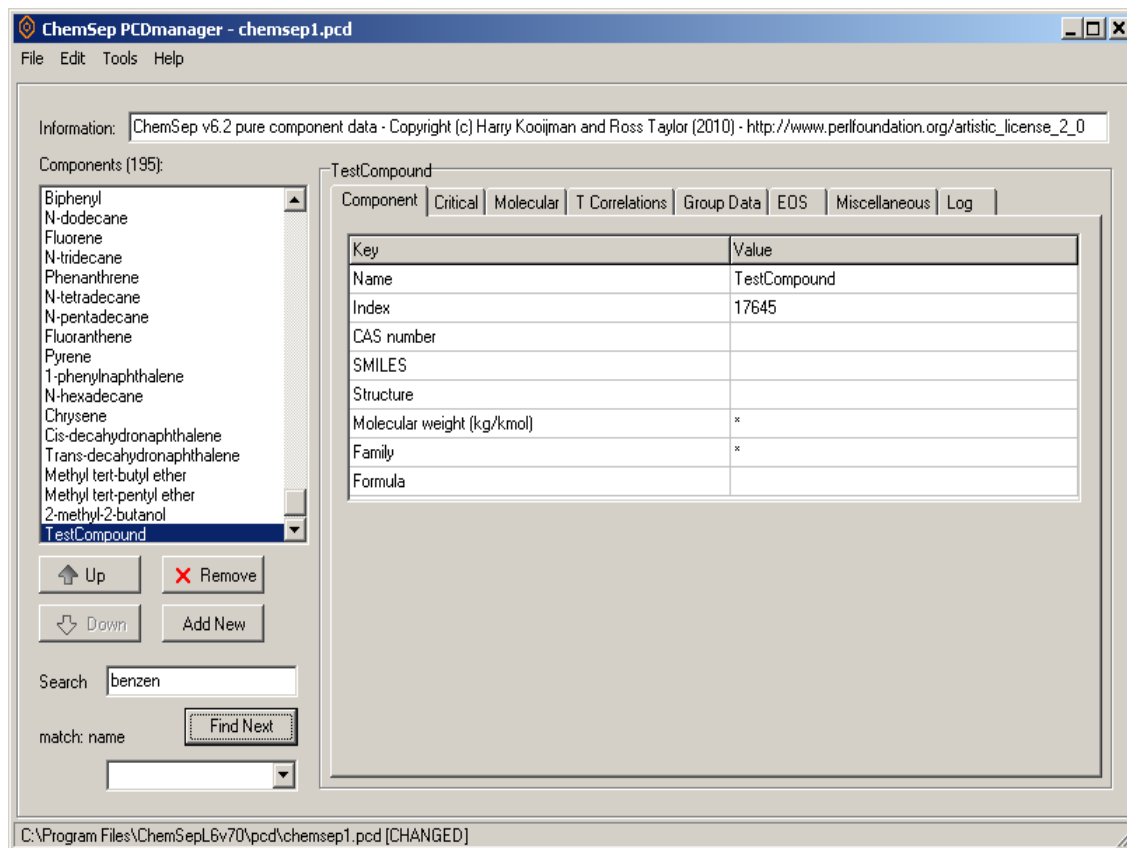
Note that the name appears in the list on the left and in the topmost cell on the data panel to the right. The name can be changed by retyping what appears on the right. An index number (created automatically by *PCDmanager*) appears below the name. This too can be changed. All of the other data panels are empty; the various constants can simply (or not so simply) be typed in to the various cells.

Do NOT forget to save the file once the record is complete.

Importing Component Data from a text file

PCDmanager can also export data one or more records to text files and, perhaps, more importantly, import pure compound data text files. This means that it is possible to add compound data from alternative sources using a semi-automated procedure. See Appendix B for more details.

Pure compound text (pct) files can be imported into *PCDmanager* from the **Edit** menu.
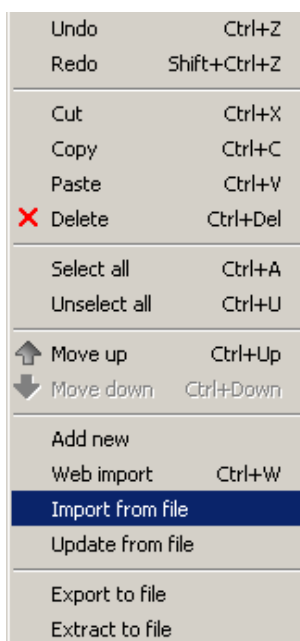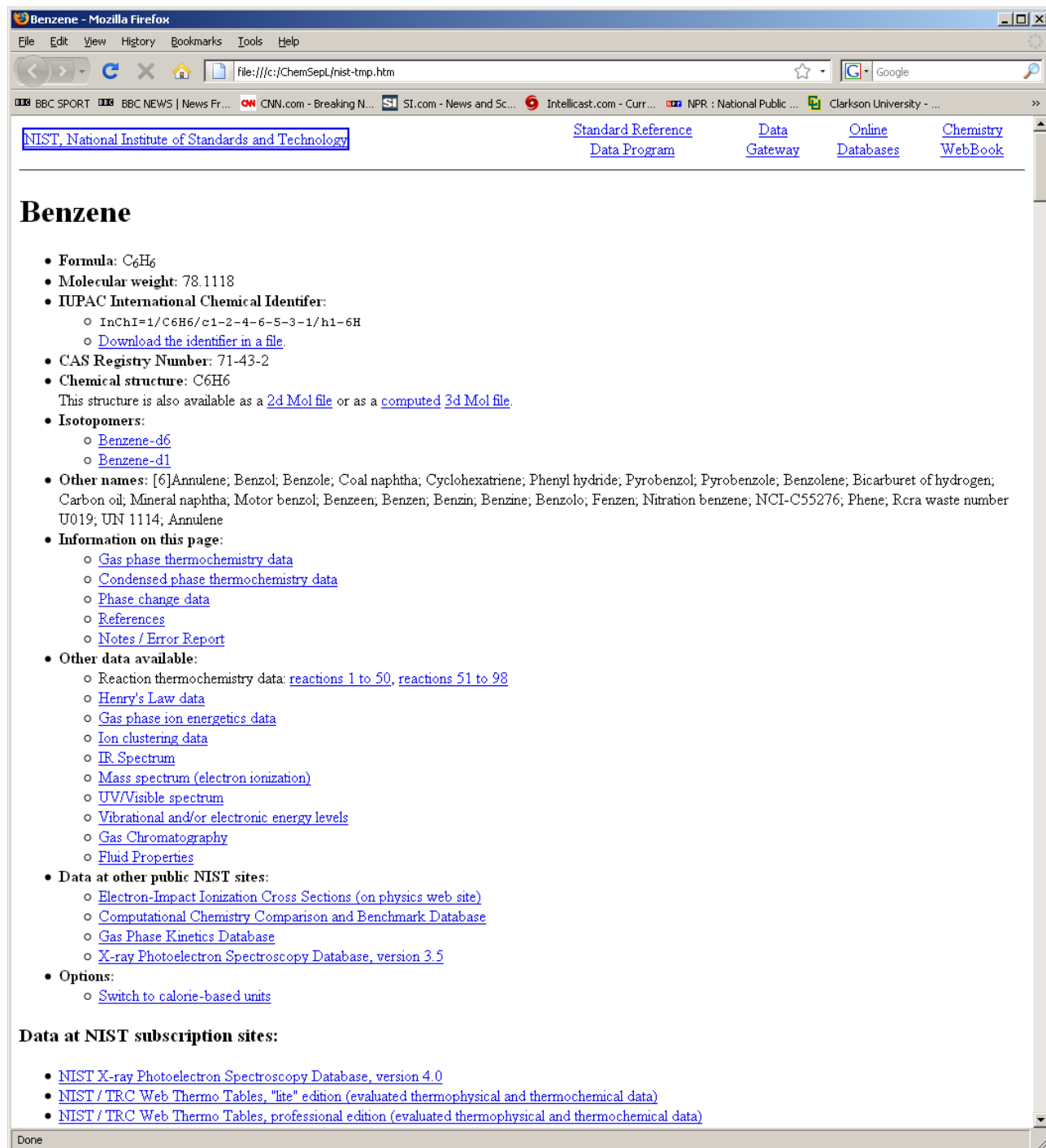
The imported text file **must** have the format specified in Appendices B and C.

