Getting started with Simulis® Thermodynamics

Use Case 5: Create pseudo-compounds from TBP and API gravity data curves

Software & Services In Process Simulation

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ProSim

About pseudo-compounds…..

Simulis® Thermodynamics oil characterization environment enables you to characterize petroleum fluids using experimental data.

The oil will be characterized by a set of pseudo-compounds (or pseudo-components) in order to reduce the computational effort.

Each pseudo-compound will be defined by physical properties just like usual compounds. These properties are automatically generated from experimental data and used in the fluid thermodynamic package.

This document presents the different steps to follow in order to generate pseudo-compounds from a crude oil TBP 760 curve and an API gravity data curve.

The following steps will be followed:

- **Step 1: Select the light ends (when necessary)**
- **Step 2: Enter assay characterization data**
- **Step 3: Generate the pseudo-compounds**
- **Step 4: Analyze the results**

Before studying this chapter, it is recommended to consult "Getting Started with Simulis® Thermodynamic: Use Case 1" .

About pseudo-compounds…..

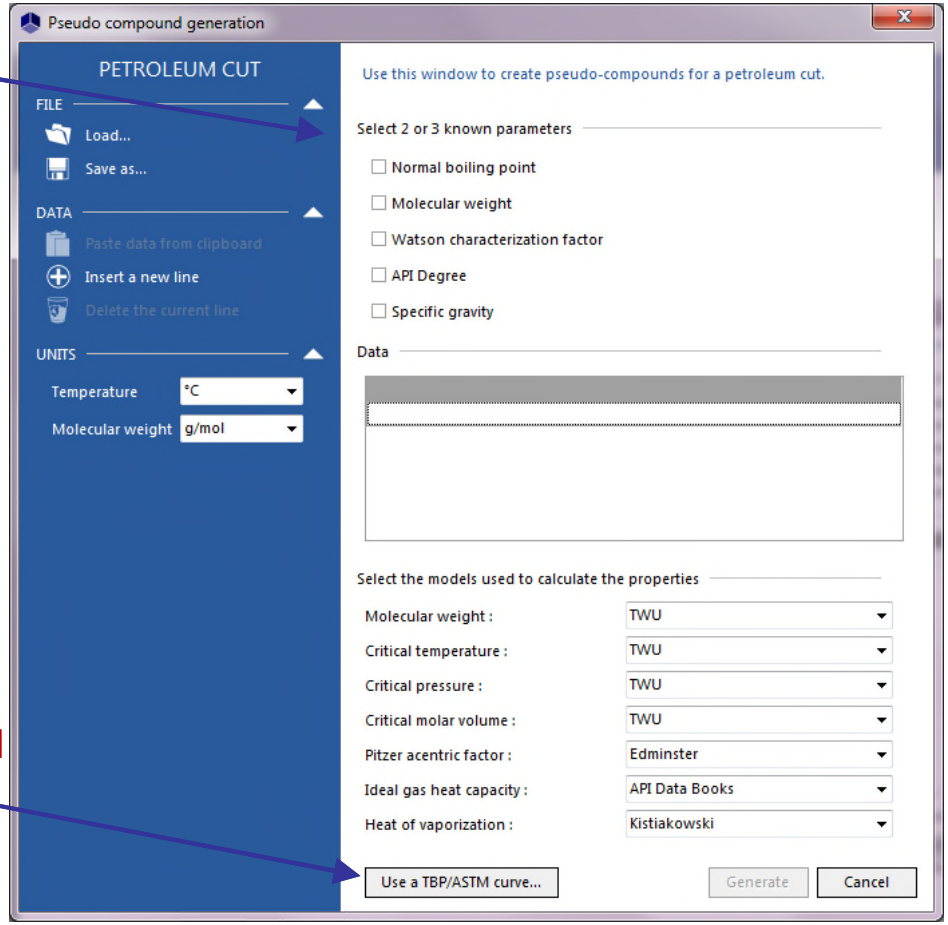
Method 1:

A petroleum cut can be characterized by selecting two or three of the following properties:

- **Normal boiling point.**
- **Molecular weight.**
- **Watson characterization factor.**
- **API degree.**
- **Specific gravity .**

Method 2:

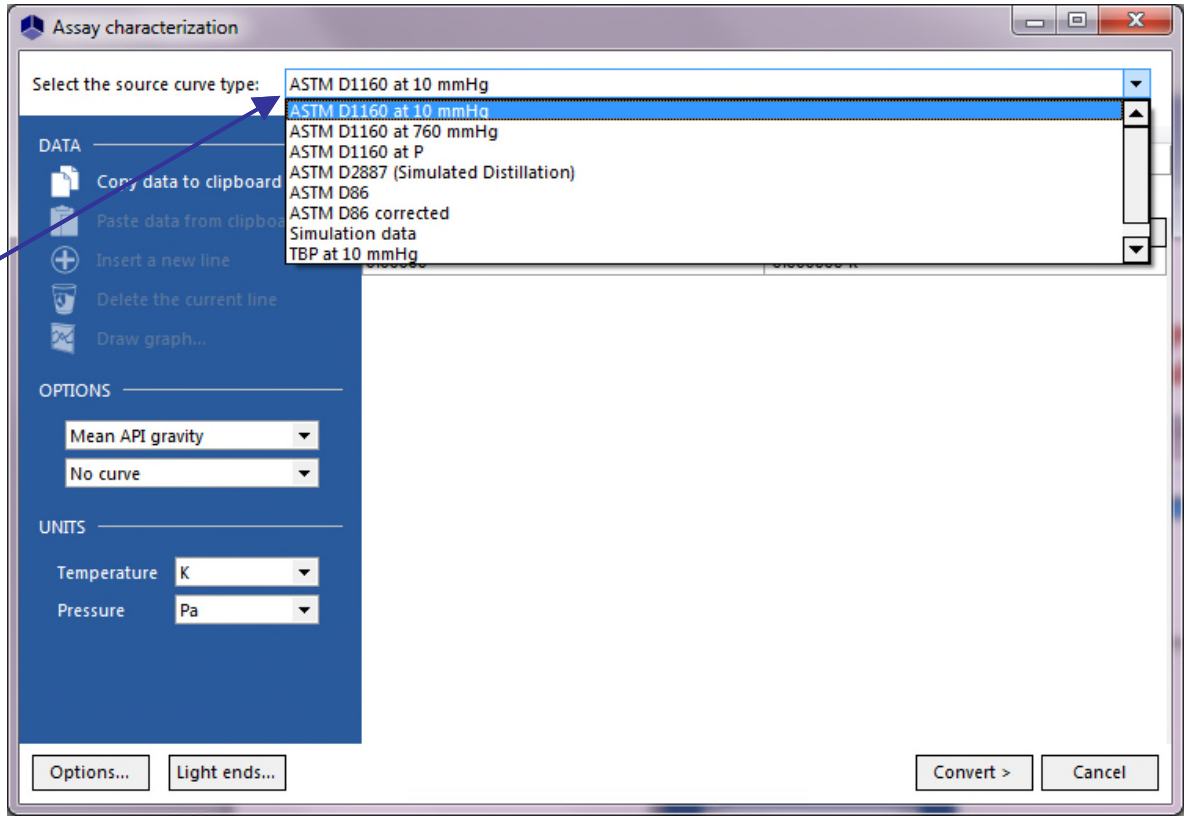
It can also be characterized by experimental distillation curve and gravity (or density) data (TBP or ASTM curves).



About pseudo-compounds…

All physical properties are calculated from an internally generated TBP curve at atmospheric conditions. All other curves are automatically converted into TBP curve.

Access the different types of curve.



Preparation of the data

Prepare the required information in an Excel spreadsheet.

1. TBP distillation curve.

TBP distillation	
LV percent	°F
3.83	98
5	125
10	167
20	227
30	291
40	370
50	460
60	552
70	643
80	799
90	1023
100	1440

2. API gravity curve.

API gravity	
Mid LV percent	°API
12	66.7
19	55.3
40	37.6
62	27
82	19

Mean API gravity 35

Light Ends, LV Percent on Crude	
Propane	0.18
i-Butane	0.3
n-Butane	0.69

3. Light ends list and volume % on crude (if any light ends are identified).

TBPCUTS :		
Tstart	Tend	Nb pseudos
50	150	4
150	550	16
550	750	4
750	1250	5

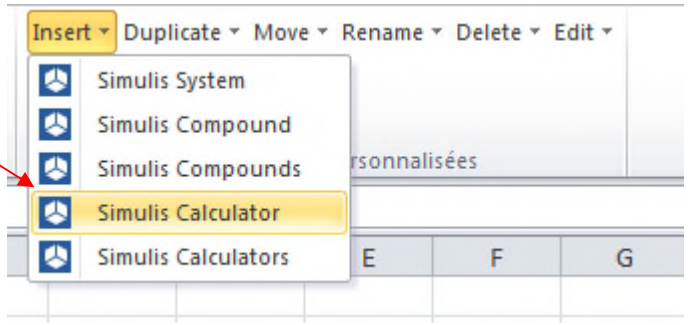
4. Number of required pseudo-compounds (optional).

