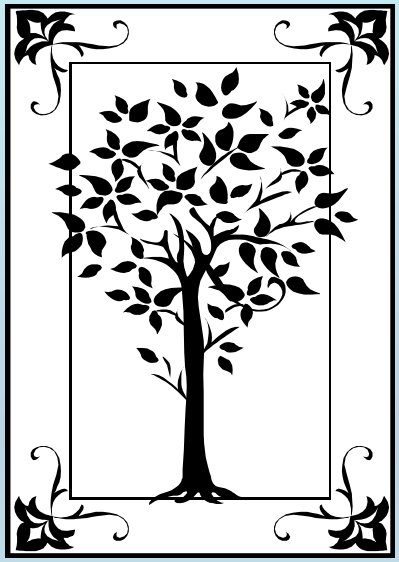
METADATA AND NUMERICAL DATA CAPTURE:
AZEOTROPIC pressure, *p*
(2 components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
AZEOTROPIC pressure *p*
(2 Components)
with the Guided Data Capture (GDC) software.

NOTE:

The tutorials proceed sequentially to ease the descriptions. It is not necessary to enter *all* compounds before entering *all* samples, etc.

Compounds, samples, properties, etc., can be added or modified at any time.

However, the hierarchy must be maintained (i.e., a property cannot be entered, if there is no associated sample or compound.)

The experimental data used in this example are from:

J. Chem. Eng. Data 2001, *46*, 535−540

Isothermal Vapor−Liquid Equilibrium of 1-Chlorobutane with Ethanol or 1-Hexanol at Ten Temperatures between 278.15 K and 323.15 K

Santiago Martínez, Rosa Carriga, Pascual Pérez, and Mariano Gracia*

Departamento de Química Orgánica y Química Física (Área de Química Física), Facultad de Ciencias, Universidad de Zaragoza, 50009-Zaragoza, Spain

Vapor pressures of (1-chlorobutane + ethanol or 1-hexanol) at 10 temperatures between 278.15 and 323.15 K were measured by a static method. The reduction of the vapor pressures to obtain activity coefficients and excess molar Gibbs energies was carried out by fitting the vapor pressure data to the Wilson equation according to Barker's method. In the 1-chlorobutane + ethanol system, azeotropic mixtures with a minimum boiling point temperature were observed over the whole temperature range.

AZEOTROPIC pressure for 1-chlorobutane + ethanol

Table 4. Azeotropic Pressures and Mole Fractions for the System {(1 − z) 1-Chlorobutane + z Ethanol}