Importing Component Data from the Web

If, when you click on OK after typing in a compound name and your computer is connected to the Internet *ChemSep* will do two things, it will search the databank of NIST (National Institute of Science and Technology) for data and load what is available into a new data record. You will also be given the option of displaying the NIST data page in a we browser. The images below are screen shots from the NIST page for benzene.

One important caveat: for some compounds NIST does not use a simple polynomial for the ideal gas heat capacity. In those cases, the program does not load the NIST parameters.

Phase change data

Go To: Top, Gas phase thermochemistry data, Condensed phase thermochemistry data, References, Notes / Error Report

Data compilation copyright by the U.S. Secretary of Commerce on behalf of the U.S.A. All rights reserved.

Data compiled as indicated in comments:
TRC - Thermodynamics Research Center, NIST Boulder Laboratories, M. Frenkel director
BS - R.L. Brown and S.E. Stein
ALS - H.Y. Afeefy, J.F. Liebman, and S.E. Stein
DRB - D.R. Burgess
C - J.S. Chickos
DH - E.S. Domalski and E.D. Hearing

Quantity	Value	Units	Method	Reference	Comment
T_{boil}	353.3 ± 0.1	K	AVG	N/A	Average of 147 out of 183 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
T_{fus}	278.64 ± 0.08	K	AVG	N/A	Average of 57 out of 69 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
T_{triple}	278.5 ± 0.6	K	AVG	N/A	Average of 9 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
T_c	562.0 ± 0.8	K	AVG	N/A	Average of 36 out of 41 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
P_c	48.9 ± 0.4	bar	AVG	N/A	Average of 24 out of 26 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
V_c	0.25 ± 0.03	l/mol	AVG	N/A	Average of 6 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
ρ_c	3.9 ± 0.2	mol/l	AVG	N/A	Average of 12 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
$\Delta_{vap}H°$	$33. \pm 2.$	kJ/mol	AVG	N/A	Average of 6 values; Individual data points

Enthalpy of vaporization

$\Delta_{vap}H$ (kJ/mol)	Temperature (K)	Reference	Comment
30.72	353.3	Majer and Svoboda, 1985	

Enthalpy of vaporization

$\Delta_{vap}H° = A \exp(-\alpha T_r) (1 - T_r)^\beta$
$\quad \Delta_{vap}H° = $ Enthalpy of vaporization (kJ/mol)
$\quad T_r = $ reduced temperature (T / T_c)

View plot Requires a Java capable browser.

Importing Data from the DIPPR Compilation

ChemSep is not supplied with the DIPPR databank so you must have a separate license from DIPPR. If that is the case you can use *PCDmanager* to make a databank that ChemSep can read. Proceed as shown below.