Step 1: Select the light ends

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

- **<u>If you are using Simulis Thermodynamics in Excel</u>:**

Create the calculator object in a spreadsheet



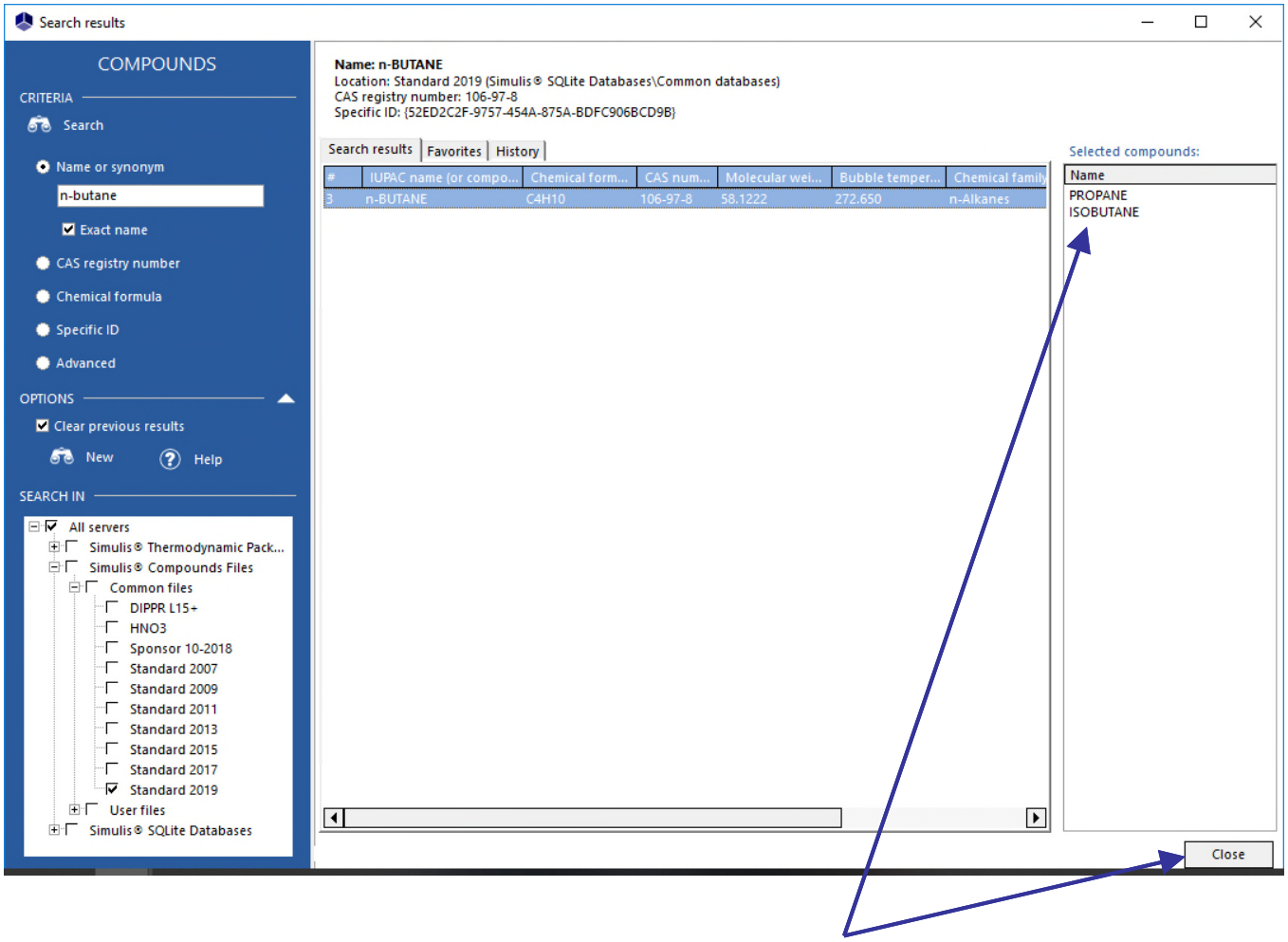
- **<u>If you are using Simulis Thermodynamics within another ProSim environnement</u> (ProSimPlus, BatchReactor, BatchColumn etc…):**

Click on the thermodynamic icon to open the calculator editor:

or

Simulis Thermodynamics is a « software component » that you can integrate into different applications: ProSim software, Excel, Matlab, your own software, etc…

Step 1: Select the light ends

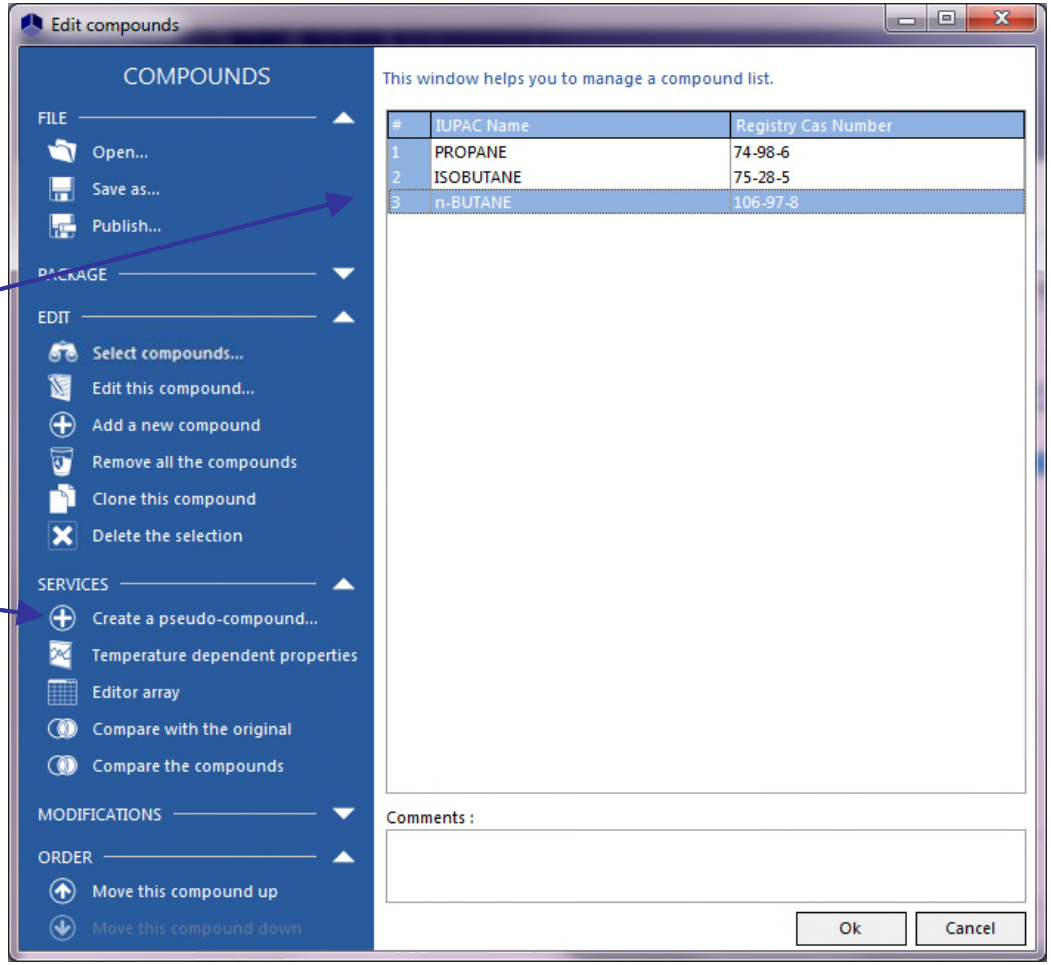


Define light ends: Import Propane, Isobutane and n-Butane from the database and close the window.

Step 1: Select the light ends

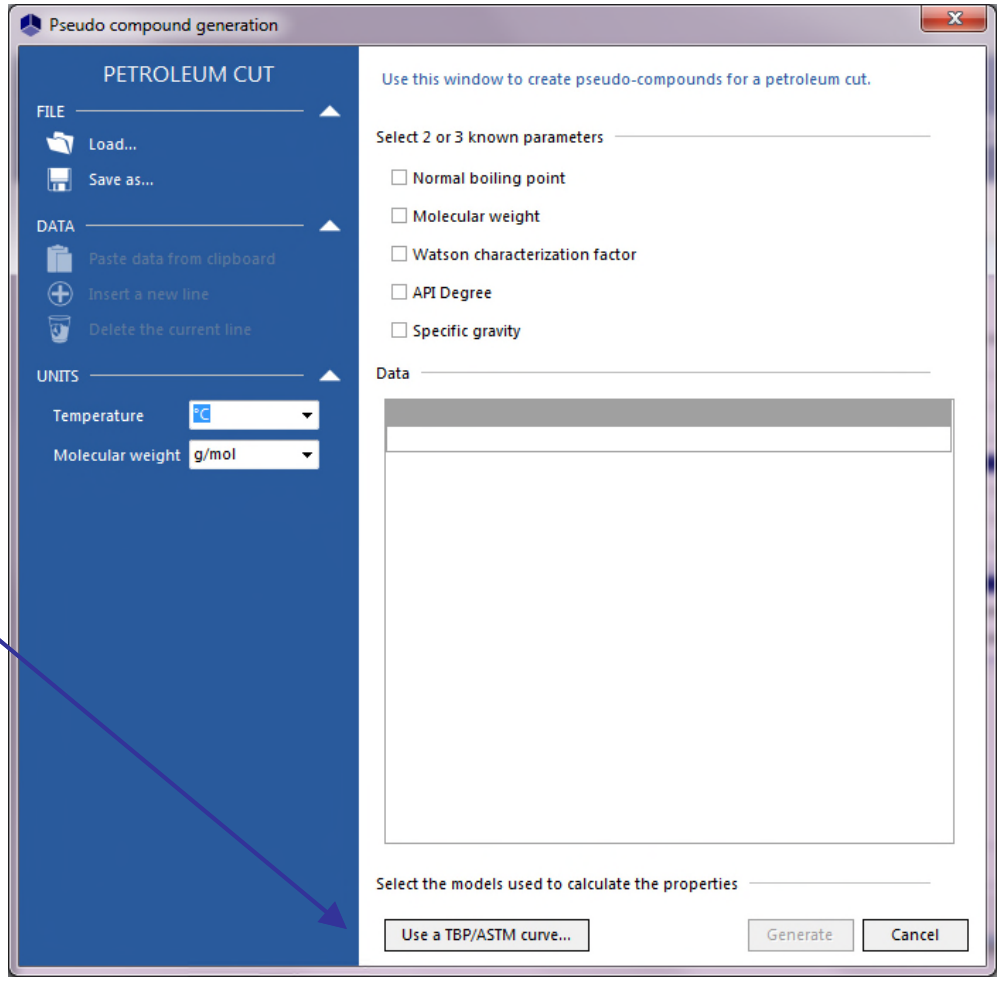
Your list of light ends is defined…

…click on "*Create a pseudo-compound*".