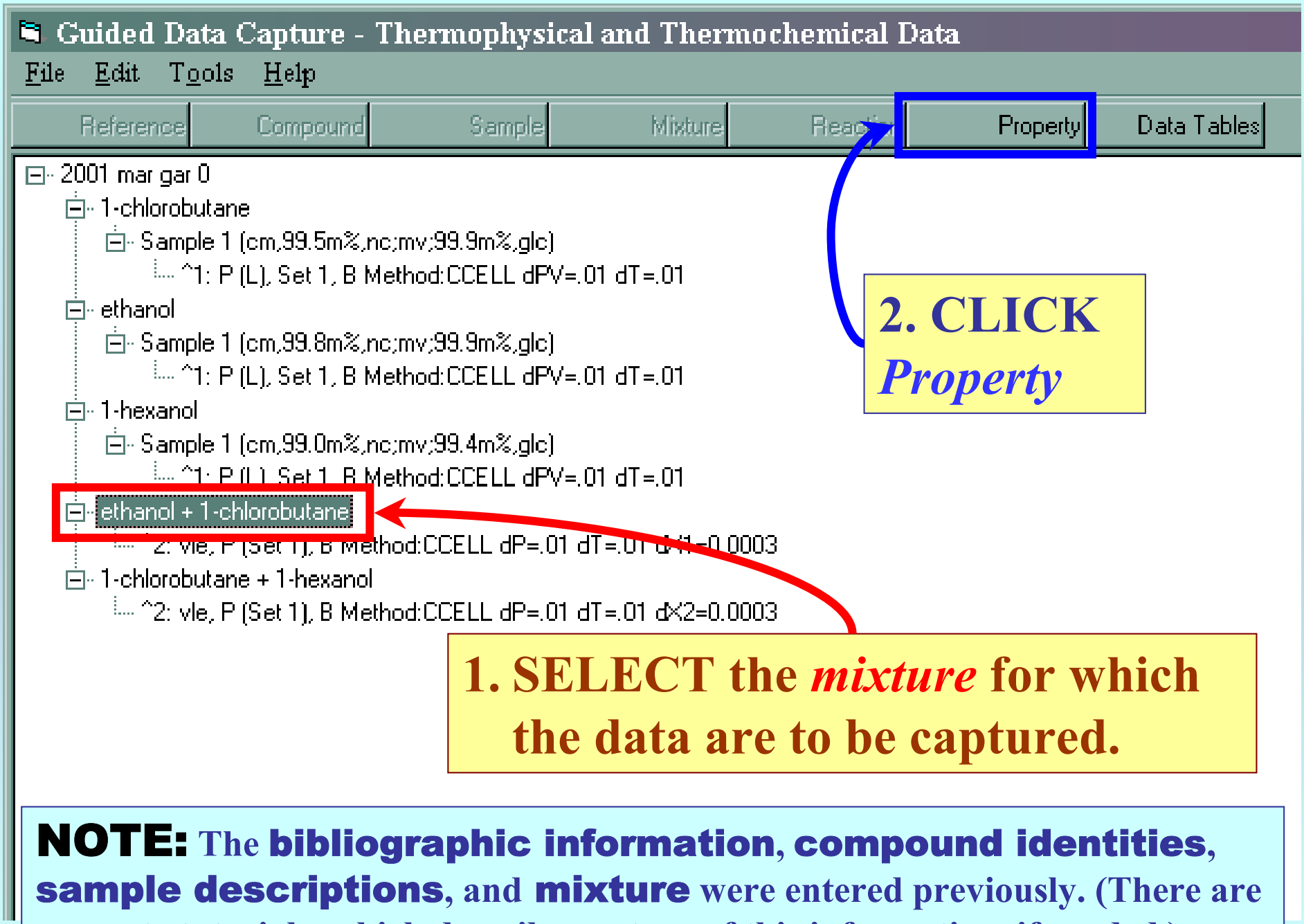
T/K	z(exptl)	P_z(exptl)/kPa	z(calcd from eq 11)	P_z(calcd from eq 13)/kPa
278.15	0.245	6.172	0.244	6.213
283.15	0.259	8.166	0.259	8.167
288.15	0.274	10.640	0.274	10.633
293.15	0.288	13.756	0.289	13.720
298.15	0.304	17.612	0.304	17.553
303.15	0.318	22.383	0.319	22.274
308.15	0.334	28.128	0.334	28.047
313.15	0.349	35.086	0.349	35.058
318.15	0.364	43.410	0.364	43.516
323.15	0.379	53.328	0.379	53.654

This data set is considered here.

