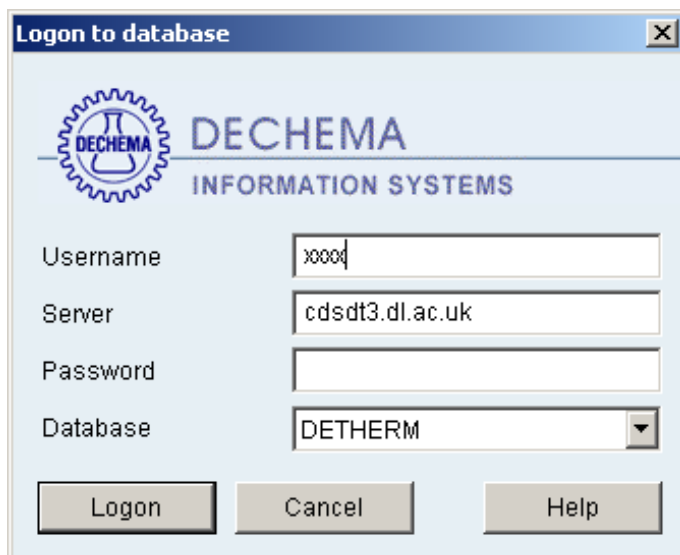


Detherm 2.1 training examples

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 octafluoronaphthalene, 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

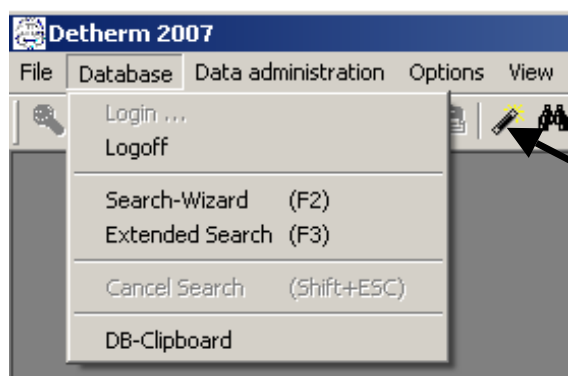
Server – **cdsdt3.dl.ac.uk**

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.

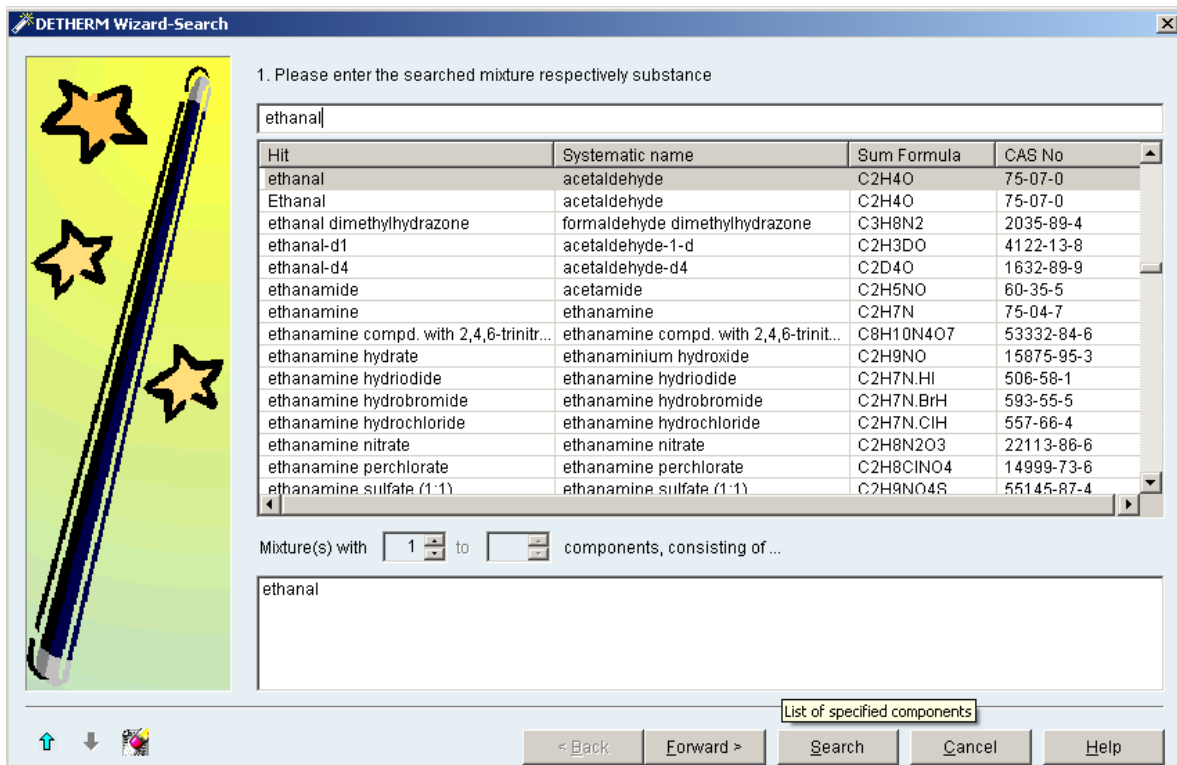
To start the Search Wizard, EITHER:

- 1) Select Search-Wizard from the **Database** menu **OR**
- 2) Press the **F2** key.



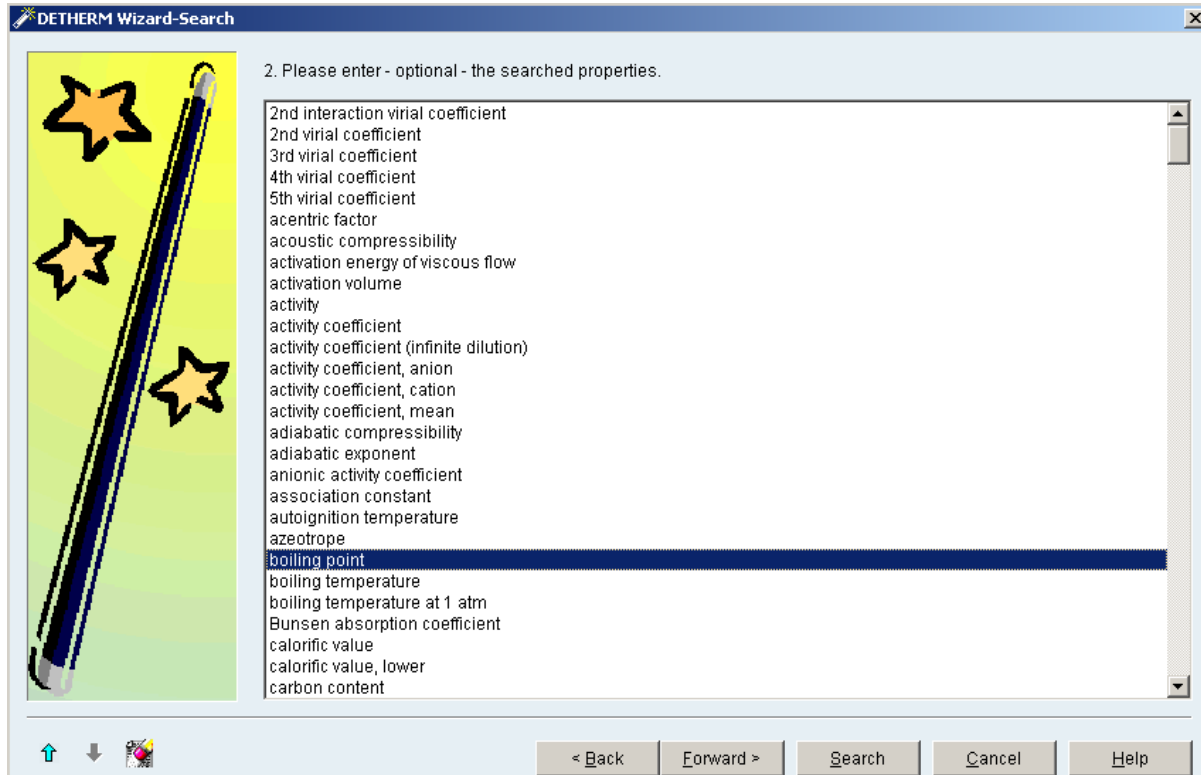
OR

- 3) Click the **Wand** icon

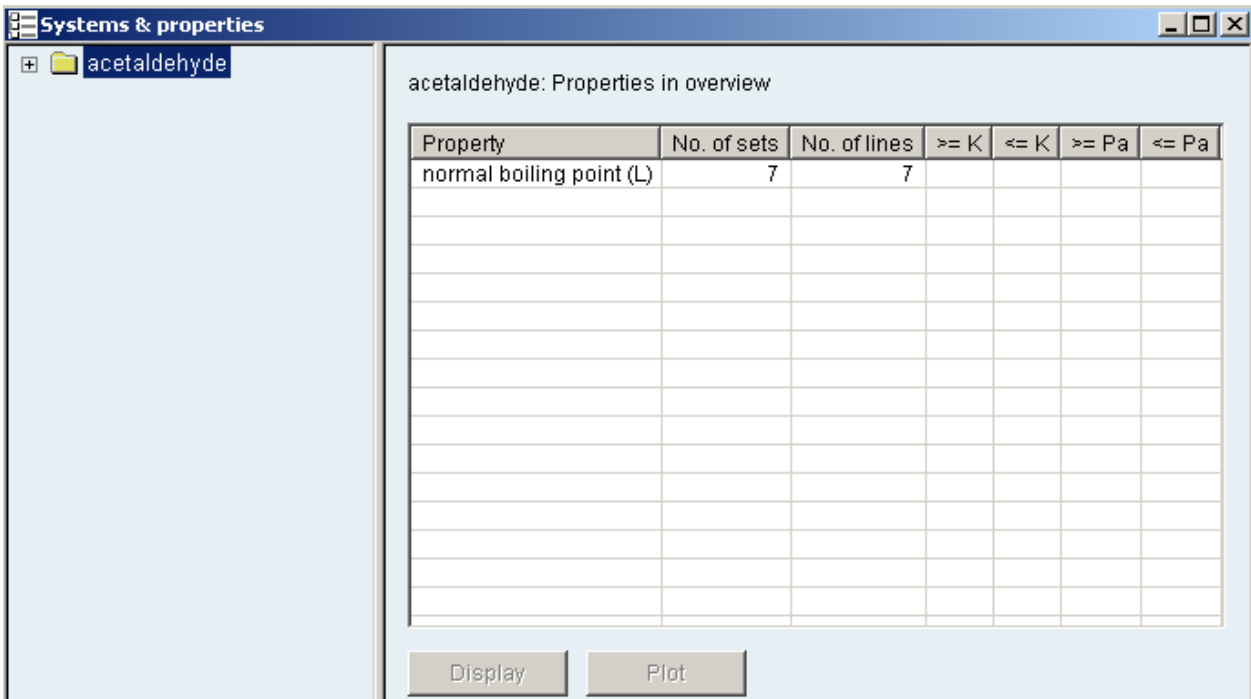


Type **ethanal** in the top box of the Search Wizard. The main part of the