Step 2: Enter assay characterization data

Select "*Use a TBP/ASTM curve*".

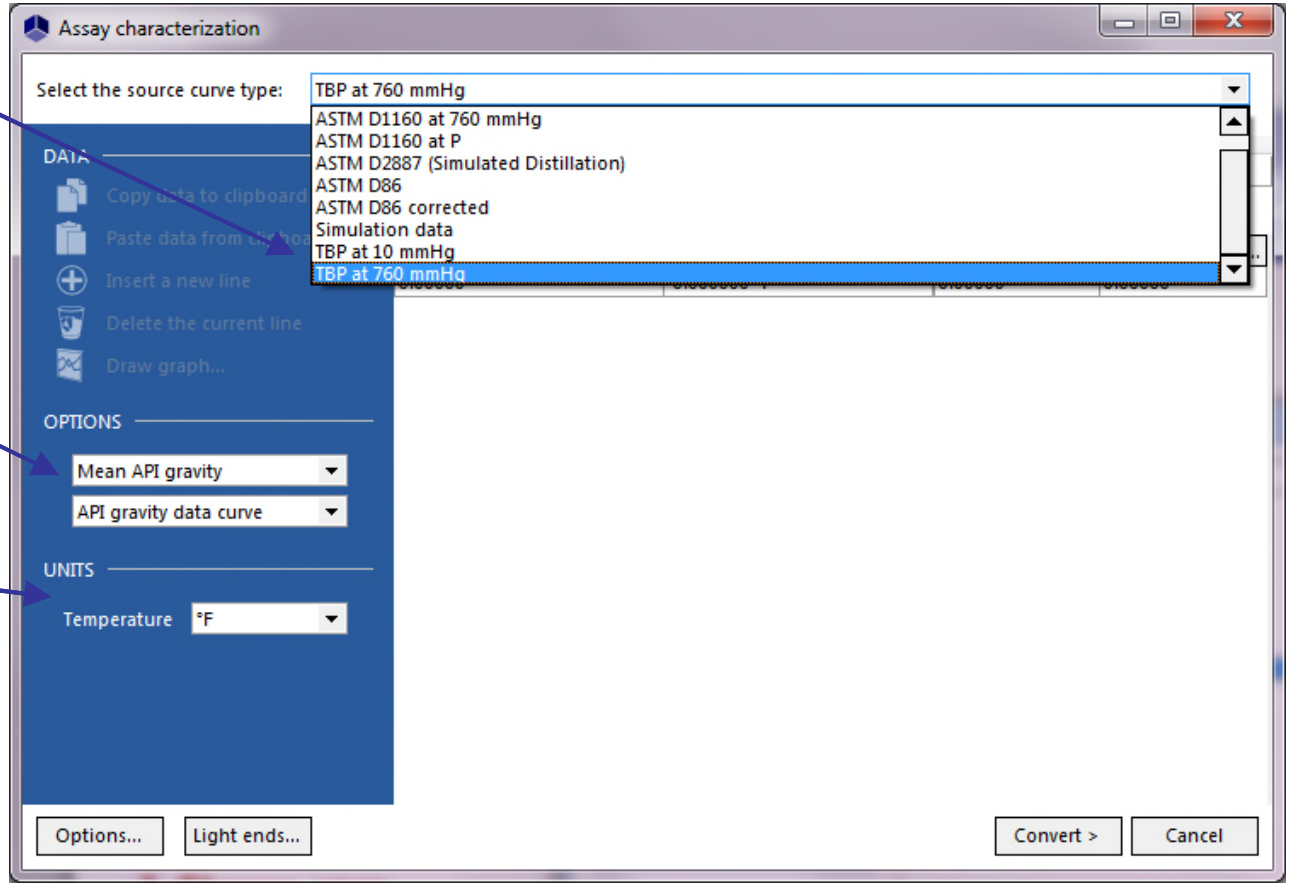


Step 2: Enter assay characterization data

1. **Select a type of curve (“*TBP at 760 mmHg*” in this example).**

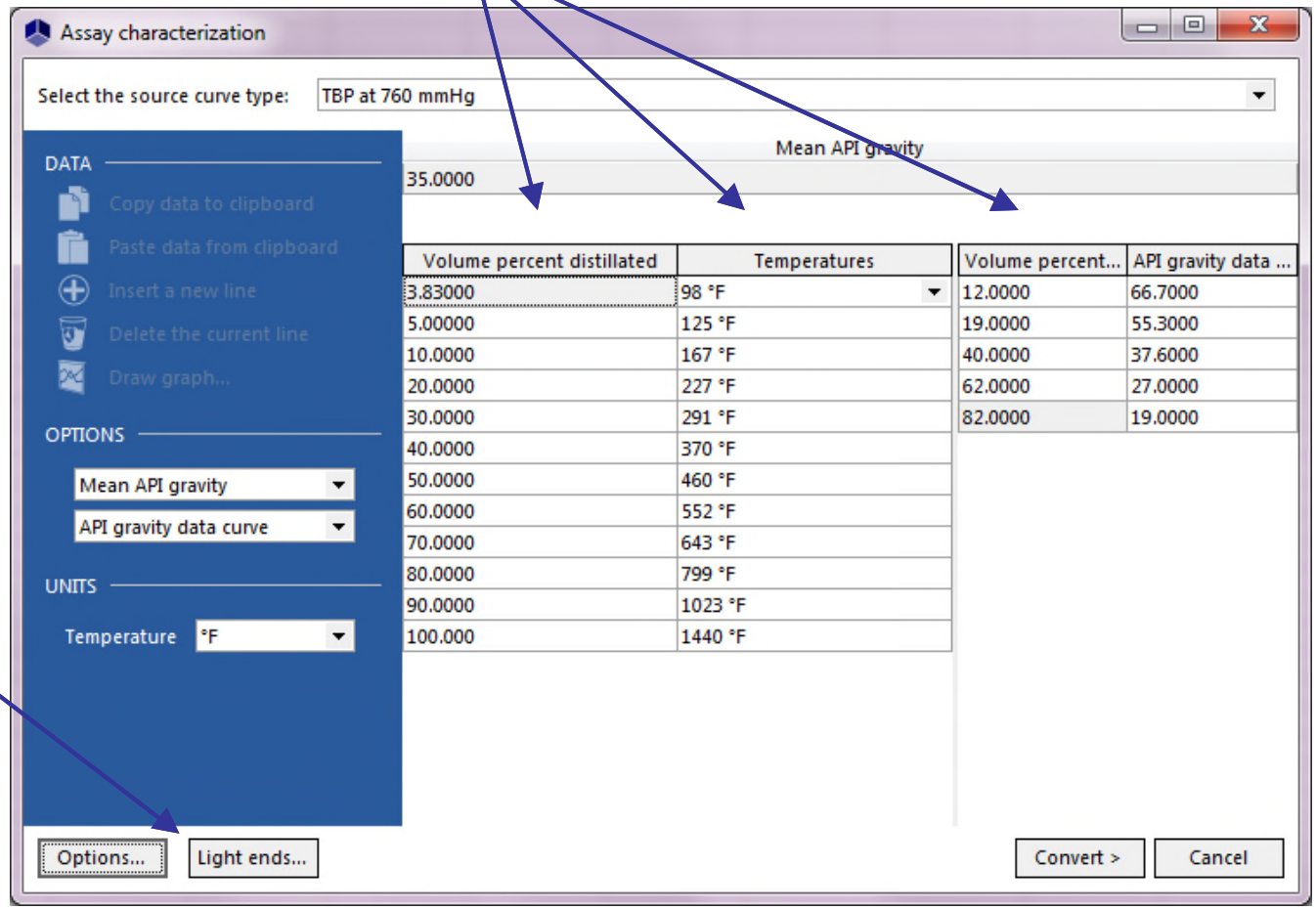
2. **Select your options for defining the gravity.**