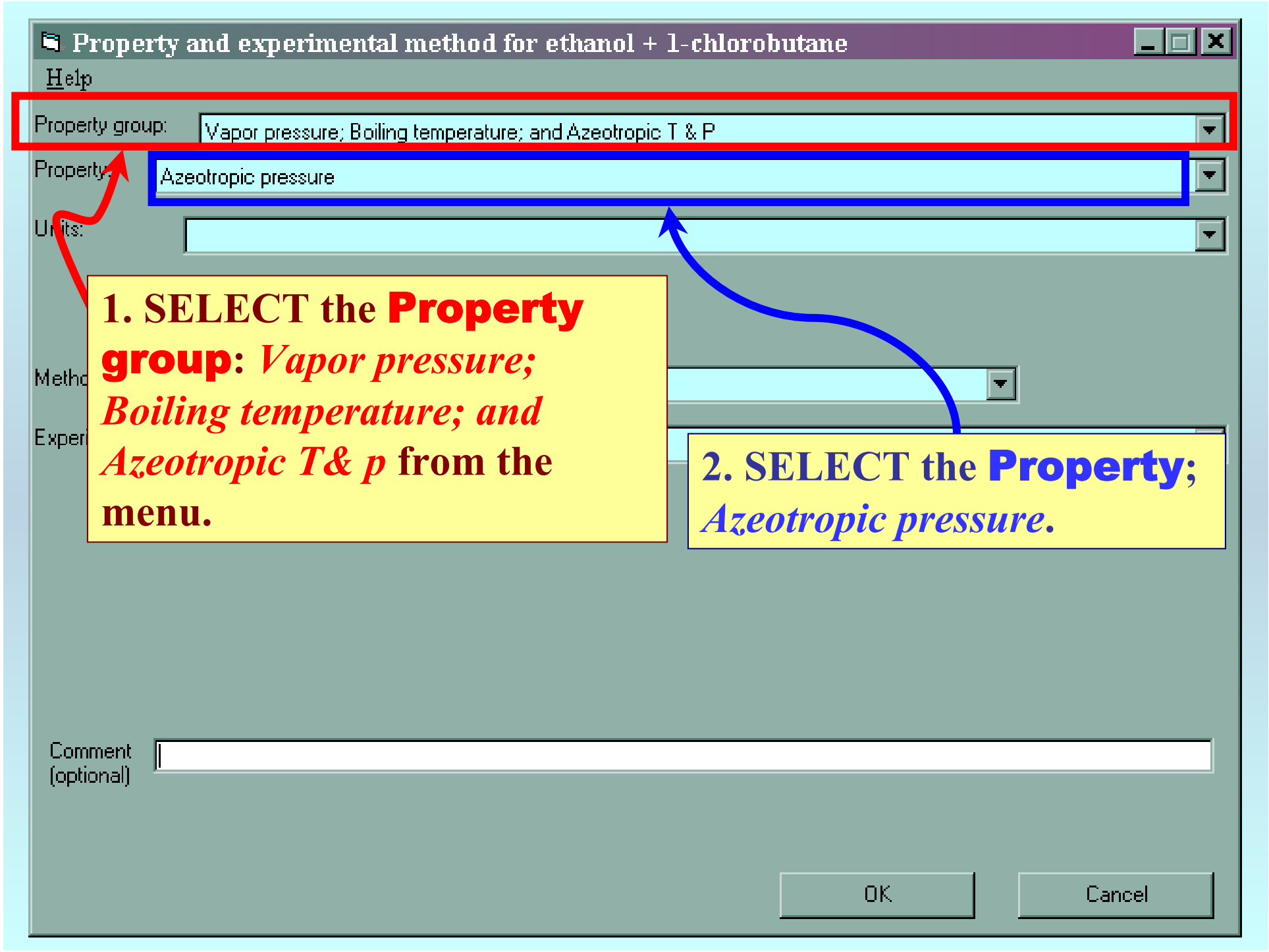
Method Information:

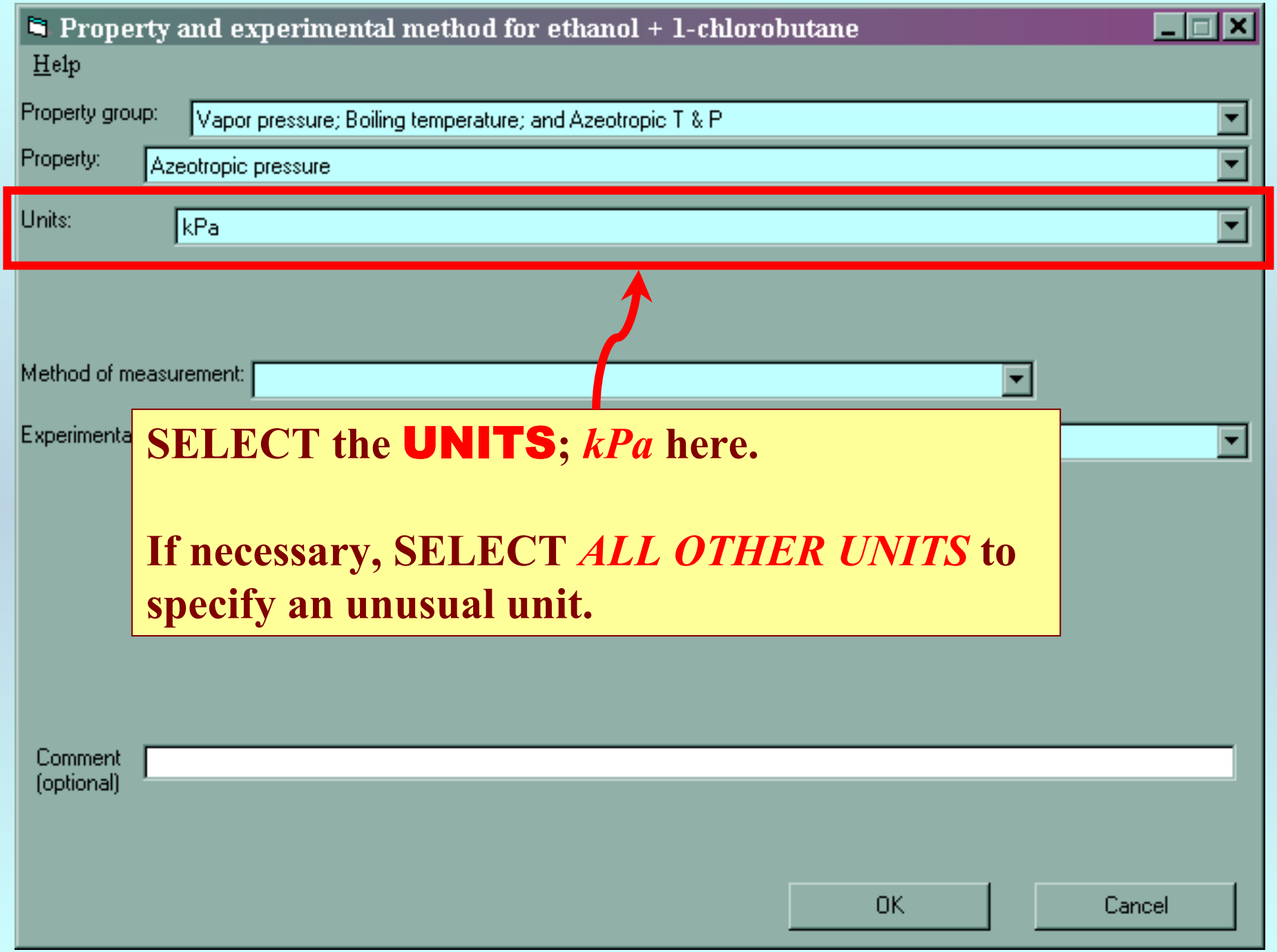
For (1-chlorobutane + ethanol), azeotropic mixtures with a minimum boiling temperature were observed over the whole range of temperature. Azeotropic mole fractions z were graphically calculated, assuming ideal behavior of the vapor, from the well-known equation, $\gamma_1/\gamma_2 = P_2^o/P_1^o$.