1. Start *PCDmanager*.
2. Click on *File*, click on *New* to create a new databank.
3. Click on *Edit*, select *Import from file*
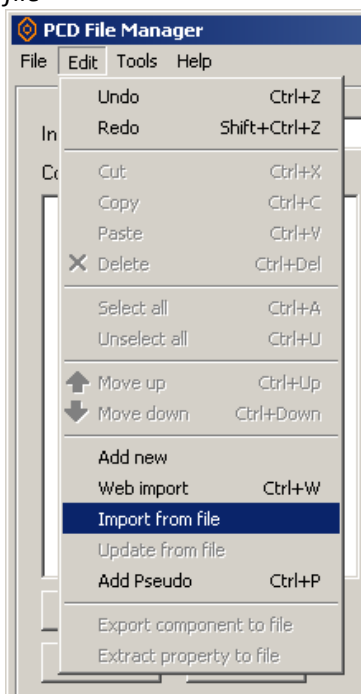
4. Click on *Files of type* pull down list and select *DIPPR files*:
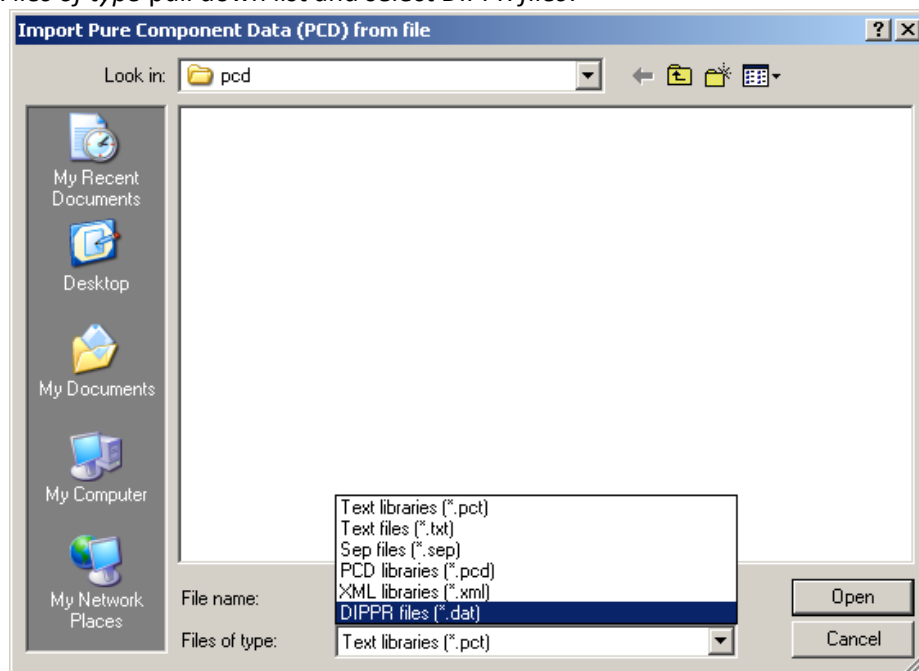
5. Search for the file **source.dat** in the DIPPR databank installation on your computer.
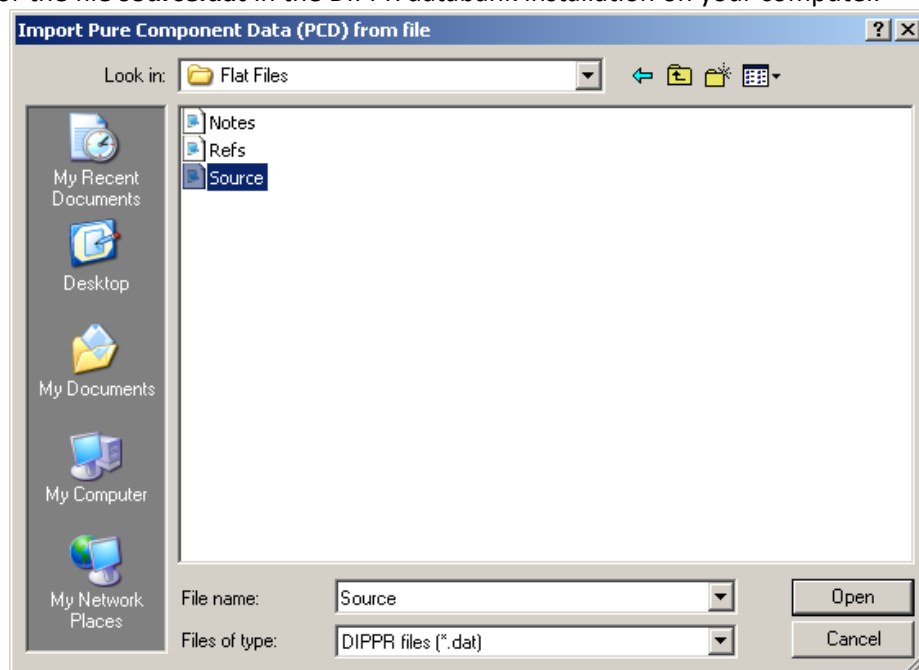
6. Click *Open*.
7. Answer the question posed on the window that pops up:
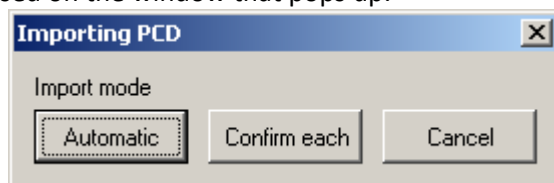
We recommend *Automatic*, otherwise you might need to accept or reject a great many compounds. If you follow our advice you will see this:
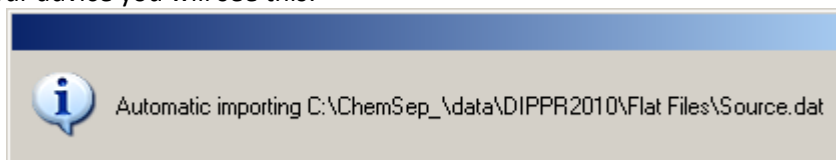
Importing all compounds from DIPPR can take a while depending on the speed of your computer, because there may be more than two thousand compounds in the latest DIPPR compilation.

8. When the import is complete make sure to save the file (Click on *File* and select *Save As*. We suggest that you save the file somewhere *other* than the *ChemSep* pcd folder and copy it to that folder for ease of use with *ChemSep*.

IMPORTANT: *ChemSep* rate-based simulations may need some properties that are not available in the DIPPR data bank. A good example is the Fuller diffusion volume (see *Miscellaneous Properties* tab page). PCDmanager contains methods to estimate many of the properties that are not included in DIPPR. We recommend that after importing the DIPPR databank that you review each panel to see what properties are missing and to assess whether or not they might be needed in your particular simulations.

For more information please see Appendix A.

Estimating Missing Properties

In this subsection we demonstrate how to estimate properties that might be missing from the original data source.

To add the new compound click on the *Add new* button as shown above. Type in a name for the compound. We willustrate with a hypothetical compound to which we give the unimaginative name shown below:
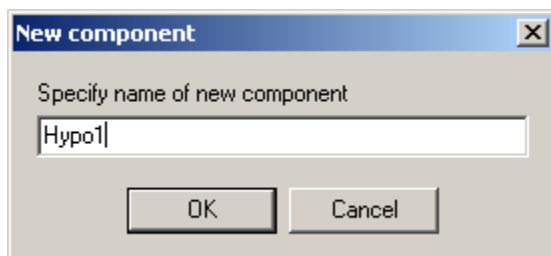
Click *OK*.