window should display an alphabetical list of compounds starting with ones which match ethanal. **Double click** on the required compound – the name should then appear in the lower box.

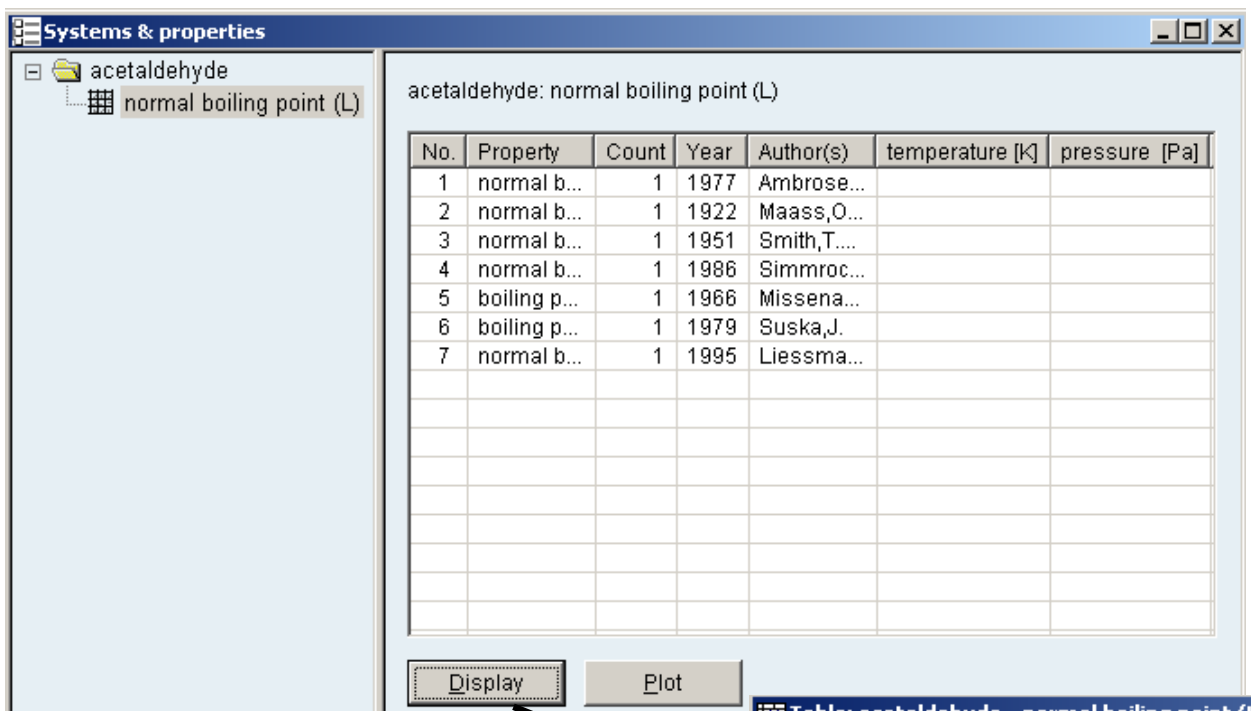
Click the **Forward>** button at the bottom of the window.



