Detherm 2.1 training examples

1. Start the Detherm client and logon:

2. Use the Search Wizard to find the boiling point of ethanal in Kelvin.

3. Find the most recent determination for question 2, and convert the units to Centigrade.

4. Build a plot of vapour pressure verses temperature for octafluoronapthalene, C10F8.

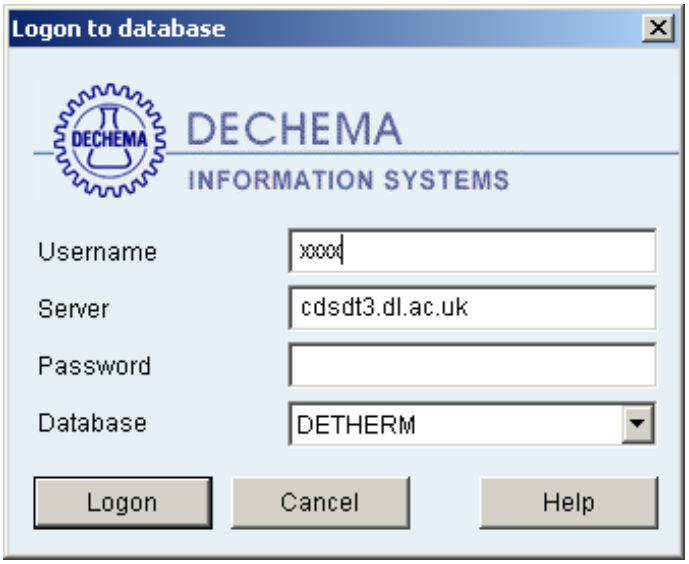
5. Find the entropy for liquid methanol at 50 °C and around 200 atmospheres pressure.

6. Find some three component azeotropes containing pyridine and water.

7. Return to question 5 and check for data at 60 °C.

Solutions to Detherm training examples

1. Start the Detherm 2007 client and enter the following details into the logon box.



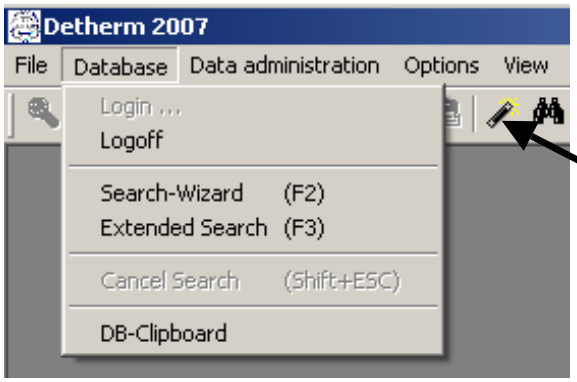
Username – your CDS id

Server – **cdsdt3.dl.ac.uk**

Password – your CDS password

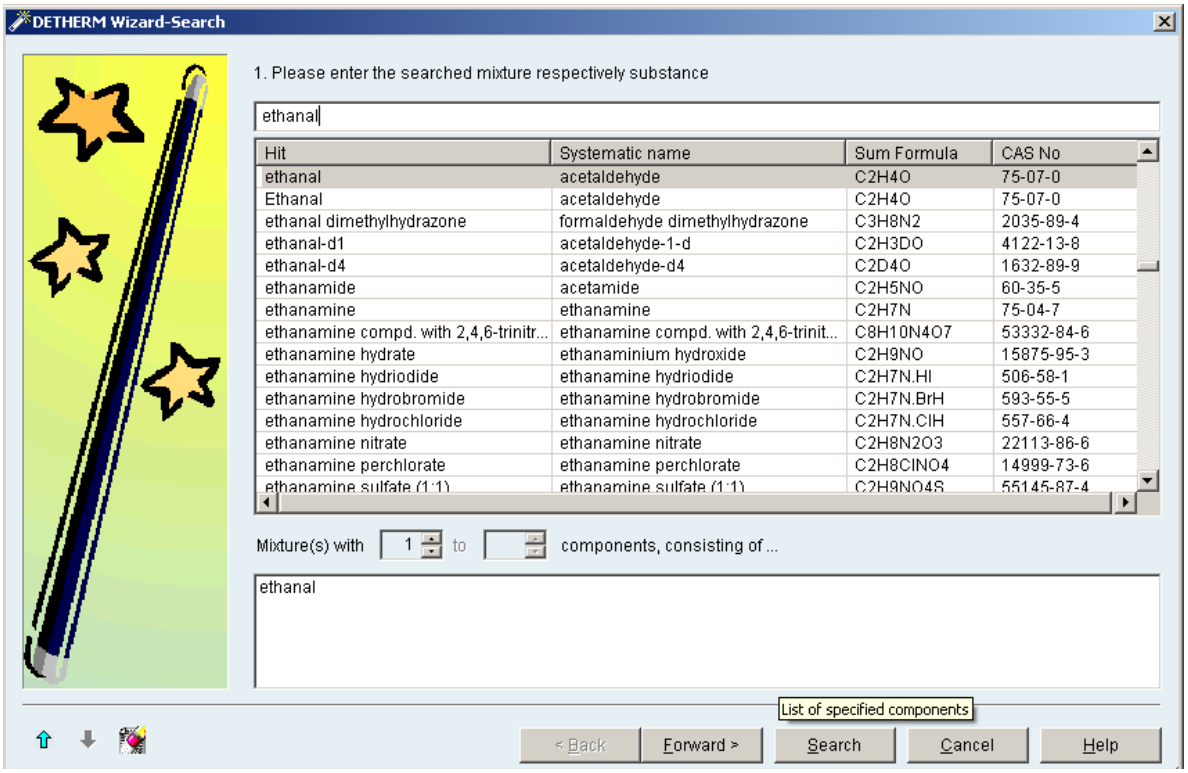
2. All of the following examples have been done with the Search Wizard, but this is not the only way to perform these searches.