You should now see the name and an ID number that has been automatically assigned to this compound appear in the *Component* panel.
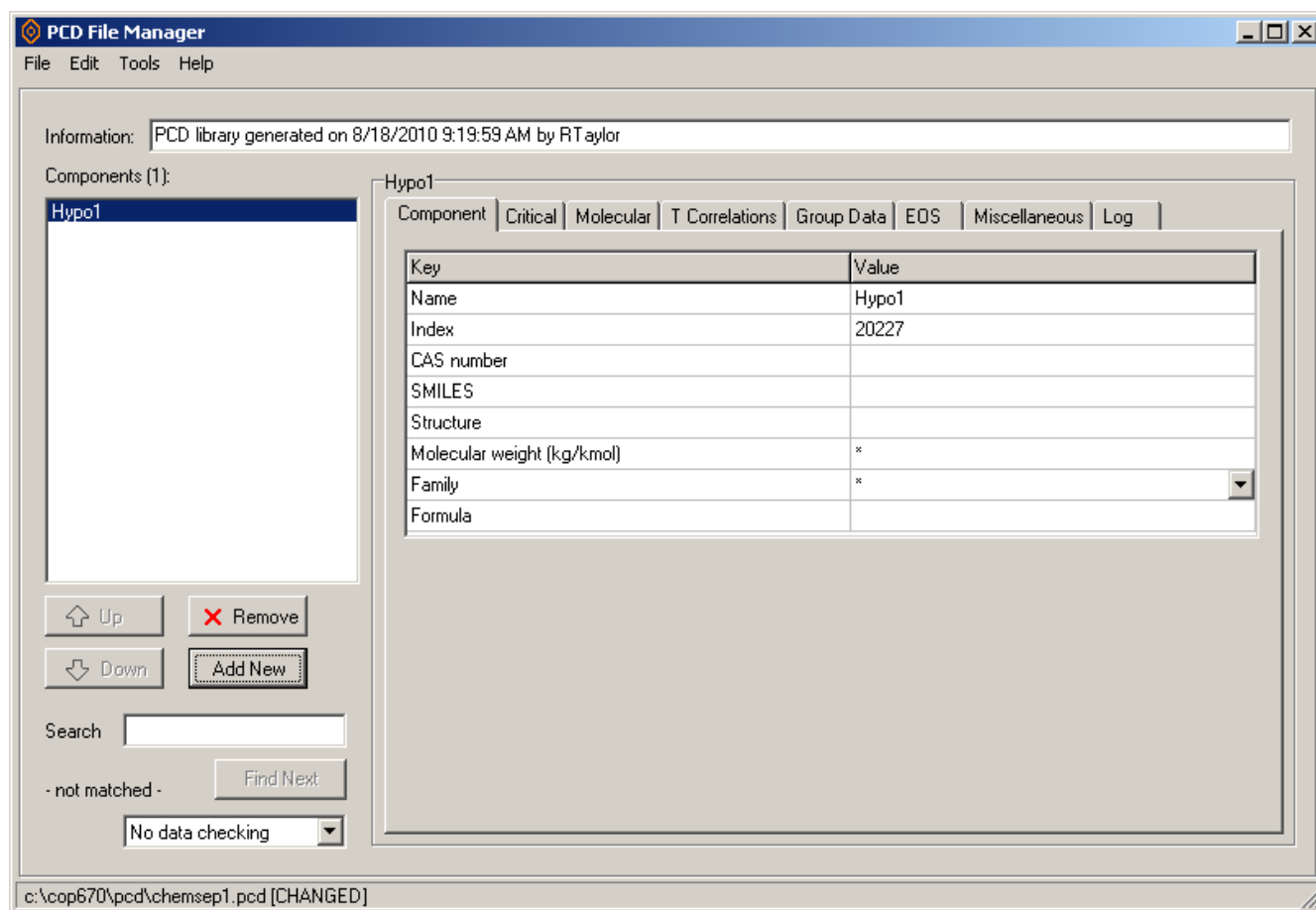
We now proceed to enter a few key properties as shown in the screen images that follow.

1. The Normal Boiling Point in the *Critical* panel (Note: if you know the temperature in Celcius simply type in the value followed by a C as shown).

Key	Value
Critical temperature (K)	×
Critical pressure (Pa)	×
Critical volume (m3/kmol)	×
Critical compressibility factor ( )	×
Normal boiling point (K)	80C
Melting point (K)	×
Triple point temperature (K)	×
Triple point pressure (Pa)	×

Component | Critical | Molecular | T Correlations | Group Data | EOS | Miscellaneous | Log

Hypo1

Press enter when complete and the value will be automatically converted to the units used for display purposes.

Normal boiling point (K)	353.150

2. If you have them available then you can enter the critical properties on the same panel. These are extrememly important properties and **must** be recorded in the databank. We shall proceed here as though we do not have them available.

3. The specific gravity on the *Miscellaneous* panel.

Hypo1

Component | Critical | Molecular | T Correlations | Group Data | EOS | Miscellaneous | Log

Key	Value
COSTLD characteristic volume (V*) (m3/kmol)	×
Lennard Jones diameter (m)	×
Lennard Jones energy (K)	×
Rackett parameter ( )	×
Fuller et al. diffusion volume ( )	×
Surface tension at normal boiling point (N/m)	×
Parachor (kg1/4.m3/s1/2/kmol)	×
Specific gravity ( )	0.700000
Charge ( )	×
Wilson volume (m3/kmol)	×
UNIQUAC r ( )	×
UNIQUAC q ( )	×
UNIQUAC q' ( )	×

4. Return to the *Critical* panel and click on *Estimate* at the bottom of the spreadsheet. This brings up a list of properties in this panel that were estimated using the methods built in to *PCDmanager.*
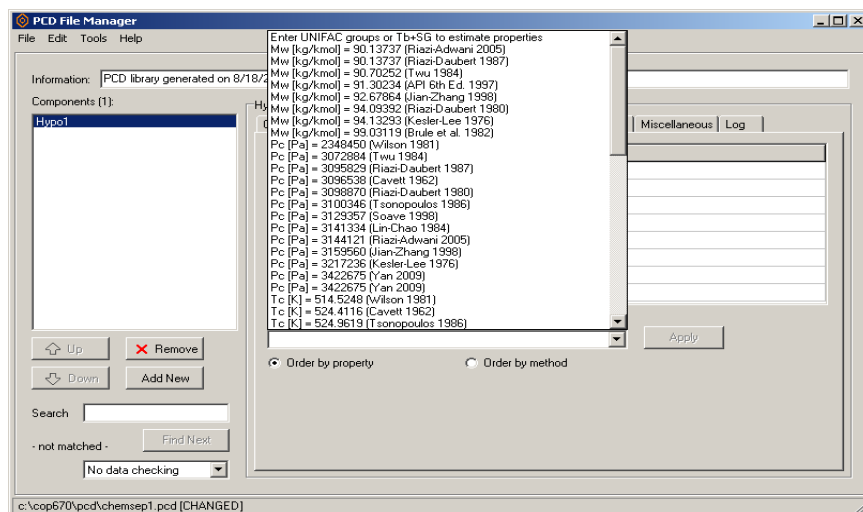
Note that for some properties there are many different estimates available because there are many different methods that have been developed for estimating these properties. Select any one of these property estimates and click on the *Apply* button. Repeat as necessary to select all the properties that you wish estimated.

5. Go to the *T-correlations* panel and if not shown, select the ideal has heat capacity. This is a very important property. If you have values for a correlation available then select the correlation and enter the values. It is very important to note that the temperature must be Kelvin and the corelation must provide values of the heat capacity in J/kmol. Unit conversions are not carried out for temperature dependent correlation constants.

If you do not have parameters for a heat capacity correlation then click on the *Estimate* list to see this (look at the lower part of the screen image below).
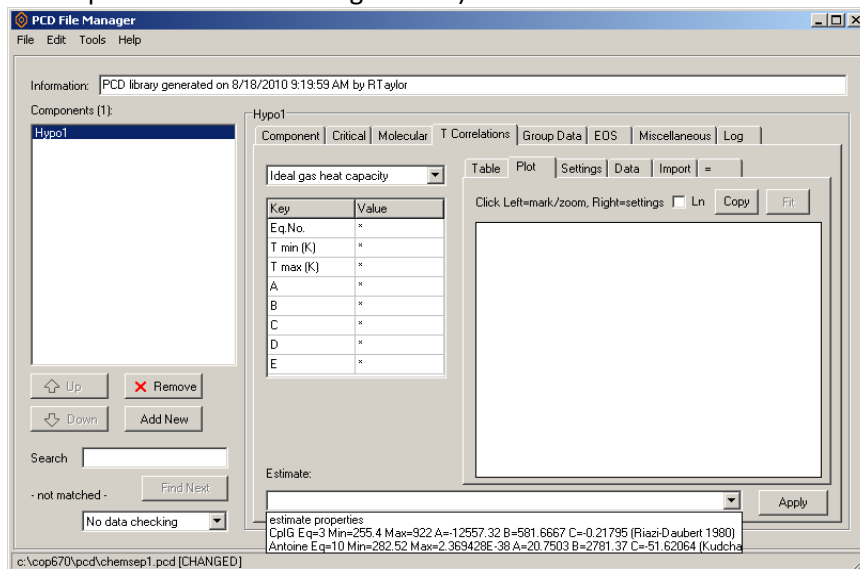
Select the ideal gas heat capacity parameters, click on the *Apply* button to the right and they will appear in the upper part of the panel, along with a plot of the heat capacity.