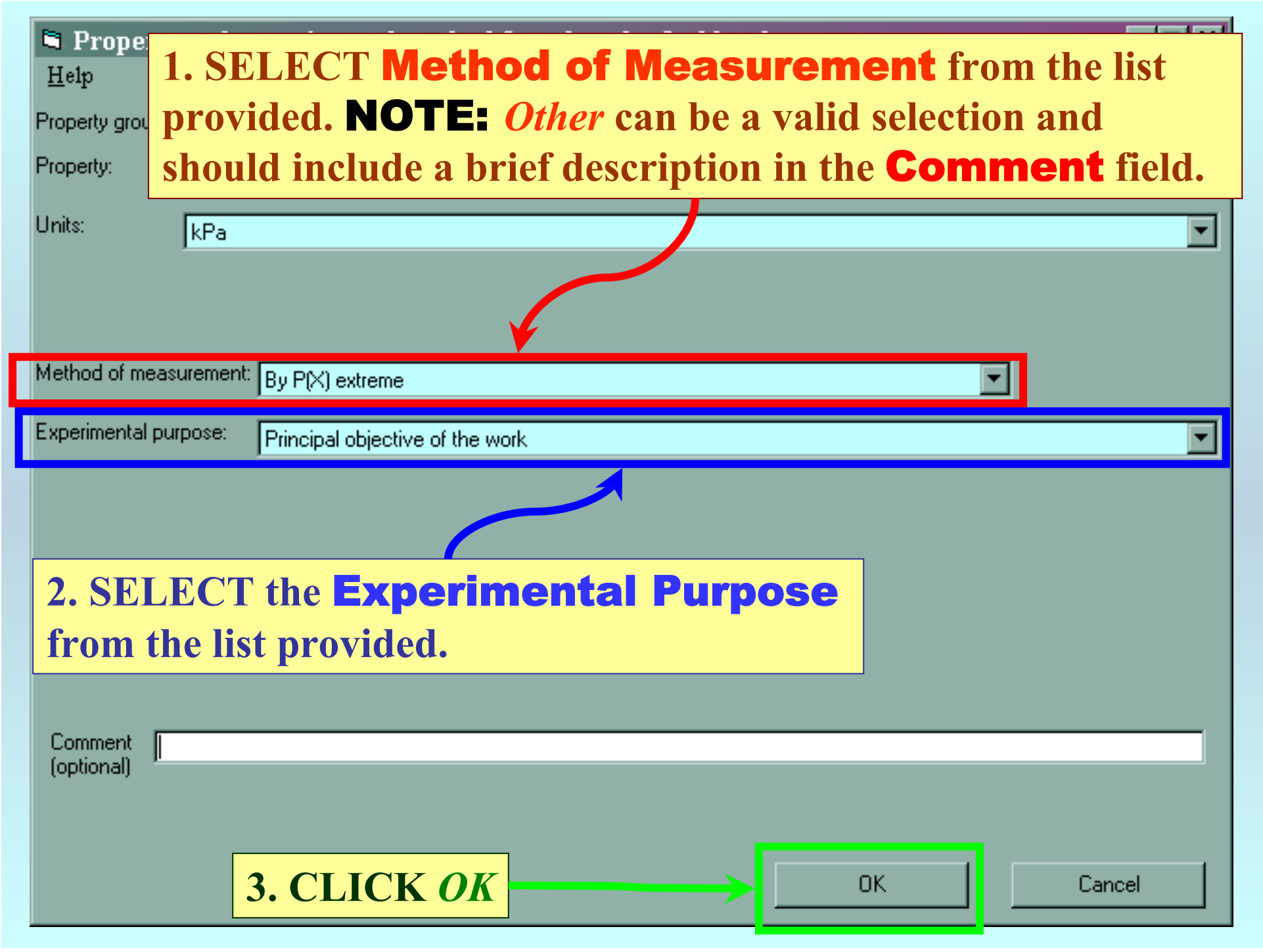
NOTE: Although the focus of the data-capture is experimentally determined values, derived azeotropic properties were considered of adequate importance to be included.



NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for ethanol + 1-chlorobutane
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Azeotropic pressure
Units:
1. SELECT the Property group: Vapor pressure; Boiling temperature; and Azeotropic T& p from the menu.
2. SELECT the Property; Azeotropic pressure.
Comment (optional)
OK
Cancel


Property and experimental method for ethanol + 1-chlorobutane
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Azeotropic pressure
Units:
kPa
Method of measurement:
Experimenta
SELECT the UNITS; kPa here.
If necessary, SELECT ALL OTHER UNITS to specify an unusual unit.
Comment (optional)
OK
Cancel