To start the Search Wizard, EITHER:
1) Select Search-Wizard from the **Database** menu **OR**
2) Press the **F2** key.



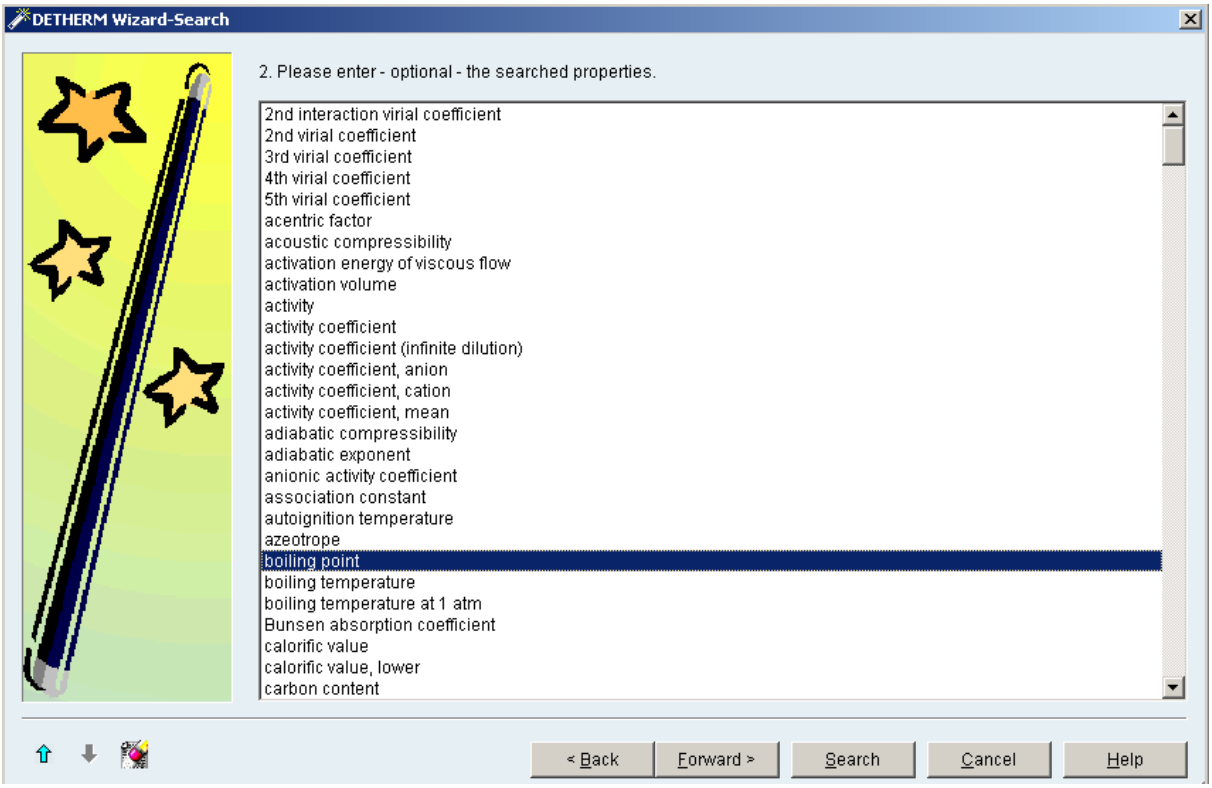
OR

3) Click the **Wand** icon

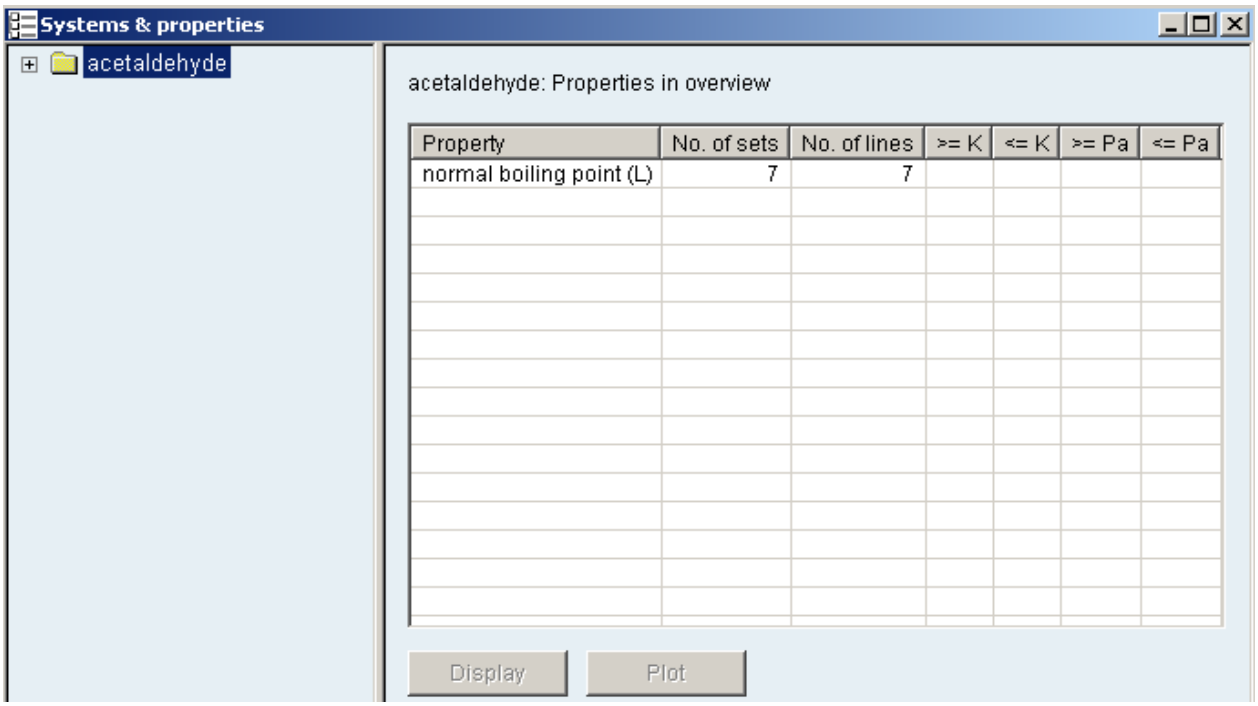


Type **ethanal** in the top box of the Search Wizard. The main