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.

Table: acetaldehyde - normal boiling point (L)

Line no.	boiling point	Table No	Source no.
	L		
	System		
	K		
1	294.00	1	1
2	293.95	2	2
3	293.31	3	3
4	293.75	4	4
5	294.00	5	5
6	293.40	6	6
7	293.31	7	7

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.

Table: acetaldehyde - normal boiling point (L)

Line no.	boiling point	Table No	Source no.
	L		
	System		
	K		
1	°C		1
	°F		
	°Reamur		
	K		
	mK		
	Rnk		

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

1. Please enter the searched mixture respectively substance

C10H8

Hit	Systematic name	Sum Formula	CAS No
C10H8	naphthalene	C10H8	91-20-3
C10H8	azulene	C10H8	275-51-4
C10H8Br2N2	2,3-bis(bromomethyl)quinoxaline	C10H8Br2N2	3138-86-1
C10H8.C6H3N3O8	naphthalene compd. with 2,4,6-trini...	C10H8.C6H3N...	D902230824
C10H8CIN	2-chloro-4-methylquinoline	C10H8CIN	634-47-9
C10H8CINO2	4-chlorobenzoic acid 2-cyanoethyl ...	C10H8CINO2	90799-61-4
C10H8CIN3O	5-amino-4-chloro-2-phenyl-3(2H)-p...	C10H8CIN3O	1698-60-8
C10H8CI2	(4,4-dichloro-1,3-butadienyl)benzene	C10H8CI2	56772-77-1
C10H8CI2	(3,3-dichloro-1-methylene-2-prope...	C10H8CI2	D003199931
C10H8CI8	(1R,3S,4S,6E)-rel-2,2,3-trichloro-6-...	C10H8CI8	165820-14-4
C10H8CI10	(1R,4S,6S,7R)-rel-2,2,5,5,6-pentac...	C10H8CI10	151183-19-6
C10H8CuF6O4	bis(1,1,1-trifluoro-2,4-pentanedion...	C10H8CuF6O4	14324-82-4
C10H8F10	decafluorodecahydronaphthalene	C10H8F10	D136902829
C10H8NNaO2	1H-indole-3-acetic acid monosodi...	C10H8NNaO2	6505-45-9
C10H8NNaO7S2	4-amino-5-hydroxy-2,7-naphthalen...	C10H8NNaO7...	5460-09-3

Mixture(s) with [] to [] components, consisting of ...

< Back Forward > Search Cancel Help

Double-click on octafluoronaphthalene, 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**.