3. **Select your temperature unit (“*°F*” in this example).**



Step 2: Enter assay characterization data

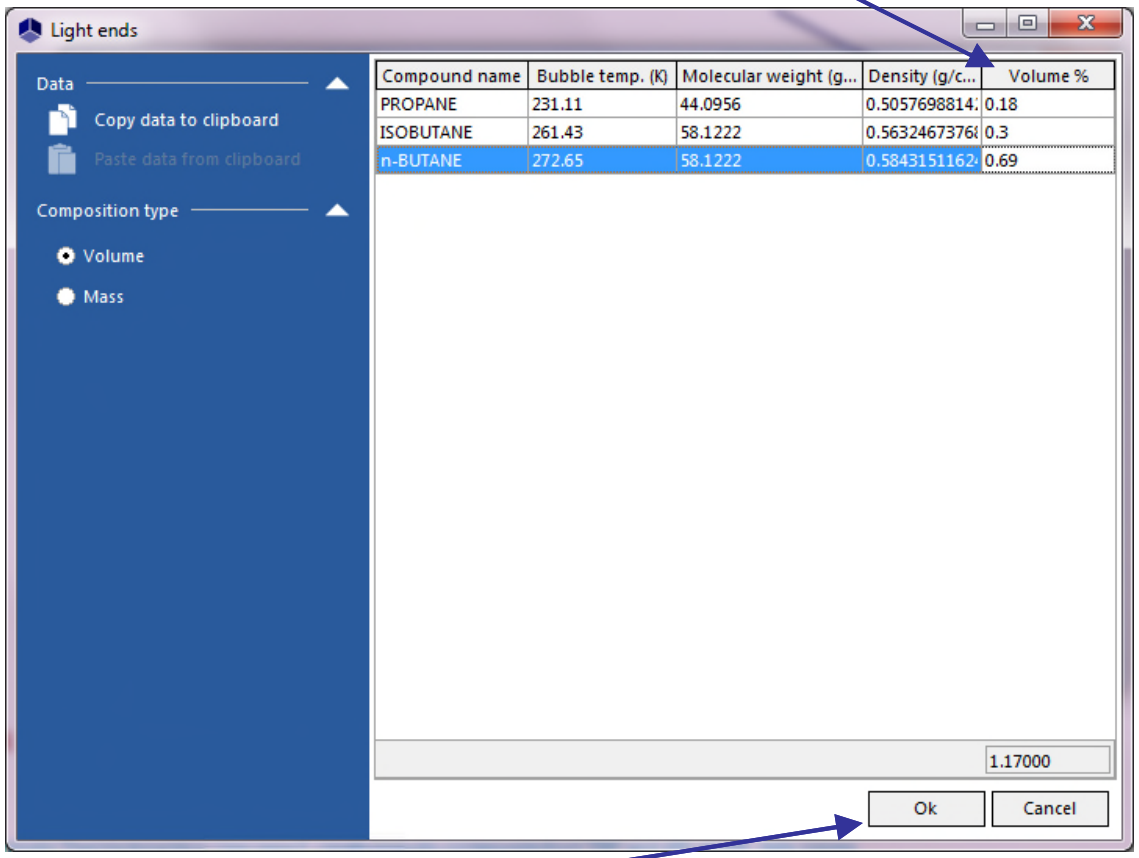
Enter your experimental values for the TBP and the API gravity.



If light ends have been selected, click on "*Light ends*".

Step 2: Enter assay characterization data

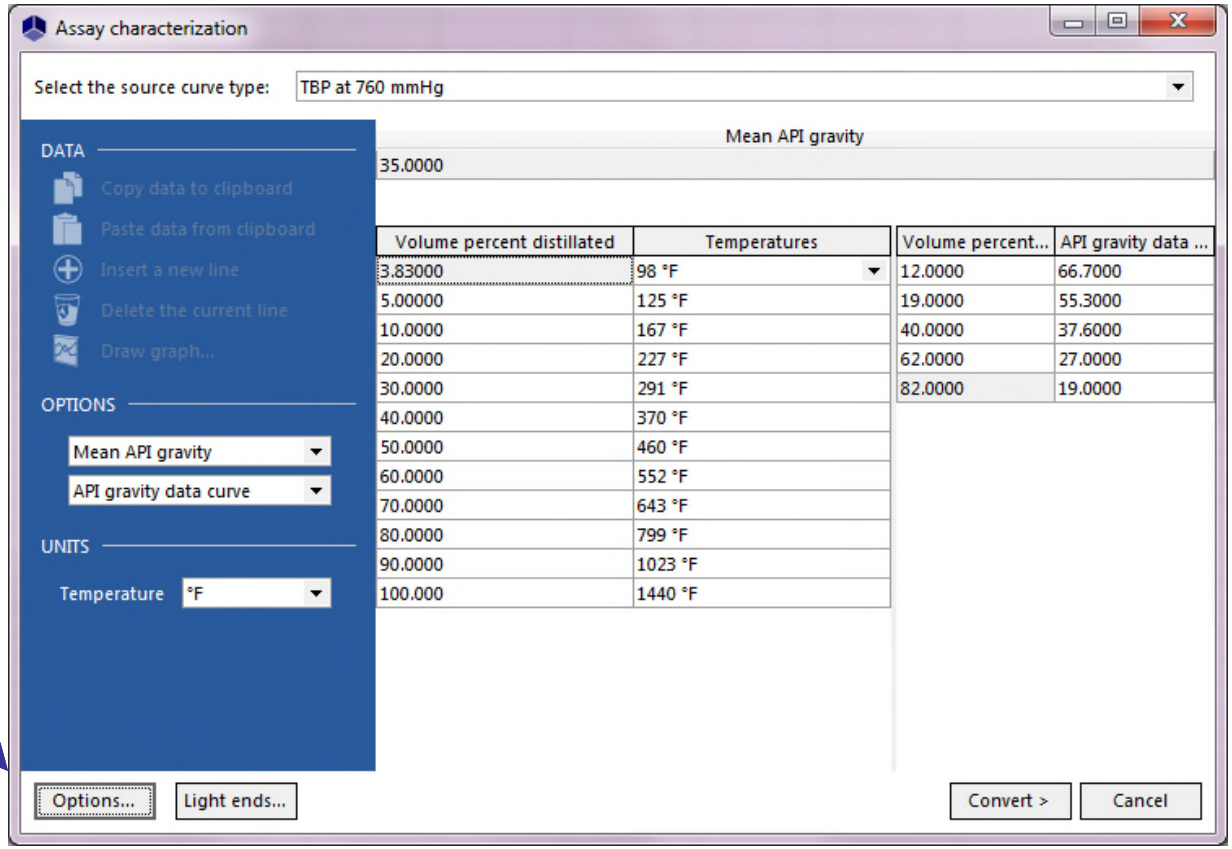
Enter your experimental values for the volume percentage of light ends.



Click on "*OK*" to confirm.

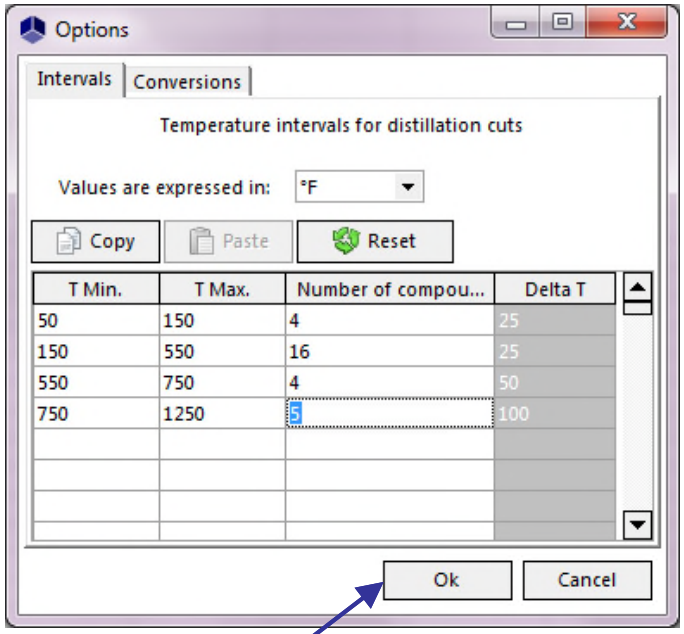
Step 2: Enter assay characterization data

Click on "*Options*".