part of the window should display an alphabetical list of compounds starting with ones which match ethanal. **Double click** on the required compound – the name should then appear in the lower box.

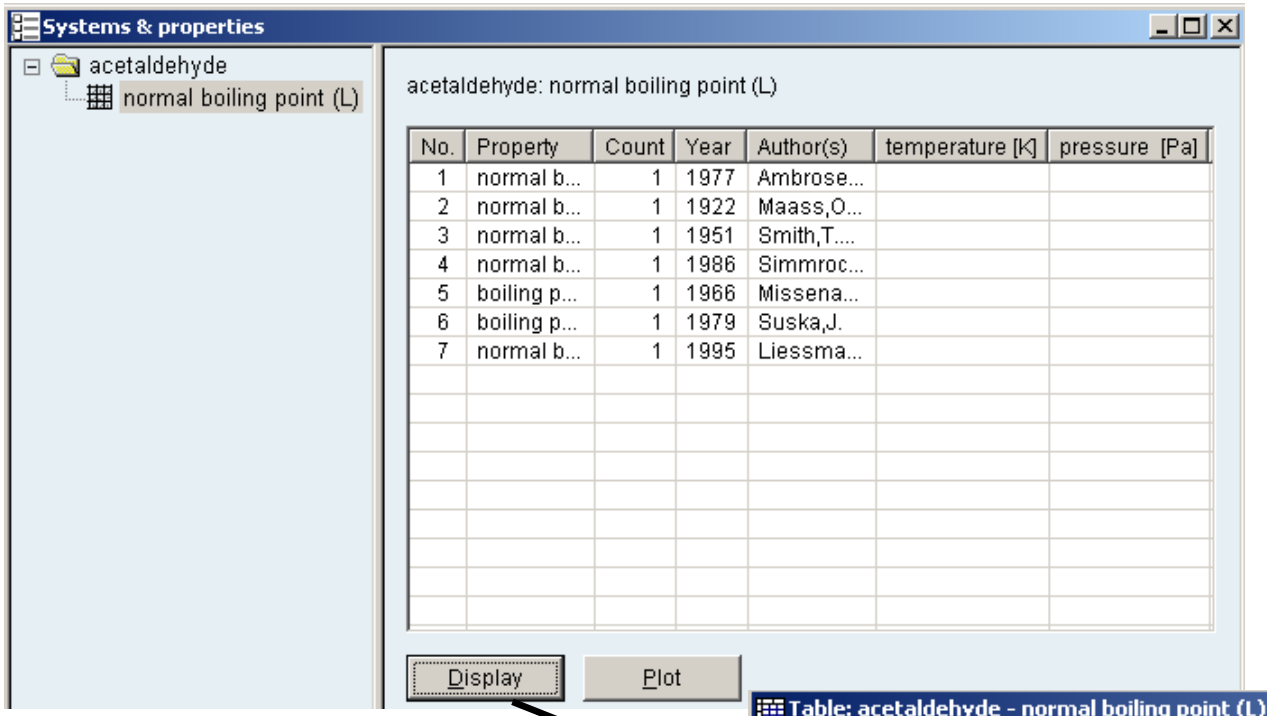
Click the **Forward>** button at the bottom of the window.