6. Review the section below concerning **Essential properties**. Remember also, that some simulations may require additional properties that cannot be estimated for hypothetical compounds without some additional data. For example: the Fuller diffusion volume can normally only be estimated once the UNIFAC structure of the molecule has been entered. If this diffusion volume is not available in the PCD file then *ChemSep* will estimate it at run time using an unpublished correlation developed by the authors.

Checking New Property Data

It is useful to know that you do not need to enter values for all of the missing properties in order to run *ChemSep*. Nevertheless, **process simulation makes extensive use of thermodynamic and physical properties, and they can have a profound influence on the simulation results.** **It is important that you assess whether or not the data you have saved is adequate for your needs.**

PCDmanager incorporates a feature that allows you to check for missing data. The check can be done on several different levels selected from the pull down list on the bottom of the left side of the *PCDmanager* window:
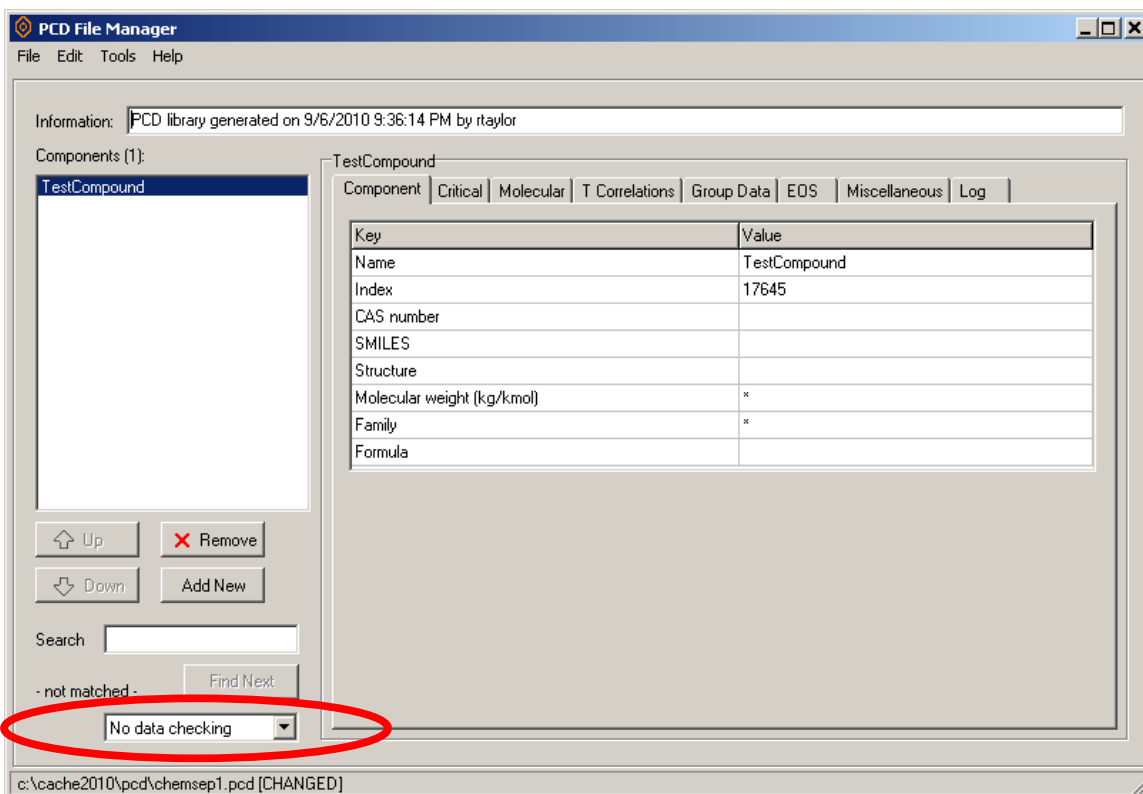
Data checking has been turned off in the illustration above.

The options available are:

- No data checking
- Check essential data
- Check preferred data
- Check reaction data
- Check all data

If we select the second of these we will see something like this:
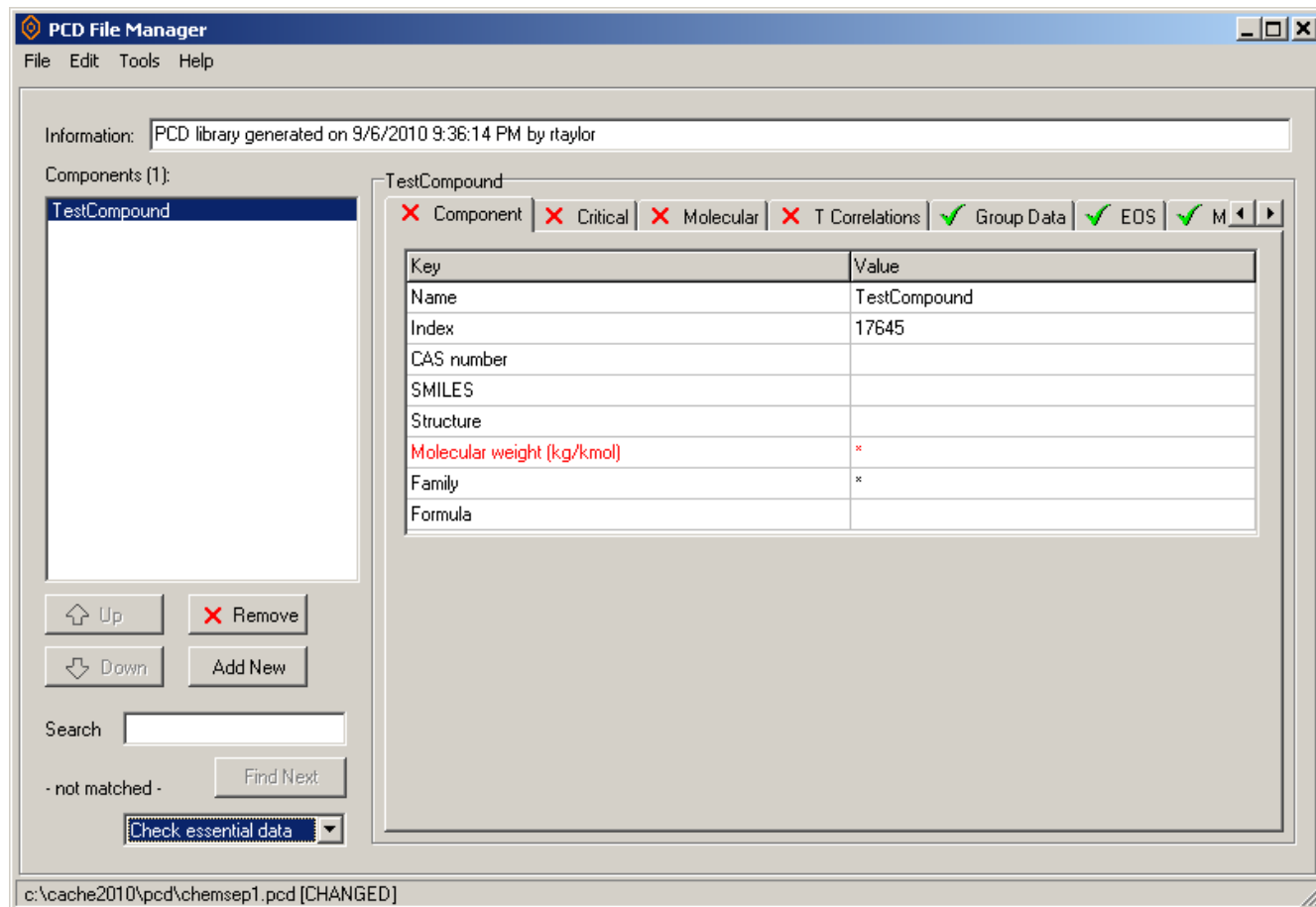
Notice the red X on four of the tab pages shown above, and the properties shown with their label in red (there are others on the other tab pages not shown in this illustration). The properties in red are those considered essential that are missing from this compounds data record.