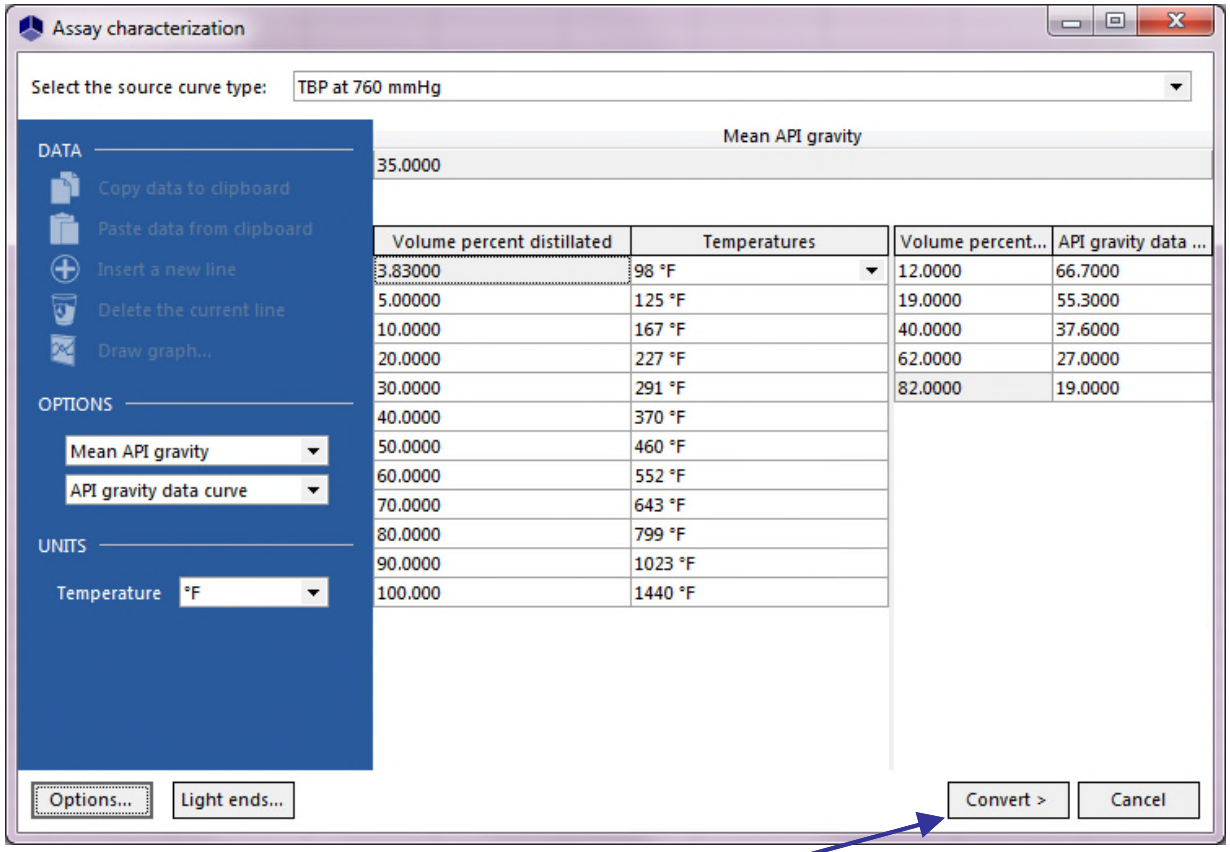
Step 2: Enter assay characterization data

Select the number of pseudo-compounds you want to generate for the different temperature ranges.
Here, 29 pseudo compounds will be generated.



Click on "*OK*" to confirm.

Step 3: Generate the pseudo-compounds

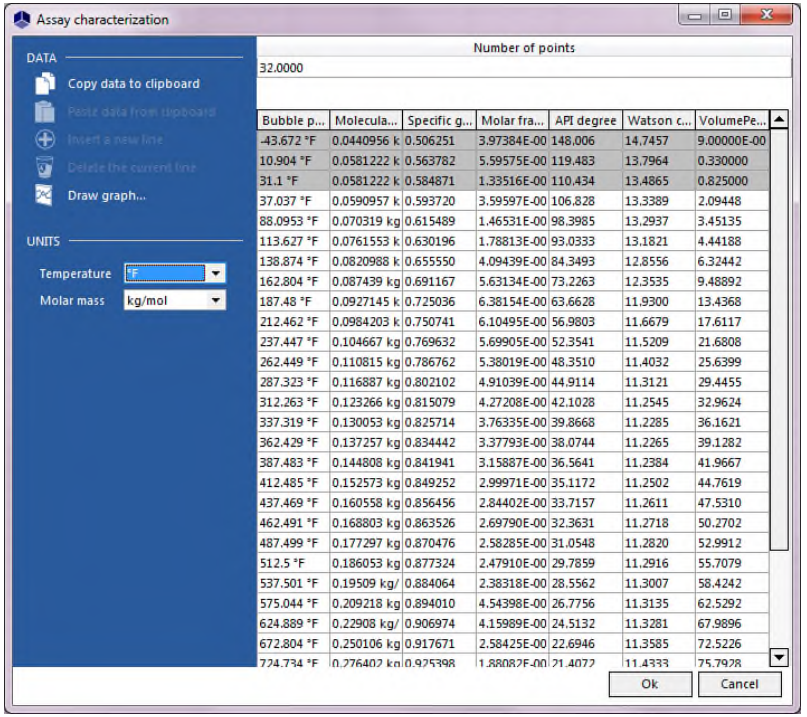


Click on "*Convert*" to generate pseudo-compounds.

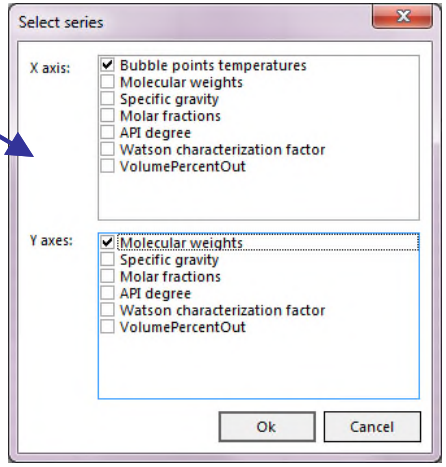
Step 3: Generate the pseudo-compounds

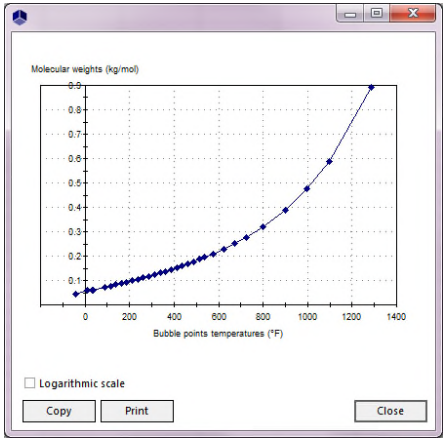
This window displays the data that was generated. 32 compounds will be taken into account:

- **3 light ends already defined (C3, iC4 and nC4).**
- **29 pseudo compounds as explained before.**



The user can plot graphs to analyze the results.





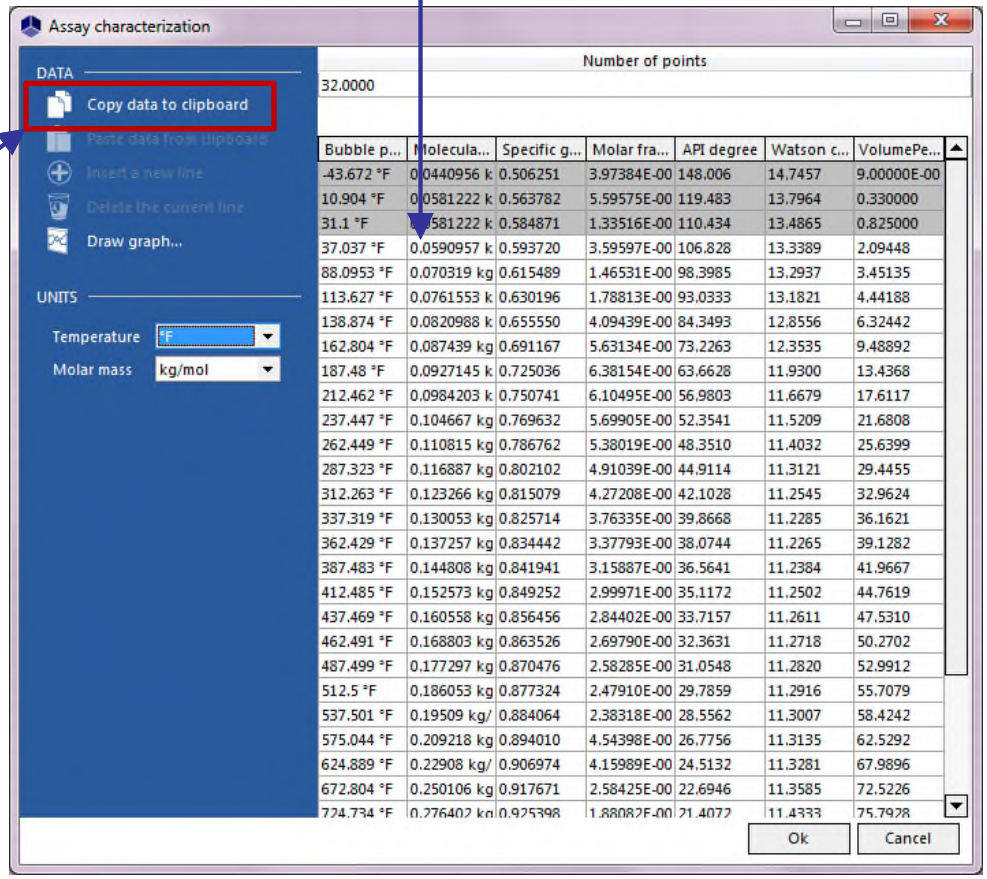
Example of graph: molecular weights (MW) vs. bubble points temperatures.

Step 3: Generate the pseudo-compounds

At this stage, it is important to save the composition of the mixture. This composition will be required afterward to carry out simulations or compute mixture properties. Once this window is closed, it will no longer be possible to access the composition.