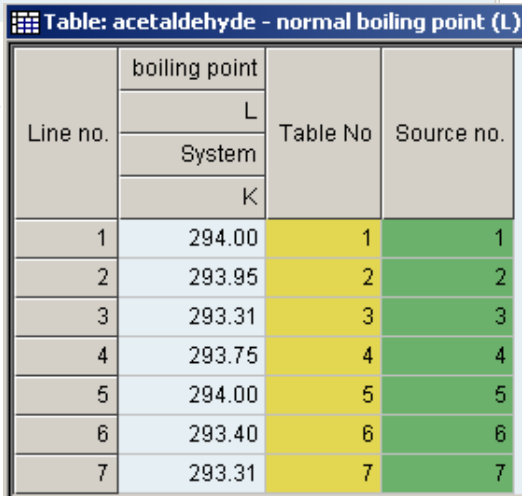
Select the required property, in this case boiling point, from the list.
Click the **Search** button and Detherm will perform the search and display the following Systems and Properties box.



Select the required property (normal boiling point) and click the **Display** button.

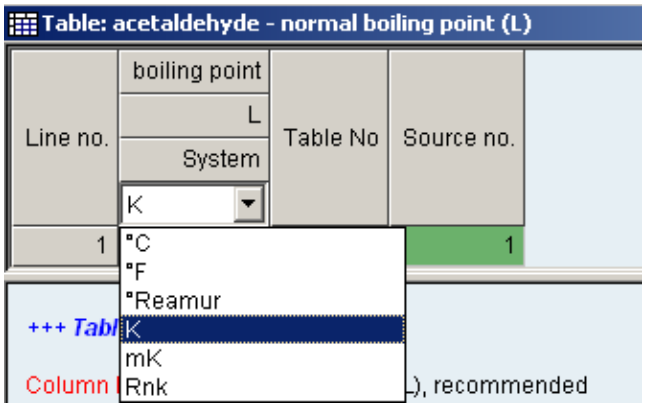


Click **Display** again to show all the actual data.