Essential Properties

Index number: anything will do as long as it is between **10000 and 30000 (see note 1)**
Critical temperature
Critical pressure
Critical compressibility (set to 0.25 if it is not supplied and cannot be calculated)
Critical volume (assumes $v_c = z_c RT_c / P_c$ if not supplied)
Acentric factor (assumes zero if absent)
Liquid molar volume at the normal boiling point (estimated at run time if not supplied)
Molecular weight
Ideal gas heat capacity (assumes $7R/2$ if not specified)

The fact that these properties are the absolute minimum that you need in order to be able to do some equilibrium calculations should not be taken to mean that the equilibrium properties will be accurate, one must also ensure that the models selected for estimating properties are appropriate, and that those models do not need data that is not available.

Many other properties can be estimated from just the properties listed above. Even more can be estimated if, in addition, the normal boiling point, specify gravity, and UNIFAC structure is provided. A list of the properties that are estimated in *PCDmanager* and/or at simulation run time is provided in Appendix A.

A special word about the liquid molar volume at the normal boiling point which is included in the list of essential properties. Strictly speaking this property is not absolutely essential because many calculations can be done without ever needing this property and because, if it is missing a value for it will be estimated at run time from an unpublished correlation developed by the authors. However, the liquid molar volume is sufficiently important in many rate-based simulations that we have included it in the list of essential properties.

Preferred Properties

In addition to the essential properties listed above we prefer that the following also be provided:

> CAS number
> SMILES
> Structural formula (see note 2)
> Chemical formula (is determined by the program from the structural formula)
> Normal boiling point
> Radius of gyration
> Solubility parameters
> Dipole moment
> Van der Waals volume
> Van der Waals area
> UNIFAC structure
> COSTLD characteristic volume (V*)
> Lennard Jones diameter
> Lennard Jones energy
> Rackett parameter
> Fuller et al. diffusion volume
> Surface tension at normal boiling point
> Parachor
> Specific gravity
> Charge
> SRK acentric factor
> Wilson volume
> UNIQUAC r
> UNIQUAC q
> UNIQUAC q'

We repeat the sentiments expressed above: **Process simulation makes extensive use of thermodynamic and physical properties, and they can have a profound influence on the simulation results.** **It is important that you assess whether or not the data you have saved is adequate for your needs.**

We end this section with another caution: Do not make up information to enter into empty cells! For example, if you do not know the structural formula leave it out, do not make up an arbitrary sequence of letters and numbers because it might turn out to be a legitimate chemical formula but have no relevance for the set of data that has been saved for this particular compound (see note 2 below).

Notes:

1. Compound index numbers should not be duplicated! It is possible, of course, to assign the same numbers to two different compounds in two different data banks. No problems will arise as long as compounds from both databanks are never involved in the same simulation. To then use compounds with the same index number from two different data banks in the same simulation is not recommended.

2. Do NOT use PS for pseudo compounds as the program will assume P to stand for phosphorous and S to mean Sulfur. Pseudo compounds have their own family, called, oddly enough, *Pseudo*.

Appendix A: Properties in PCD Files

The tables in this appendix summarize:

1. Properties recorded in *PCDmanager*
2. Properties available in the DIPPR databank
3. Properties that can be estimated by *PCDmanager* using just the boiling point and specific gravity
4. Properties that can be estimated by *PCDmanager* using the UNIFAC structure
5. Properties that are estimated at run time if they are not provided by the property databank

Pure compound Constants	In DIPPR	Can be Estimated		
		in PCDmanager with Tboil+SG	in PCDmanager with UNIFAC	At run time if absent
Index number	√			
Structural formula	√			
Family	√			
CAS Number	√			
SMILES string				
Molecular weight	√	√	√	
Critical temperature	√	√	√	
Critical pressure	√	√	√	
Critical volume	√	√	√	√
Critical compressibility factor	√	√	√	√
Normal boiling point	√		√	
Melting point	√	√		
Triple point temperature	√			
Triple point pressure	√			
Liquid molar volume at normal boiling point	√			√
Acentric factor	√	√	√	
Radius of gyration	√		√	
Solubility parameter	√		√	
Dipole moment	√			
Van der Waals volume	√		√	
Van der Waals area	√		√	
IG heat of formation	√		√	
IG Gibbs energy of formation	√		√	
IG absolute entropy	√			
Heat of fusion at melting point	√		√	
Standard net heat of combustion	√		√	

Properties in bold red and black are deemed essential.

The table below lists some additional pure compound constants that are not available in DIPPR. Some of these properties are estimated automatically by *PCDmanager* when the DIPPR source file is imported. These properties are identified by the * in column 2 of the table below.