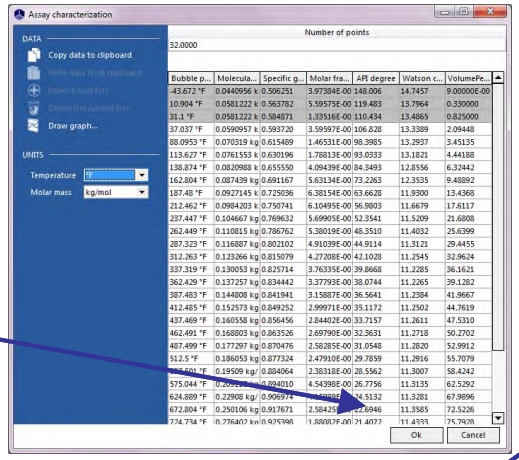
Click on the table

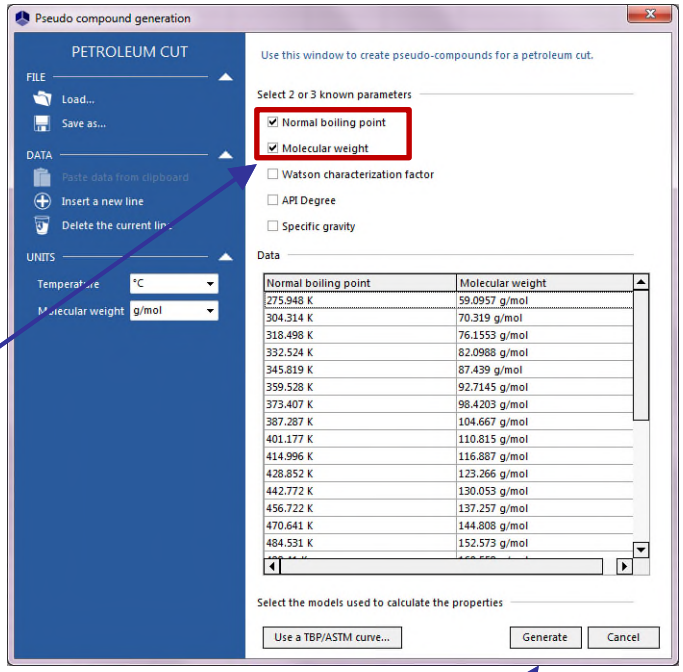
Click on « Copy data to clipboard » in order to paste the table into Excel or paste the composition into a feed module of ProSimPlus



Step 3: Generate the pseudo-compounds

Click on "*OK*" to close this window and come back to the Petroleum Cut window.





Select 2 or 3 parameters that will be used for the calculation of physical properties.
In this example, select:

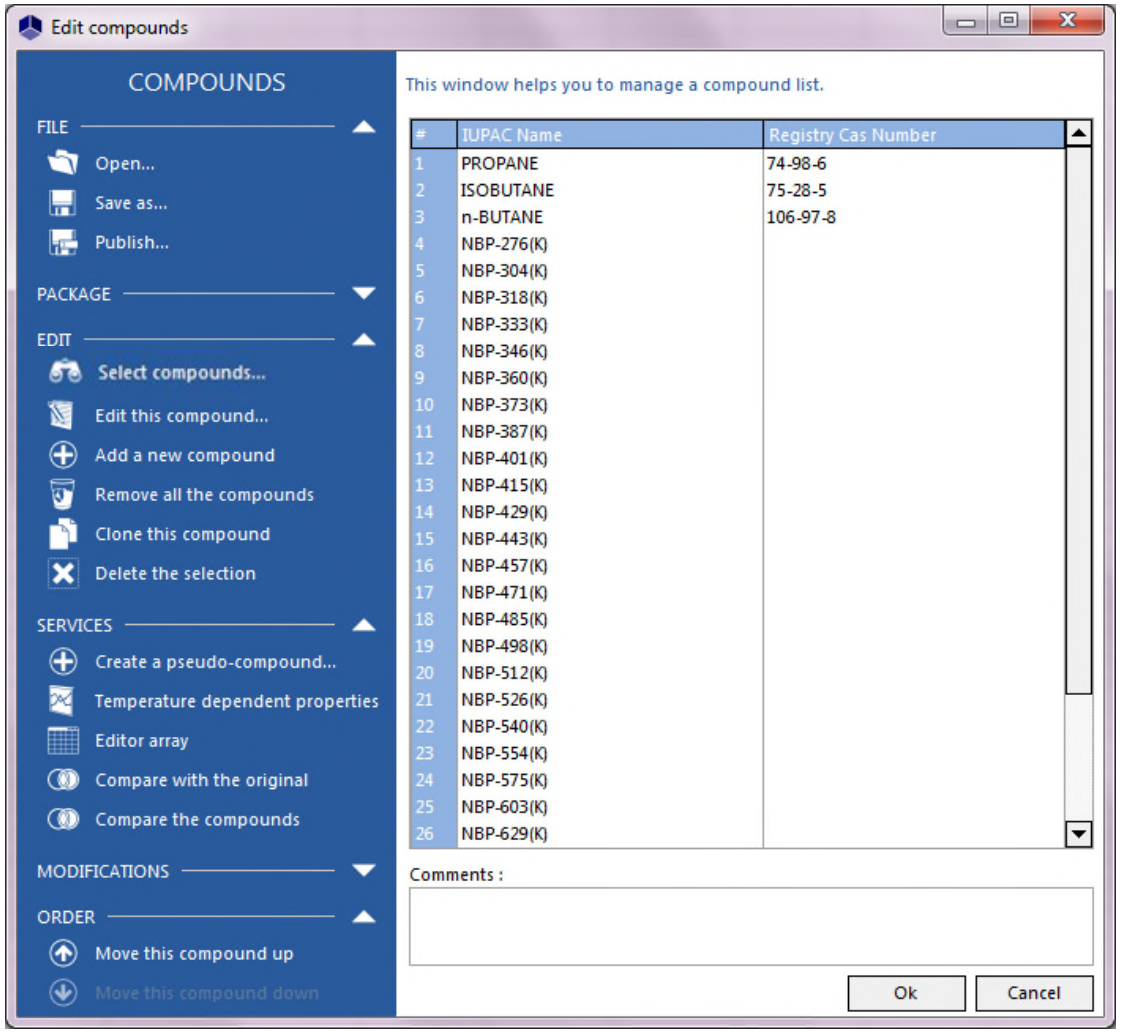
- **normal boiling point.**
- **molecular weight.**

Click on "*Generate*" to create the pseudo-compounds.

Step 3: Generate the pseudo-compounds

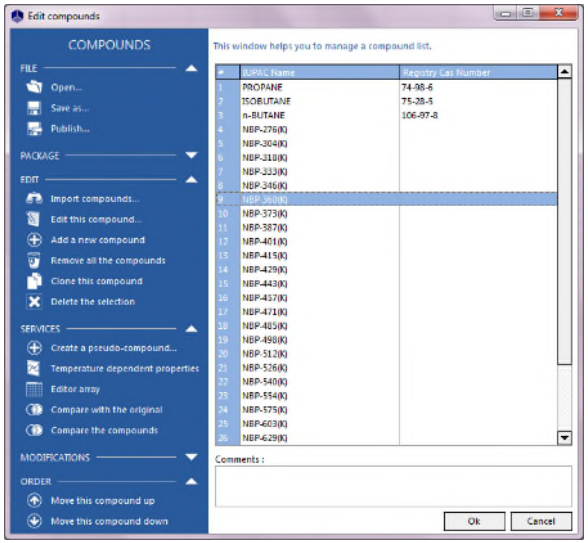
The pseudo-compounds have been automatically generated.

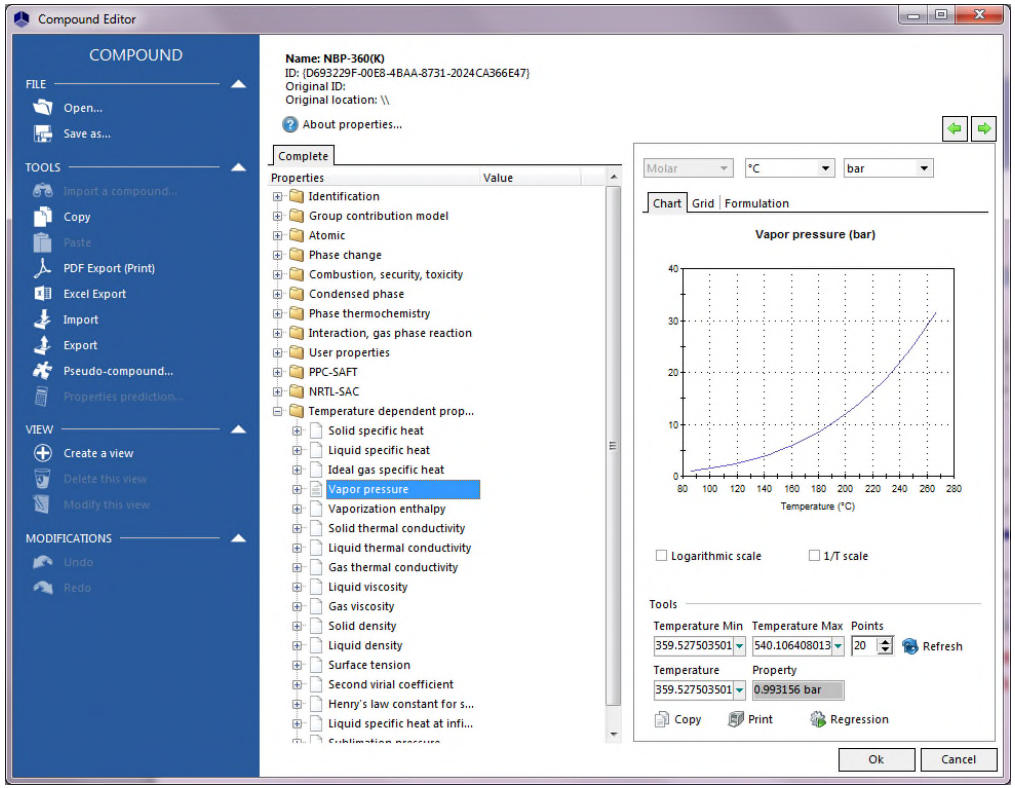
They are named “NBP-” (for Normal Boiling Point) followed by the value expressed in Kelvin.