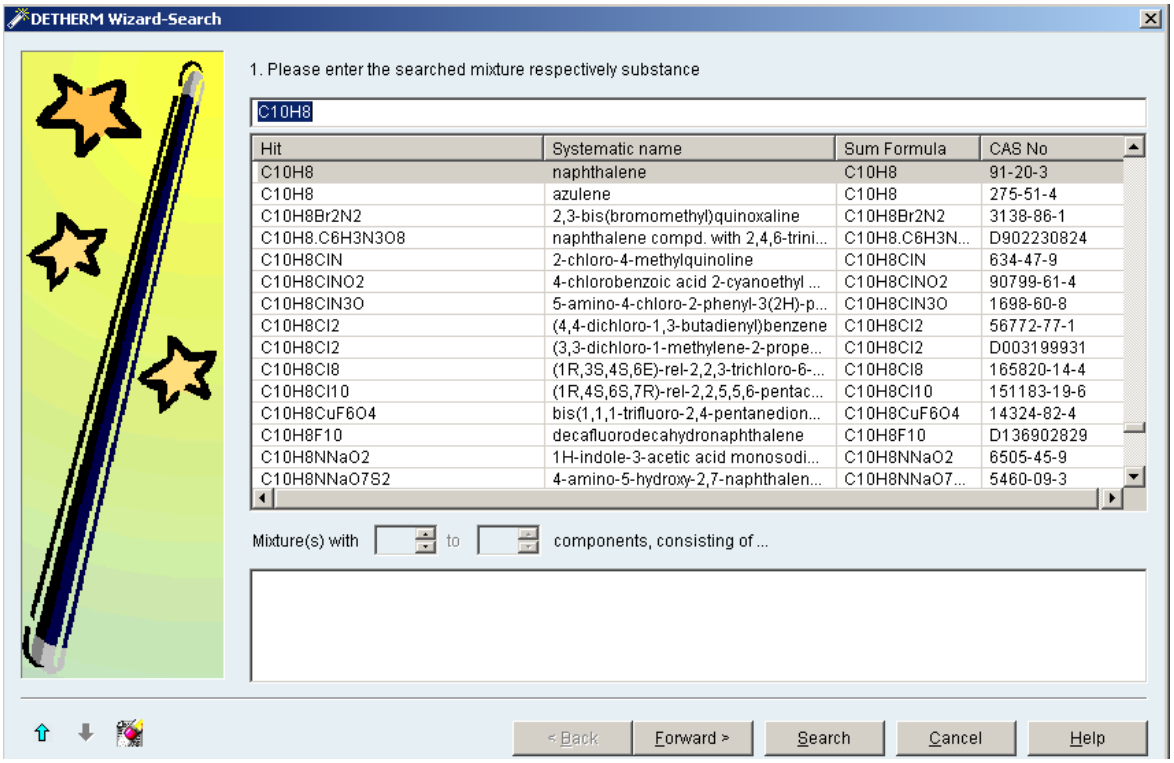


3. In the Systems and Properties box from question 2, click on the year label to sort the results by year (click again to reverse the direction of the sort).
Select the most recent data and click **Display** to view it.

To convert units, **double-click** on the unit box and select the required value from the pop-up list.

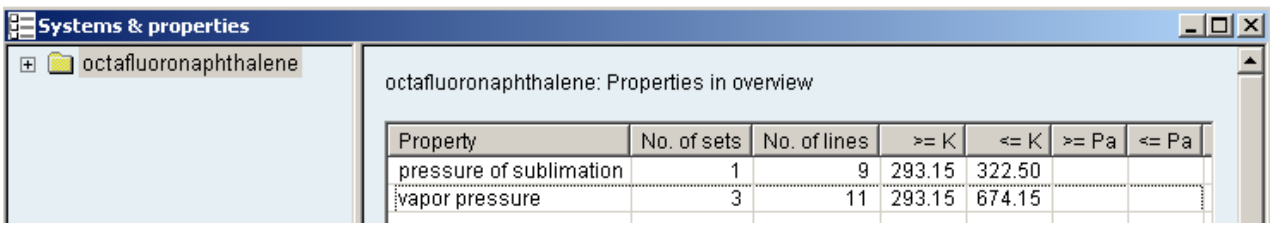


4. Starting from the Search Wizard, type C10F8 into the top box.

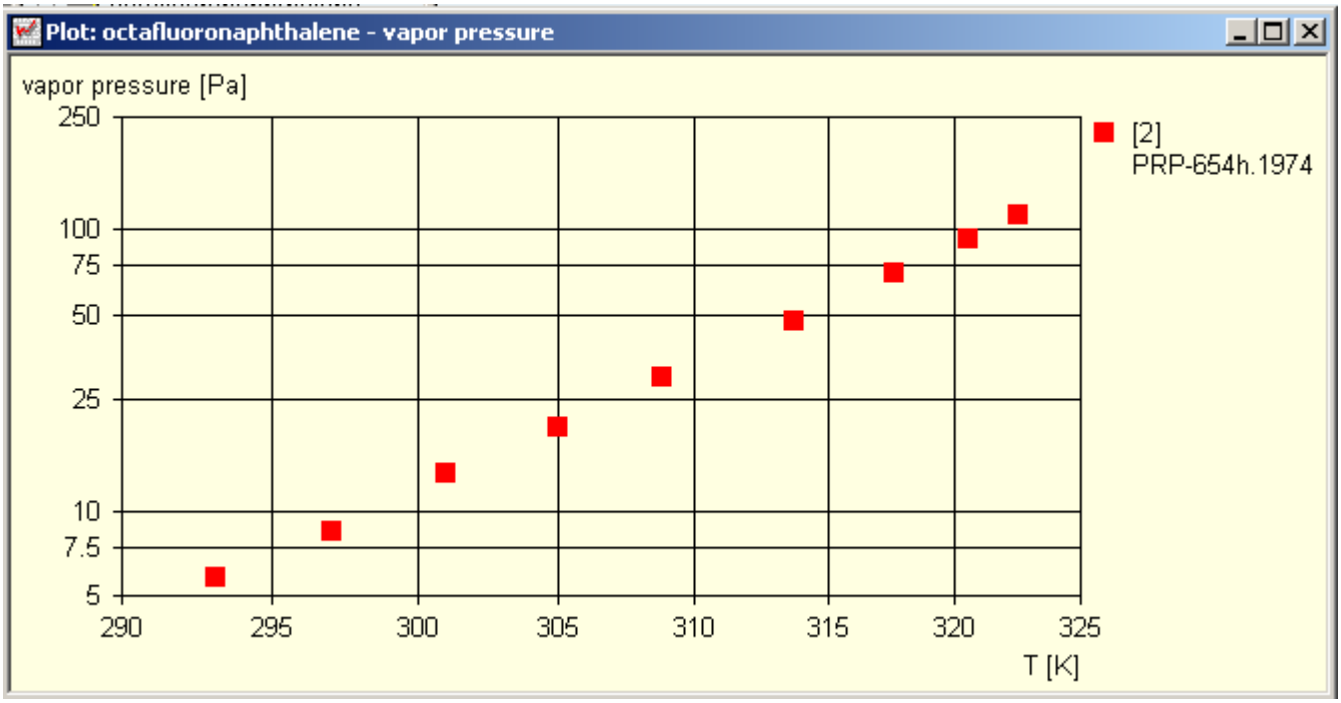


Double-click on octafluoronapthalene, and click **Forward**.
Select **vapour pressure** from the list and click **Search**.