Pure compound Constants	In DIPPR	Can be Estimated		
		in PCDmanager with Tboil+SG	in PCDmanager with other	At run time if absent
COSTLD characteristic volume (V*)	*			√
Lennard Jones diameter			√	√
Lennard Jones energy			√	√
Rackett parameter				√
Fuller et al. diffusion volume	*		√	√
Surface tension at normal boiling point			√	√
Parachor			√	√
Specific gravity				√
Charge				
SRK acentric factor	*			√
Wilson volume	*		√	√
UNIQUAC r			√	√
UNIQUAC q			√	√
UNIQUAC q'				√
API SRK s1				√
API SRK s2				√
Chao-Seader acentric factor	*			√
Chao-Seader solubility parameter	*			√
Chao-Seader liquid volume	*			√

The methodology used to assign these property values is summarized below.

1. The COSTALD characteristic volume is estimated from a published correlation. If not applicable it is set equal to the critical volume.
2. The Fuller diffusion volume is estimated from an unpublished correlation developed by the authors of ChemSep.
3. The SRK acentric factor is set equal to the standard acentric factor.
4. The Wilson volume is set equal to the molar volume at the normal boiling point.
5. The Chao-Seader acentric factor is set equal to the standard acentric factor.
6. The Chao-Seader solubility parameter is set equal to the standard solubility parameter.
7. The Chao-Seader volume is set equal to the molar volume at the normal boiling point.

The table below summarizes the temperature dependent properties that can be recorded in *PCDmanager* and those that are available in DIPPR. Note that only the ideal gas heat capacity (one of the essential properties) and the Antoine vapor pressure can be estimated with just the normal boiling point and specific gravity. Some additional properties can be estimated if more information is available (critical properties, normal boiling point etc.). Note that *ChemSep* contains methods to predict all of these properties at run time if they are needed during a simulation so it is not essential that any of these properties be estimated in *PCDmanager* other than the ideal gas heat capacity).

Temperature Dependent Properties	In DIPPR	Can be Estimated		
		in PCDmanager with Tboil+SG	in PCDmanager with other	At run time if absent
Solid density	√			
Liquid density	√			
Vapour pressure	√			
Heat of vaporization	√		√	
Solid heat capacity	√			
Liquid heat capacity	√			
Ideal gas heat capacity	√	√	√	√
Second virial coefficient	√			
Liquid viscosity	√			
Vapour viscosity	√			
Liquid thermal conductivity	√		√	
Vapour thermal conductivity	√		√	
Surface tension	√		√	
Relative static pemittivity				
Antoine vapor pressure		√		

Appendix B: Pure Compound Data Text Files

PCDmanager can export property data to text files. An advantage of text files is that they can be read (or created) by many different programs. *PCDmanager* can also import property data from a file with the correct format.

The first step is to create a template PCT file that can be edited and then imported back into *PCDmanager*. A clean template can be created as follows:

1. Start *PCDmanager* (or click on **File**, **New**)
2. Click the **Add New** button
3. Type something in the window that appears
4. Click OK
5. Select the new "compound" in the list on the left
6. Click on **Edit**, **Export to File**
7. Make sure that the file type is **pct**
8. Give the file a name and save the file somewhere that you can find it.

You have now created an empty template file that can be loaded into a text editor. The content of the text file is shown as columns 2 and 3 of the table in Appendix C (note that the spacing differs in the actual text file from that shown in the table).

To create a new pure compound record enter as much data as you can into the text file y replacing the * and 0 where appropriate. Essential properties are shown in red, desirable properties in bold face (consult the section above on **Essential Properties**). All other properties can be omitted if data is not available, but it is advisable to leave unknown parameters as *; do not replace them with a 0 – zero – as this can have serious negative consequences.

Alternatively, you can copy the data into a spreadsheet (in fact a spreadsheet was used to create the table in Appendix C). This spreadsheet template is available from the authors.

If you prefer to use the spreadsheet template fill in the data in Column 2 only (again, refer to the essential properties section as needed). Once completed (to the extent possible) proceed as follows (and repeat as needed for each new compound).

1. Copy 192 lines of column B starting from [Compound Data] (line 1) and ending with a blank line (line 192) beginning to a text editor (not Wordpad or Word)
2. Save text file with extension .pct. For example: pseduo01.pct
3. Go to **Edit** menu in *PCDmanager*
4. Select **Import from file**
5. Select pct file created in Steps 1 and 2
6. Select Confirm Each (**do NOT select automatic**)
7. Import compound
8. Click on **Stop** button
9. Go to **File** menu
10. Select **Save** (if adding to an existing file) or **Save as** (for a new databank)
11. Save as a **pcd** file

Appendix C: Pure Compound Data Text File Template

o

Line	Template	Content of cell to the left	Units	Example
1	[Component Text]	**Mandatory header**		[Component Text]
2	*	**Index**		501
3	CompoundName			Benzene
4		Structural formula		CHCHCHCHCHCH-
5	0	Family		51
6	*	**Critical temperature**	K	5.62050E+02
7	*	**Critical pressure**	Pa	4.89500E+06
8	*	**Critical volume**	m3/kmol	2.56000E-01
9	*	**Critical compressibility factor**	Ä	2.68000E-01
10	*	**Normal boiling point**	K	3.53240E+02
11	*	Melting point	K	2.78680E+02
12	*	Triple point temperature	Pa	2.78680E+02
13	*	Triple point pressure	kg/mol	4.76422E+03
14	*	**Molecular weight**		7.81140E+01
15	*	**Liquid molar volume at normal boiling point**	m3/kmol	8.94100E-02
16	*	**Acentric factor**		2.09000E-01
17	*	Radius of gyration	m	3.00400E-10
18	*	Solubility parameter	sqrt(J/m3)	1.87000E+04
19	*	Dipole moment	Coulomb.m	0.00000E+00
20	*	Van der Waals volume	m3/kmol	4.84000E-02
21	*	Van der Waals area	m2/kmol	6.00000E+08
22	*	IG heat of formation	J/kmol	8.28800E+07
23	*	IG Gibbs energy of formation	J/kmol/K	1.29600E+08
24	*	IG absolute entropy	J/kmol/K	2.69300E+05
25	*	Heat of fusion at melting point	J/kmol	9.86600E+06
26	*	Empty		*
27	*	Standard net heat of combustion	J/kmol	-3.13600E+09