Step 4: Analyze the results

You can access physical properties by double clicking on a pseudo-compound.

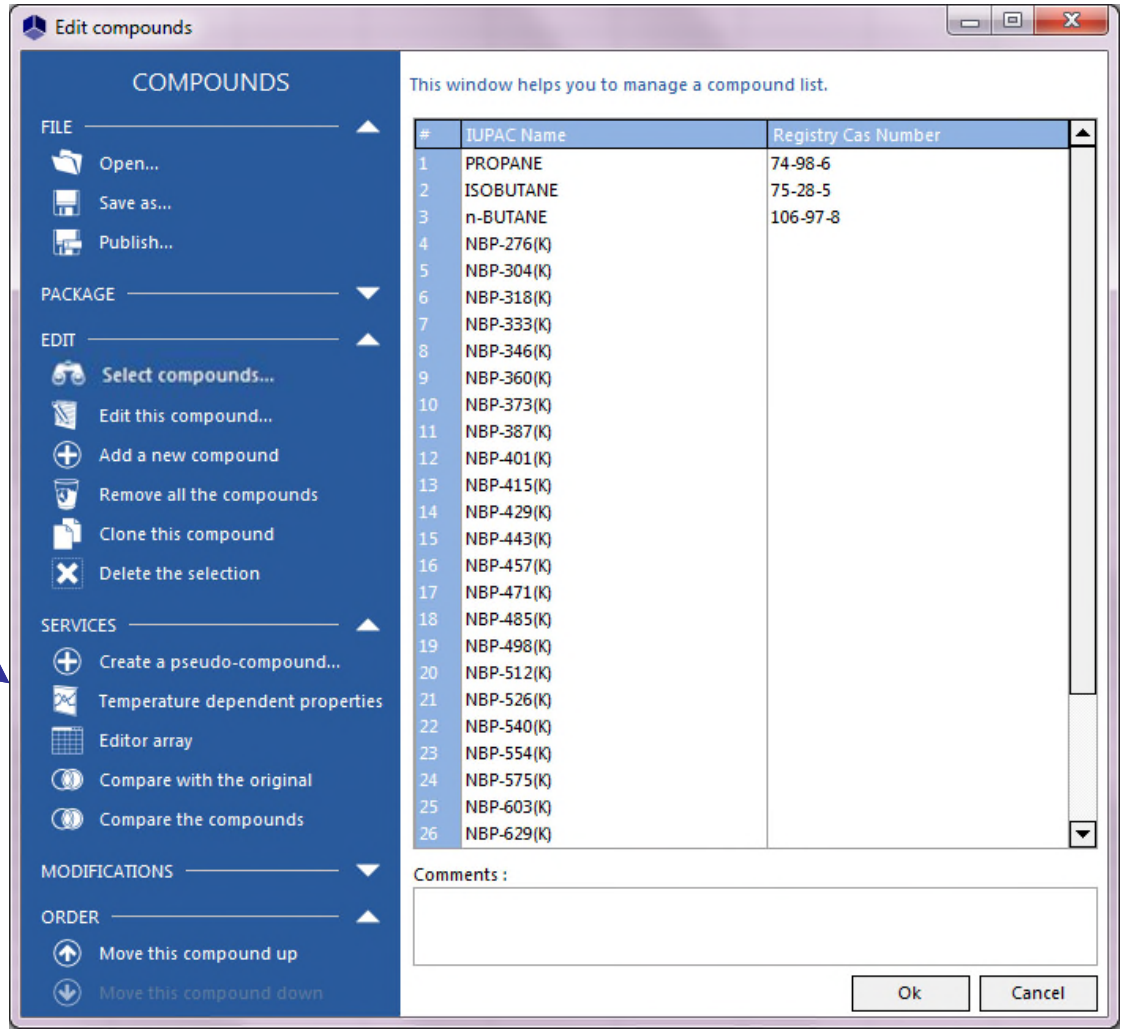




The Compound Editor window allows you to browse through the properties generated for each compound. Some properties can be plotted on a graph (in this example, the vapor pressure of the pseudo-compound NBP-360(K)).

Step 4: Analyze the results

It is also possible to compare temperature dependant properties between different compounds



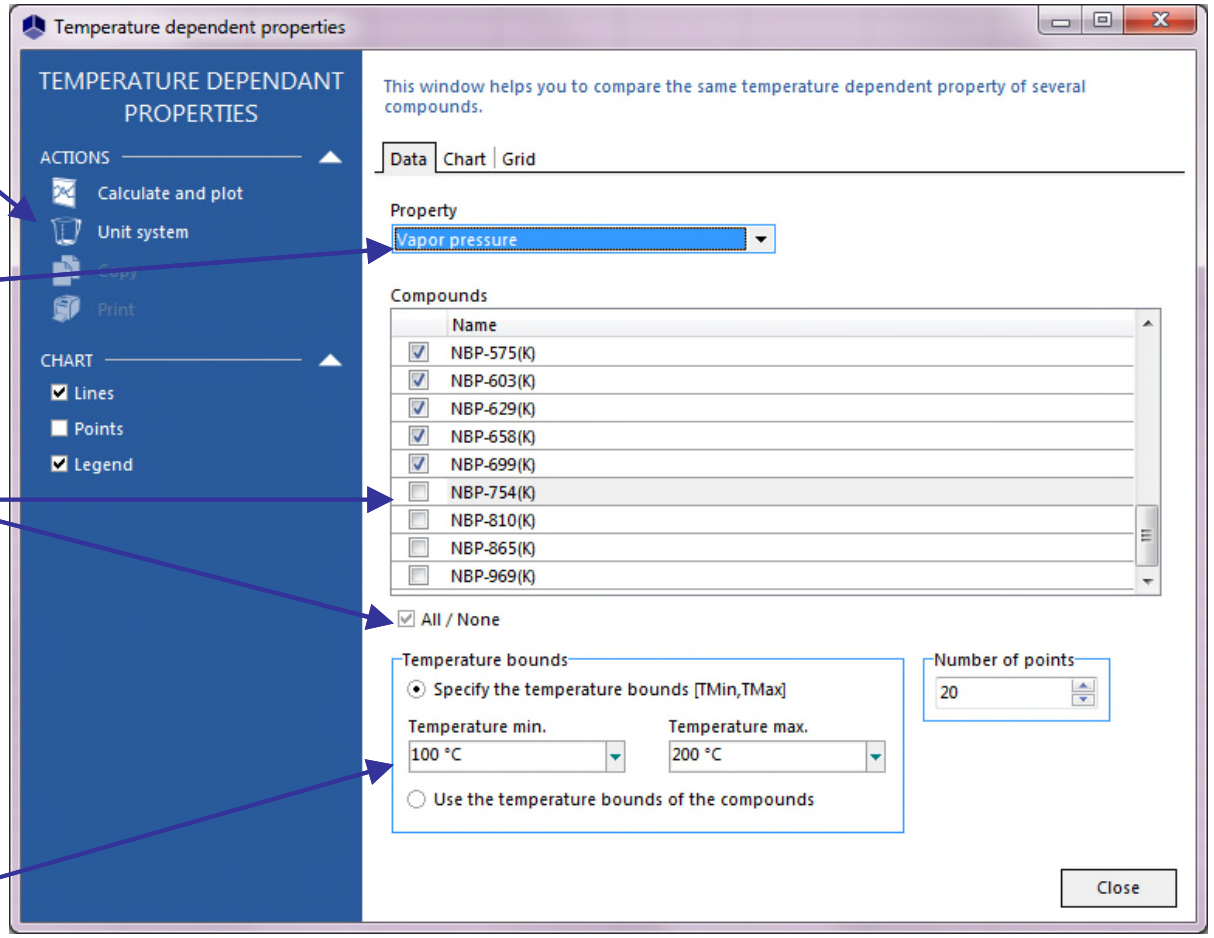
Step 4: Analyze the results

1. Select "*atm*" for pressure and "*°F*" for temperature.

2. Select "*Vapor pressure*".

3. Select the compounds that will be used for the comparison. Here we check "*All* " to select all compounds, then uncheck the four heaviest ones.