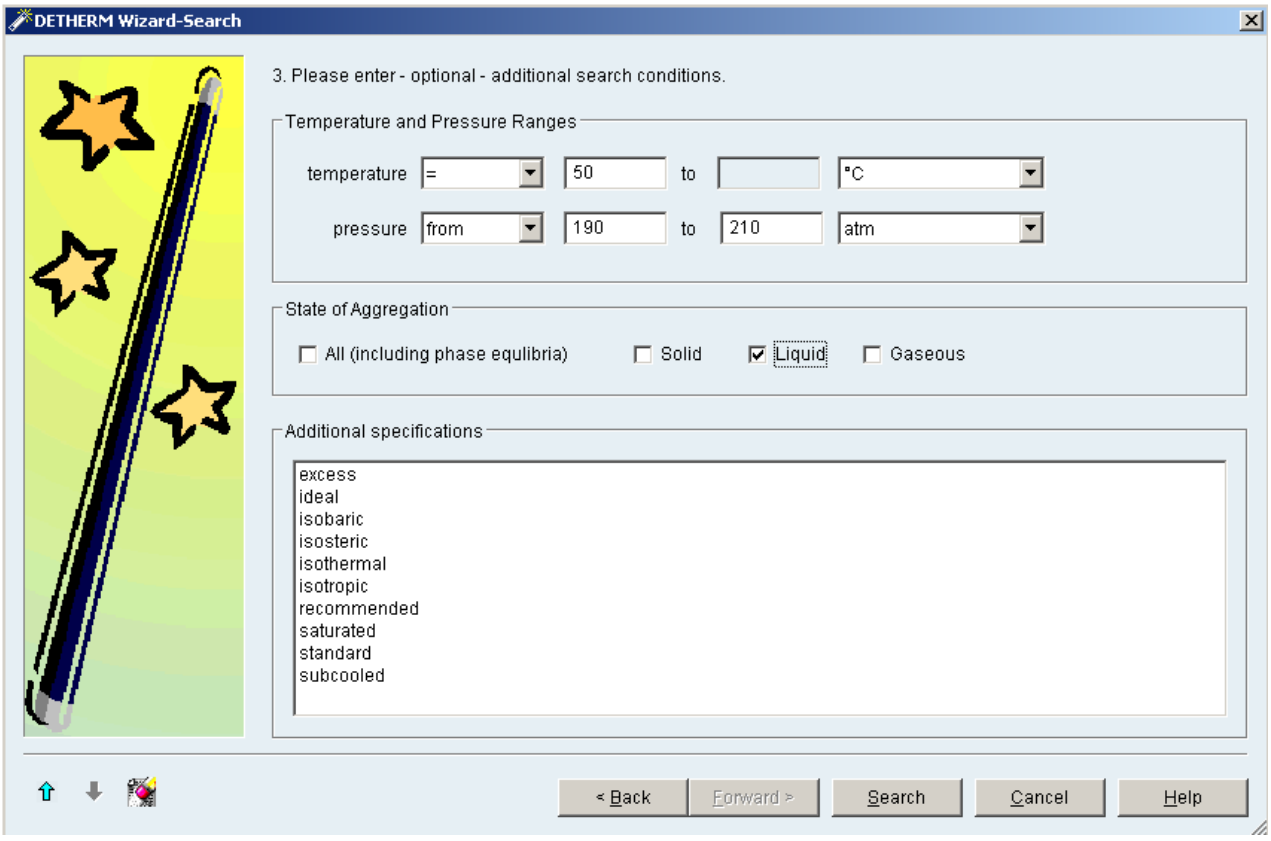
In the Systems and Properties box , which appears, double-click on **vapour pressure**.