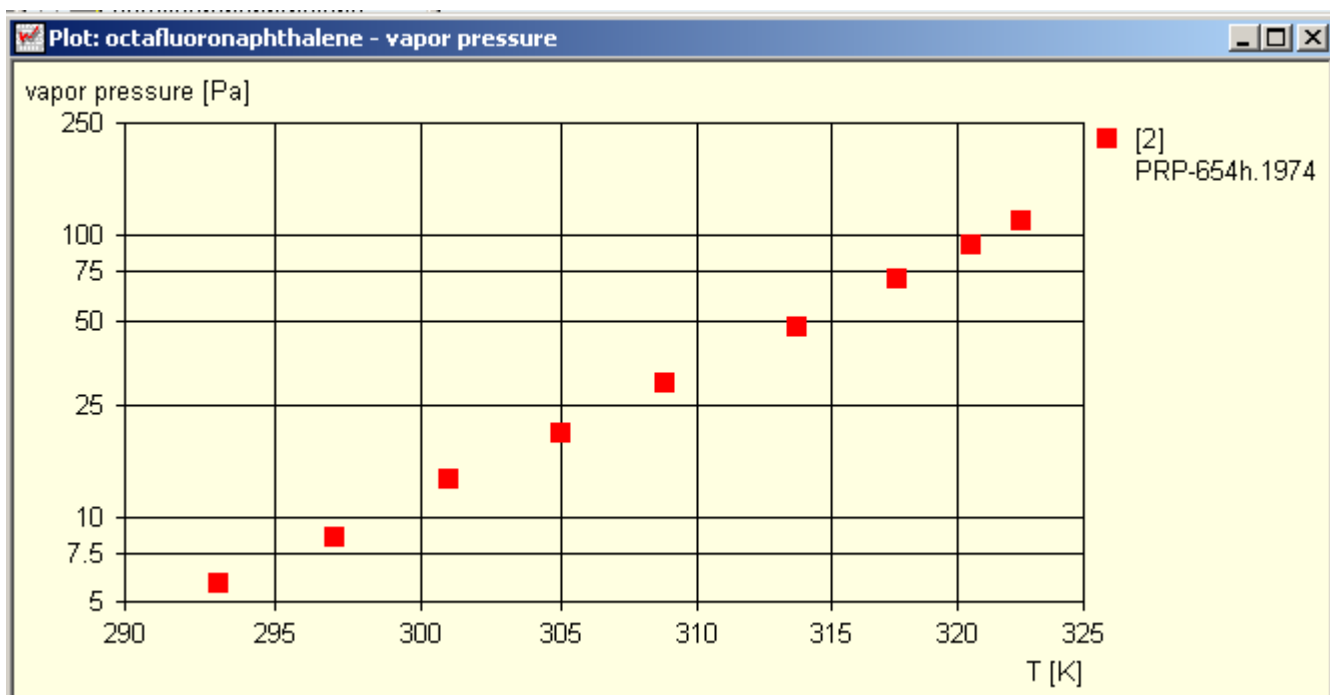
Systems & properties

octafluoronaphthalene

octafluoronaphthalene: Properties in overview

Property	No. of sets	No. of lines	>= K	<= K	>= Pa	<= Pa
pressure of sublimation	1	9	293.15	322.50		
vapor pressure	3	11	293.15	674.15		

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.

The screenshot shows the "DETERM Wizard-Search" window. The title bar reads "DETERM Wizard-Search". The main area contains the following sections:

- 3. Please enter - optional - additional search conditions.**
- Temperature and Pressure Ranges:**
 - temperature = to °C
 - pressure to atm
- State of Aggregation:**
 - All (including phase equilibria)
 - Solid
 - Liquid
 - Gaseous
- Additional specifications:**
 - excess
 - ideal
 - isobaric
 - isobaric
 - isosteric
 - isothermal
 - isotropic
 - recommended
 - saturated
 - standard
 - subcooled

At the bottom, there are navigation buttons: "< Back", "Forward >", "Search", "Cancel", and "Help".

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.

Table: methanol - entropy (L)

Line no.	T	p	S		Table No	Source no.
	L					
	System	System	System			
	°C	atm	J/kg.K			
1	50	197.4	394.39	1	1	1

+++ Bibliographic data +++

(1) ID: PRP-1800f.1988
 Language: english
 Author(s): Sun,T.; Biswas,S.N.; Trappeniers,N.J.; Seldam,C.A.T.
 Title: ACOUSTIC AND THERMODYNAMIC PROPERTIES OF METHANOL FROM 273 TO 333 K AND AT PRESSURES TO 280 MPA
 Journal: J. Chem. Eng. Data
 CODEN: JCEAAX
 Volume: 33
 Issue: 4
 published: 1988
 Pages: 395-398
 Abstract: PURITY: METHANOL: 99.8 mol
 Segment: INFOTHERM

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.

DETERM Wizard-Search

1. Please enter the searched mixture respectively substance

Hit	Systematic name	Sum Formula	CAS No
water	water	H2O	7732-18-5
water dimer	water dimer	H4O2	25655-83-8
water dimer ((H2O)2)	water dimer	H4O2	25655-83-8
water-(3)H	water-t2	OT2	14940-65-9
water-d	water-d	DH0	14940-63-7
water-d-017	water-d-017	DH0	25372-56-9
water-d-018	water-d-018	DH0	20273-01-2
water-d-t	water-d-t	DOT	20272-95-1
water-d1	water-d	DH0	14940-63-7
water-d2	water-d2	D2O	7789-20-0
water-d2-017	water-d2-017	D2O	20205-58-7
water-d2-018	water-d2-018	D2O	14674-67-0
water-017	water-017	H2O	13768-40-6
water-018	water-018	H2O	14314-42-2
water-t	water-t	HOT	13670-17-2
water-t2	water-t2	OT2	14940-65-9

Mixture(s) with to components, consisting of ...

pyridine
water

< Back Forward > Search Cancel Help