Line	Template	Content of cell to the left	Units	Example
28	0	EqNo of T correlation Solid density	kmol/m3	2
29	*	A		1.30590E+01
30	*	B		-3.48380E-04
31	*	C		*
32	*	D		*
33	*	E		*
34	*	Min.Temp.	K	2.73100E+02
35	*	Max.Temp.	K	2.82600E+02
36	0	EqNo of T correlation Liquid density	kmol/m3	105
37	*	A		9.99380E-01
38	*	B		2.63480E-01
39	*	C		5.62050E+02
40	*	D		2.78560E-01
41	*	E		*
42	*	Min.Temp.	K	2.73100E+02
43	*	Max.Temp.	K	5.62050E+02
44	0	EqNo of T correlation Vapour pressure	Pa	101
45	*	A		8.83680E+01
46	*	B		-6.71290E+03
47	*	C		-1.00220E+01
48	*	D		7.69400E-06
49	*	E		2.00000E+00
50	*	Min.Temp.	K	2.72040E+02
51	*	Max.Temp.	K	5.62160E+02
52	0	EqNo of T correlation Heat of vaporization	J/kmol	106
53	*	A		4.88100E+07
54	*	B		6.10660E-01
55	*	C		-2.58820E-01
56	*	D		3.22380E-02
57	*	E		2.24750E-02
58	*	Min.Temp.	K	2.73100E+02
59	*	Max.Temp.	K	5.62050E+02
60	0	EqNo of T correlation Solid heat capacity	J/kmol/K	100
61	*	A		-1.24610E+02
62	*	B		9.09020E+02
63	*	C		-6.04900E+00
64	*	D		2.28850E-02
65	*	E		-2.46380E-05
66	*	Min.Temp.	K	4.00000E+01
67	*	Max.Temp.	K	2.78700E+02

34

Line	Template	Content of cell to the left	Units	Example
68	0	EqNo of T correlation Liquid heat capacity	J/kmol/K	16
69	*	A		1.11460E+05
70	*	B		-1.85430E+03
71	*	C		2.23990E+01
72	*	D		-2.89360E-02
73	*	E		2.89910E-05
74	*	Min.Temp.	K	2.78680E+02
75	*	Max.Temp.	K	5.00000E+02
76	0	**EqNo of T correlation Ideal gas heat capacity**	J/kmol/K	16
77	*	**A**		3.53450E+04
78	*	**B**		-6.05220E+02
79	*	**C**		1.28470E+01
80	*	**D**		-2.10290E-04
81	*	**E**		4.88000E-08
82	*	Min.Temp.	K	2.00000E+02
83	*	Max.Temp.	K	1.50000E+03
84	0	EqNo of T correlation Second virial coefficient	m3/kmol	104
85	*	A		1.75070E-01
86	*	B		-2.20130E+02
87	*	C		-1.80850E+01
88	*	D		-7.40460E+03
89	*	E		1.66900E+04
90	*	Min.Temp.	K	2.81020E+02
91	*	Max.Temp.	K	1.96700E+03
92	0	EqNo of T correlation Liquid viscosity	Pa s	101
93	*	A		-2.46100E+01
94	*	B		1.57650E+03
95	*	C		2.16980E+00
96	*	D		-5.13660E-06
97	*	E		2.00000E+00
98	*	Min.Temp.	K	2.78680E+02
99	*	Max.Temp.	K	5.45000E+02
100	0	EqNo of T correlation Vapour viscosity	Pa s	102
101	*	A		3.13660E-08
102	*	B		9.67500E-01
103	*	C		8.02850E+00
104	*	D		-3.56290E+01
105	*	E		*
106	*	Min.Temp.	K	2.73100E+02
107	*	Max.Temp.	K	1.00000E+03

Line	Template	Content of cell to the left	Units	Example
108	0	EqNo of T correlation Liquid thermal conductivity	W/m K	16
109	*	A		4.95390E-02
110	*	B		-1.77970E+02
111	*	C		1.94750E-01
112	*	D		-7.38050E-03
113	*	E		2.79380E-06
114	*	Min.Temp.	K	2.73100E+02
115	*	Max.Temp.	K	4.13100E+02
116	0	EqNo of T correlation Vapour thermal conductivity	W/m K	102
117	*	A		4.95490E-06
118	*	B		1.45190E+00
119	*	C		1.54140E+02
120	*	D		2.62020E+04
121	*	E		*
122	*	Min.Temp.	K	2.50000E+02
123	*	Max.Temp.	K	1.00000E+03
124	0	EqNo of T correlation Surface tension	N/m	16
125	*	A		-2.57500E-02
126	*	B		-2.12190E+02
127	*	C		-6.20890E-01
128	*	D		-5.97380E-03
129	*	E		2.17710E-06
130	*	Min.Temp.	K	2.73100E+02
131	*	Max.Temp.	K	5.62050E+02
132	0	EqNo of T correlation Ideal gas heat capacity (PGL)	J/kmol/K	100
133	*	A		2.95250E+04
134	*	B		-5.14170E+01
135	*	C		1.19440E+00
136	*	D		-1.64680E-03
137	*	E		6.84610E-07
138	*	Min.Temp.	K	5.00000E+01
139	*	Max.Temp.	K	1.00000E+03
140	0	EqNo of T correlation Relative permittivity		0
141	*	A		*
142	*	B		*
143	*	C		*
144	*	D		*
145	*	E		*
146	*	Min.Temp.	K	*
147	*	Max.Temp.	K	*

Template	Content of cell to the left	Units	Example
0	EqNo of T correlation Antoine (Pa)	Pa	10
*	A		2.10750E+01
*	B		2.97730E+03
*	C		-4.15050E+01
*	D		*
*	E		*
*	Min.Temp.	K	3.38000E+02
*	Max.Temp.	K	5.05400E+02
0	EqNo of T correlation Liquid viscosity (PGL)	Pa s	13
*	A		-2.71900E+00
*	B		-1.97340E-02
*	C		1.32630E-05
*	D		*
*	E		*
*	Min.Temp.	K	2.78680E+02
*	Max.Temp.	K	5.45000E+02
*	COSTLD characteristic volume (V*)	m3/kmol	2.56390E-01
*	Lennard Jones diameter	m	5.75303E-10
*	Lennard Jones energy	K	3.20607E+02
*	Rackett parameter		2.69600E-01
*	Fuller et al. diffusion volume	cm3	9.09600E+01
*	Surface tension at normal boiling point	N/m	2.11083E-02
*	Parachor (kg¬.m3/s«/k)		3.67000E-02
*	**Specific gravity**		8.82619E-01
*	Charge		*
*	SRK acentric factor		2.13670E-01
*	Wilson volume	m3/kmol	8.94100E-02
*	UNIQUAC r		3.18780E+00
*	UNIQUAC q		2.40000E+00
*	UNIQUAC q'		2.40000E+00
*	API-SRK s1		*
*	API-SRK s2		-3.18000E-04
*	Empty 2		*
*	Chao-Seader acentric factor		2.13000E-01
*	Chao-Seader solubility parameter	sqrt(J/m3)	1.87368E+04
*	Chao-Seader liquid volume	m3/kmol	8.94000E-02
0 0 0 0 0 0 0 0 0 0 0 0	**UNIFAC**		10 6 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0	UNIFAC-LLE		10 6 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0	ASOG		0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0	GC EOS		10 6 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0	UMR		10 6 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0	Modified UNIFAC		10 6 0 0 0 0 0 0 0 0 0 0
	CAS Number		1-43-2
	SMILES string		1ccccc1
	Empty line - must be present		