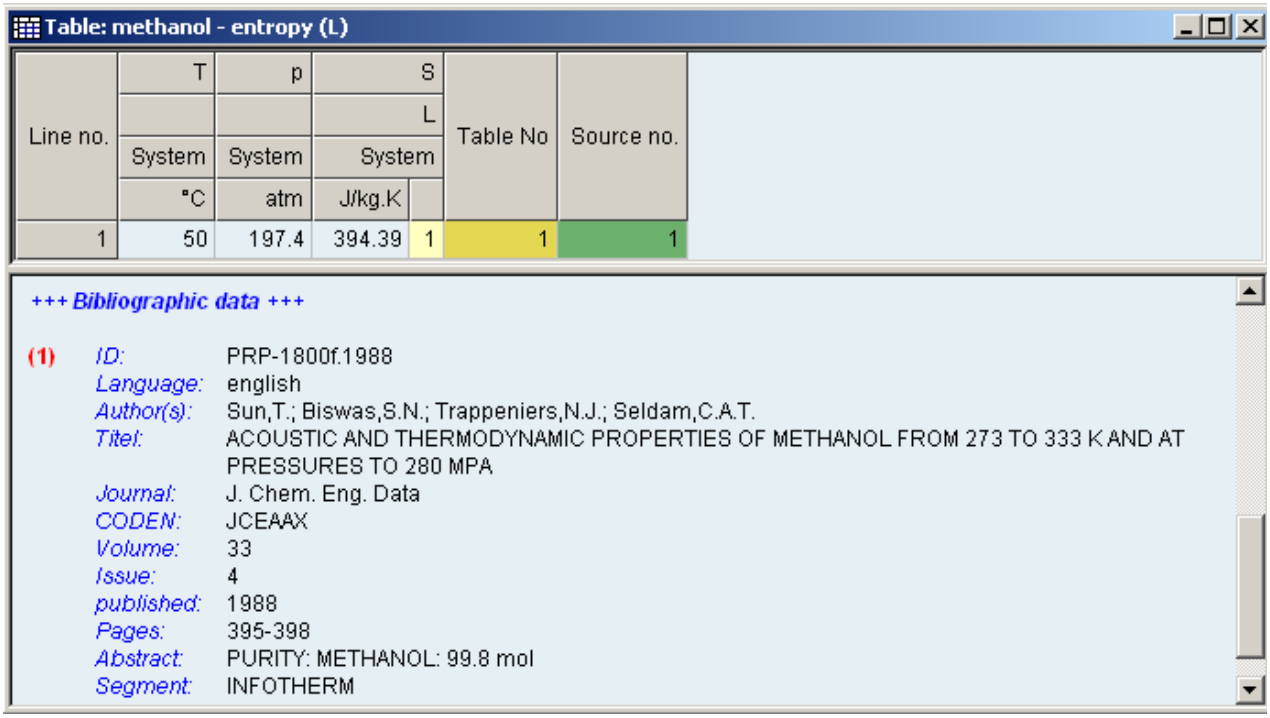
Then click on **Plot** to display the following graph, using all of the available data.



5. In the Search Wizard, select methanol and click Forward. Select the property entropy and click Forward. In the third screen, set temperature = 50 °C and pressure from 190 to 210 atm. Check the Liquid box under State of Aggregation and then press the Search button.