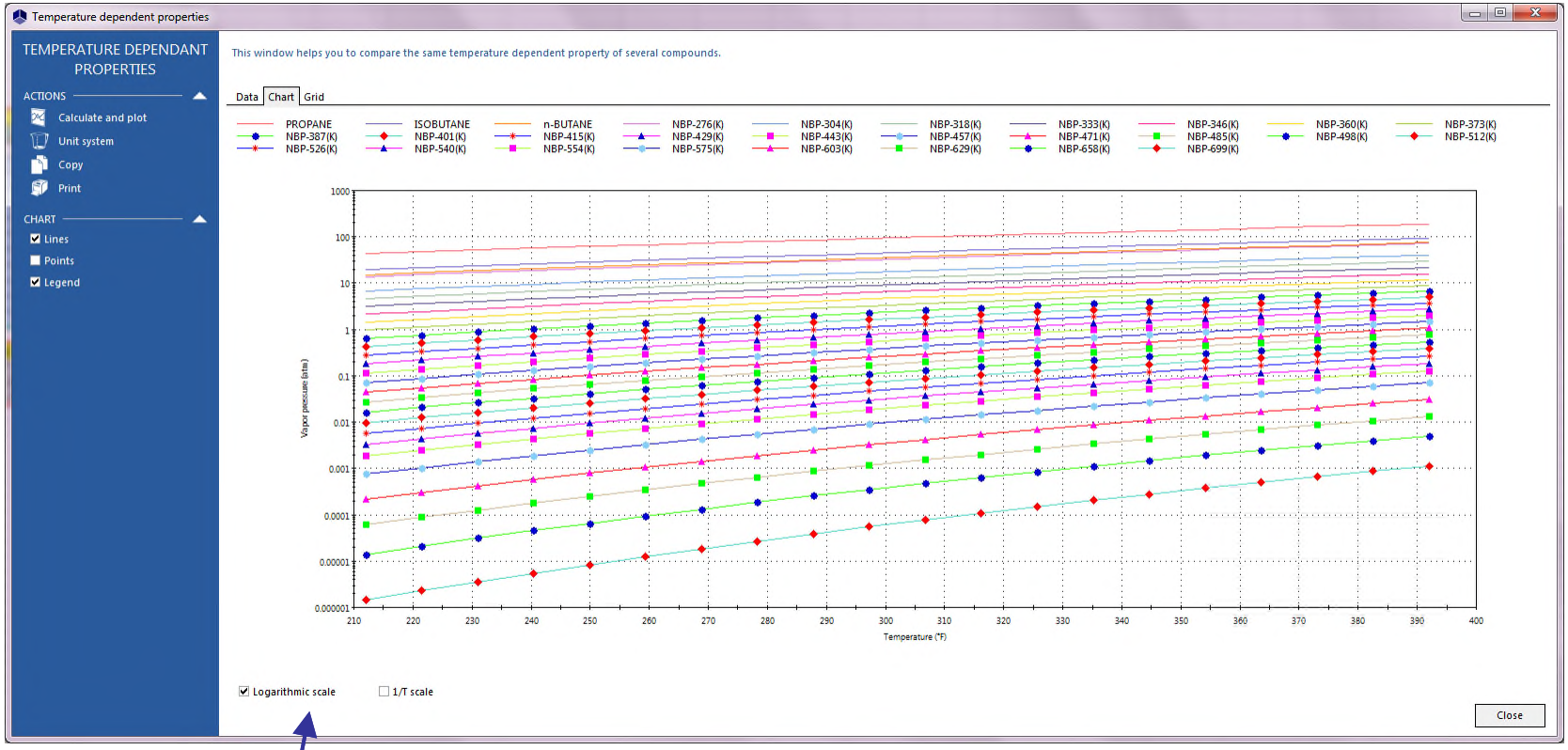
4. Enter the temperature range: 100°C to 200°C.



5. When all parameters are defined, click on "*Calculate and plot*".

Step 4: Analyze the results

Click on the "*Chart*" tab to view the graph.



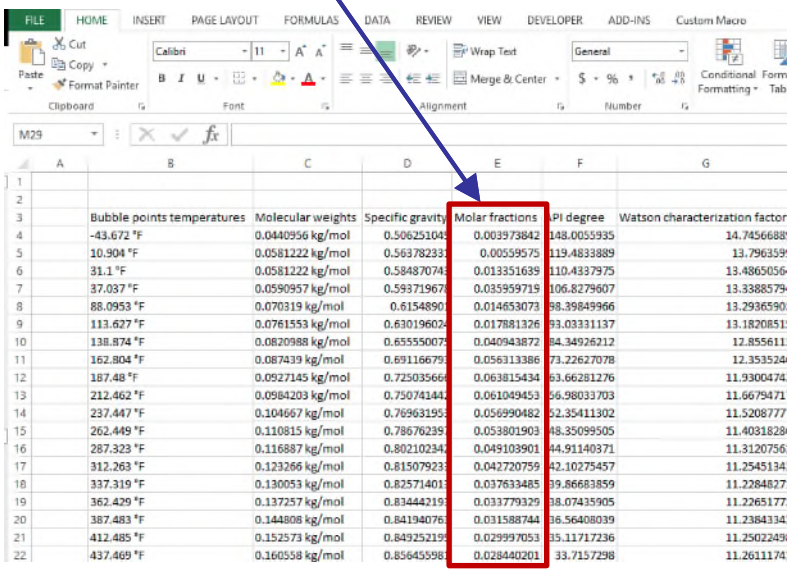
Check the "*Logarithmic scale*" option.

Step 5: Paste the mixture composition into the application that is used

The table that includes the mixture composition has been copied in the step 3. You can now paste it into the application you are using.

- **<u>If you are using Simulis Thermodynamics in Excel</u>:**

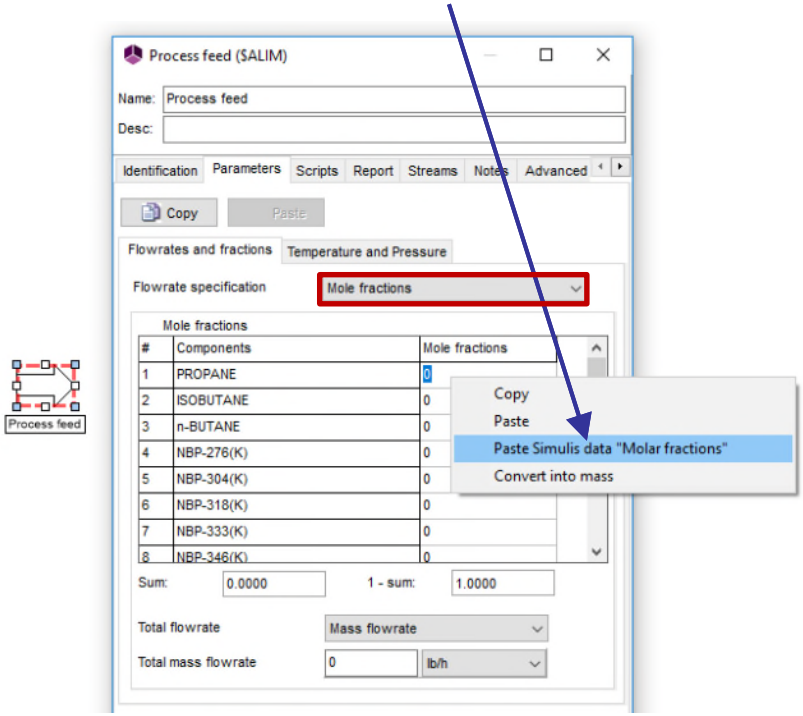
Copy the table into the Excel spreadsheet. The "Molar fractions" column corresponds to the mixture composition.



	Bubble points temperatures	Molecular weights	Specific gravity	Molar fractions	API degree	Watson characterization factor
4	-43.672 °F	0.0440956 kg/mol	0.506251045	0.003973842	148.0055935	14.7456688
5	10.904 °F	0.0581222 kg/mol	0.563782331	0.00559575	119.4833889	13.796359
6	31.1 °F	0.0581222 kg/mol	0.584870743	0.013351639	110.4337975	13.4865056
7	37.037 °F	0.0590957 kg/mol	0.593719671	0.035959719	106.8279607	13.3388579
8	88.0953 °F	0.070319 kg/mol	0.61548901	0.014653073	88.39849966	13.2936590
9	113.627 °F	0.0761553 kg/mol	0.630196024	0.017881326	93.03331137	13.1820851
10	138.874 °F	0.0820988 kg/mol	0.655550075	0.040943872	84.34926212	12.855611
11	162.804 °F	0.087439 kg/mol	0.691166791	0.056313386	73.22627078	12.3535240
12	187.48 °F	0.0927145 kg/mol	0.725035666	0.063815434	63.66281276	11.9300474
13	212.462 °F	0.0984203 kg/mol	0.750741441	0.061049453	56.98033703	11.6679471
14	237.447 °F	0.104667 kg/mol	0.769631953	0.056990482	52.35411302	11.5208777
15	262.449 °F	0.110815 kg/mol	0.786762391	0.053801903	48.35099505	11.4031828
16	287.323 °F	0.116887 kg/mol	0.802102342	0.049103901	44.91140371	11.3120756
17	312.263 °F	0.123266 kg/mol	0.815079233	0.042720759	42.10275457	11.2545134
18	337.319 °F	0.130053 kg/mol	0.825714013	0.037633485	39.86683859	11.2284827
19	362.429 °F	0.137257 kg/mol	0.834442193	0.033779329	38.07435905	11.2265177
20	387.483 °F	0.144808 kg/mol	0.841940763	0.031588744	36.56408039	11.2384334
21	412.485 °F	0.152573 kg/mol	0.849252195	0.029997053	35.11717236	11.2502249
22	437.469 °F	0.160558 kg/mol	0.856455981	0.028440201	33.7157298	11.2611174

- **<u>If you are using Simulis Thermodynamics within ProSimPlus:</u>**

In the configuration window of the feed module, select "Mole fractions" for the flowrate specification, then right click in the table to paste the mixture composition.



ProSim

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