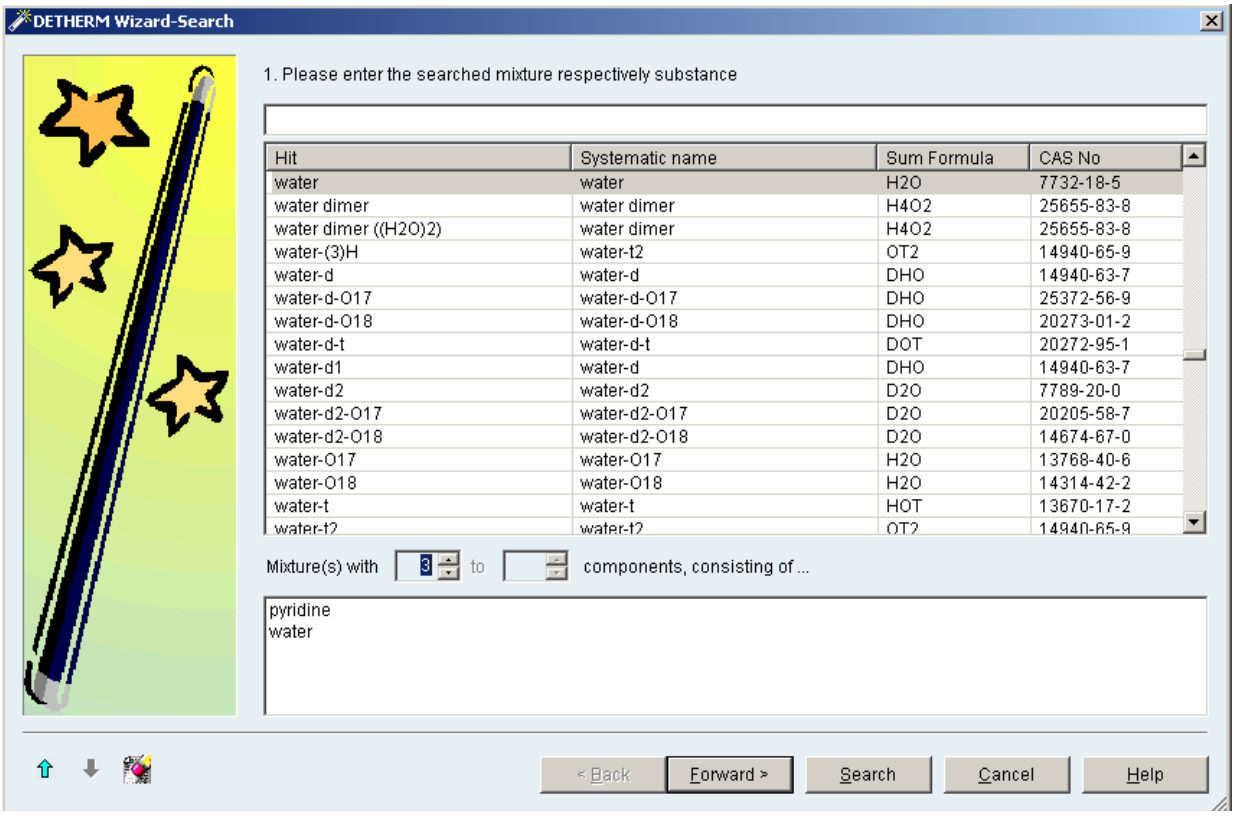


From the Systems and Properties box, **double-click** on entropy(L) and then click Display to show the data.
The bottom part of the window can be resized or scrolled to show the bibliographic source of the experimental data.

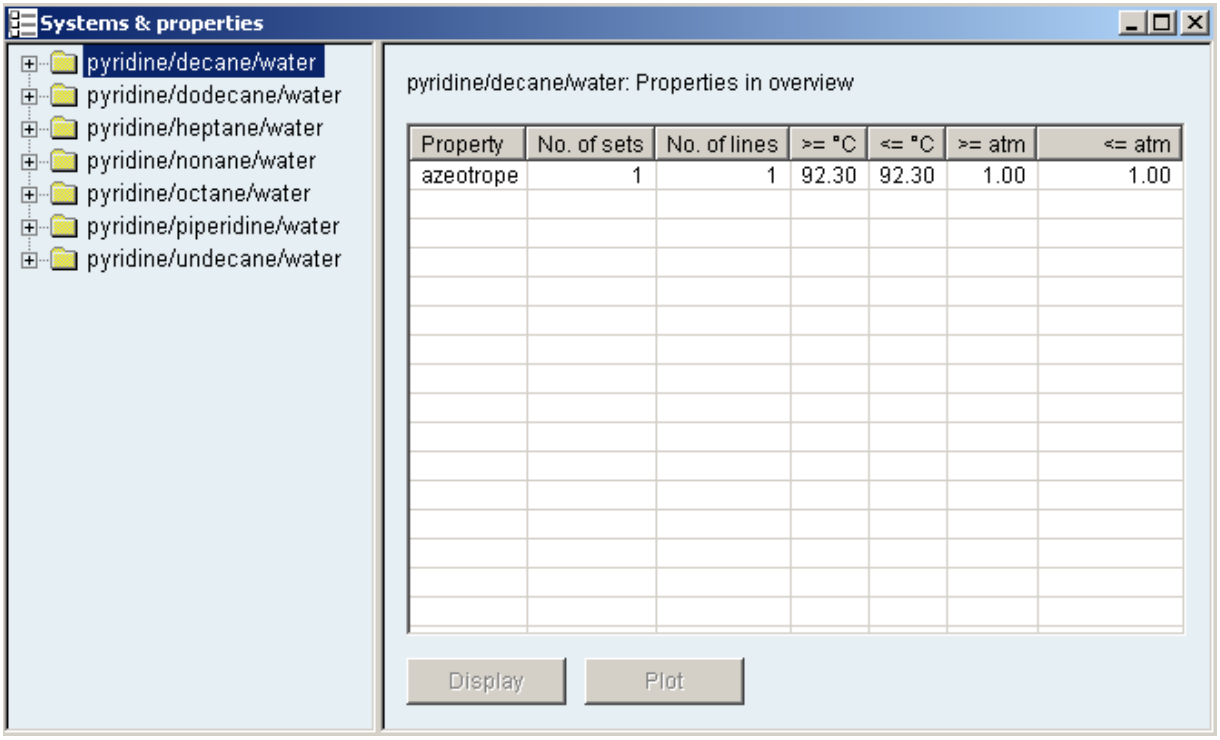


6. From the Search Wizard, select pyridine and then select water (the bottom box should show both).

Near the bottom, increase the number to show Mixture(s) with 3 components.



Press the **Forward >** button, select the property azeotrope and click



The results window shows 7 different 3 component systems.

7. In the **Search Wizard** window, click the up arrow in the bottom left corner and it will bring up the details of the last search. Click again for the search before that. Click Forward twice, change the temperature and press Search.