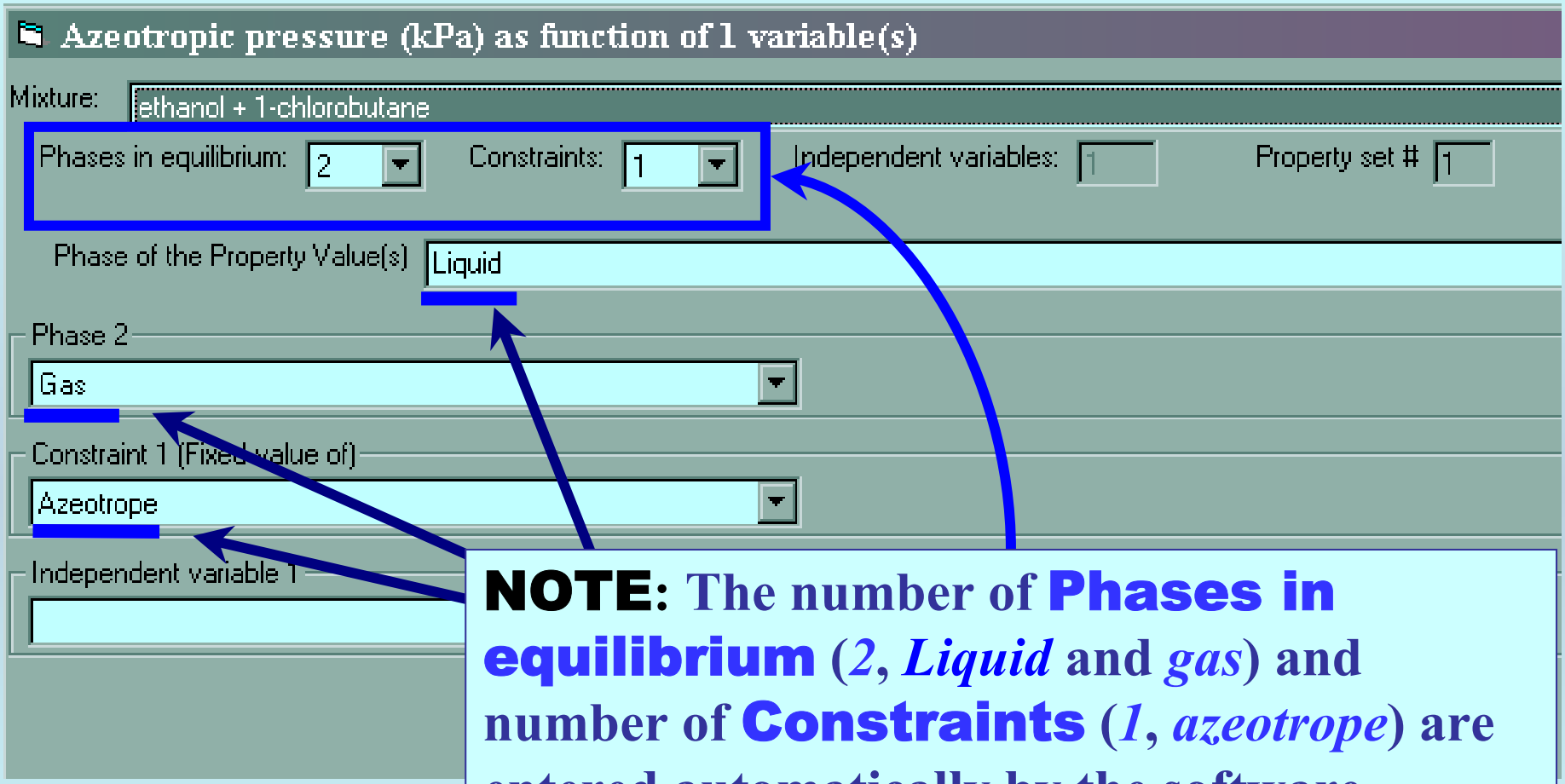


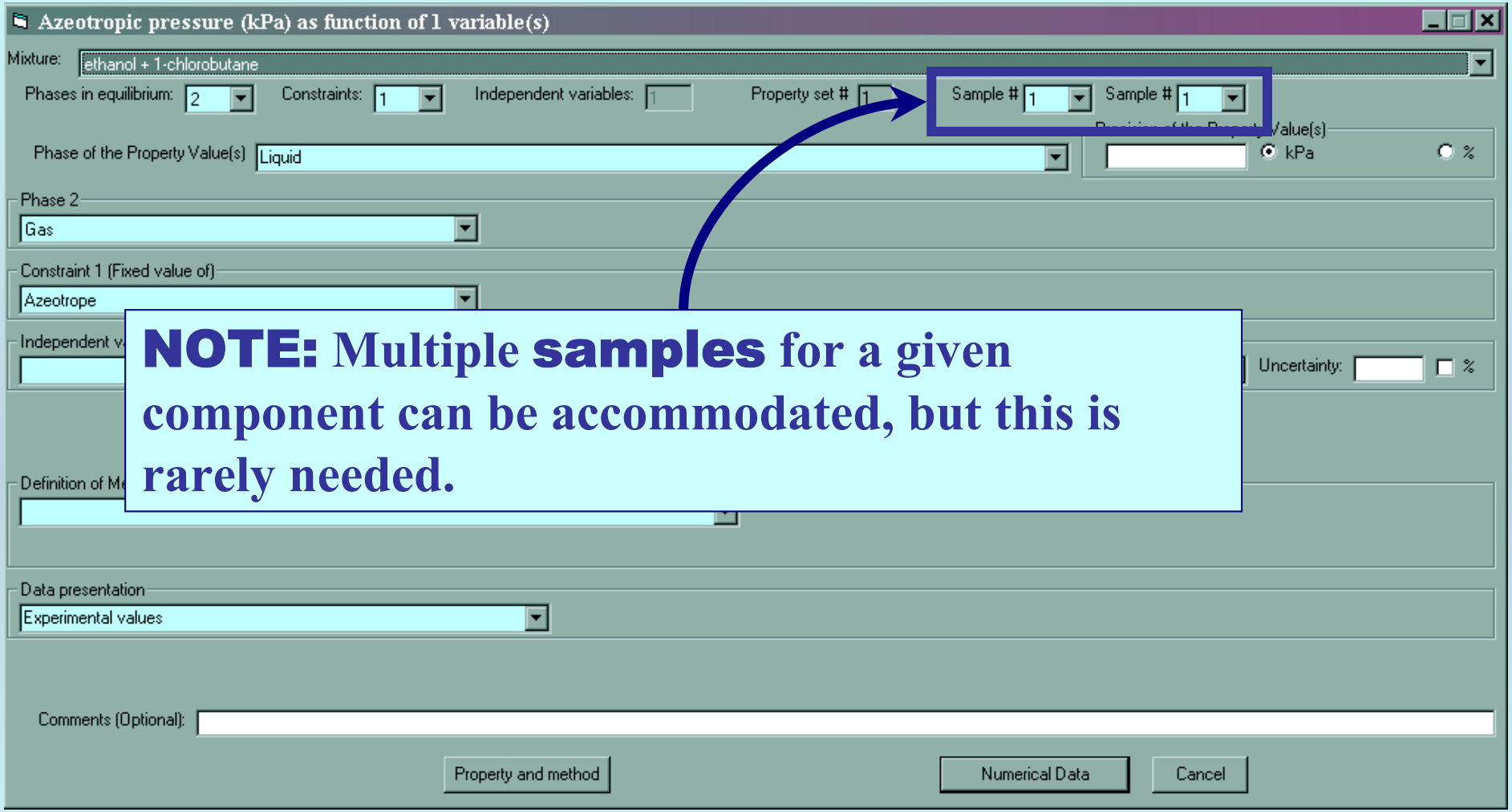
1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

2. SELECT the **Experimental Purpose** from the list provided.

3. CLICK *OK*

Specification of # of Phases in Equilibrium and # of Constraints

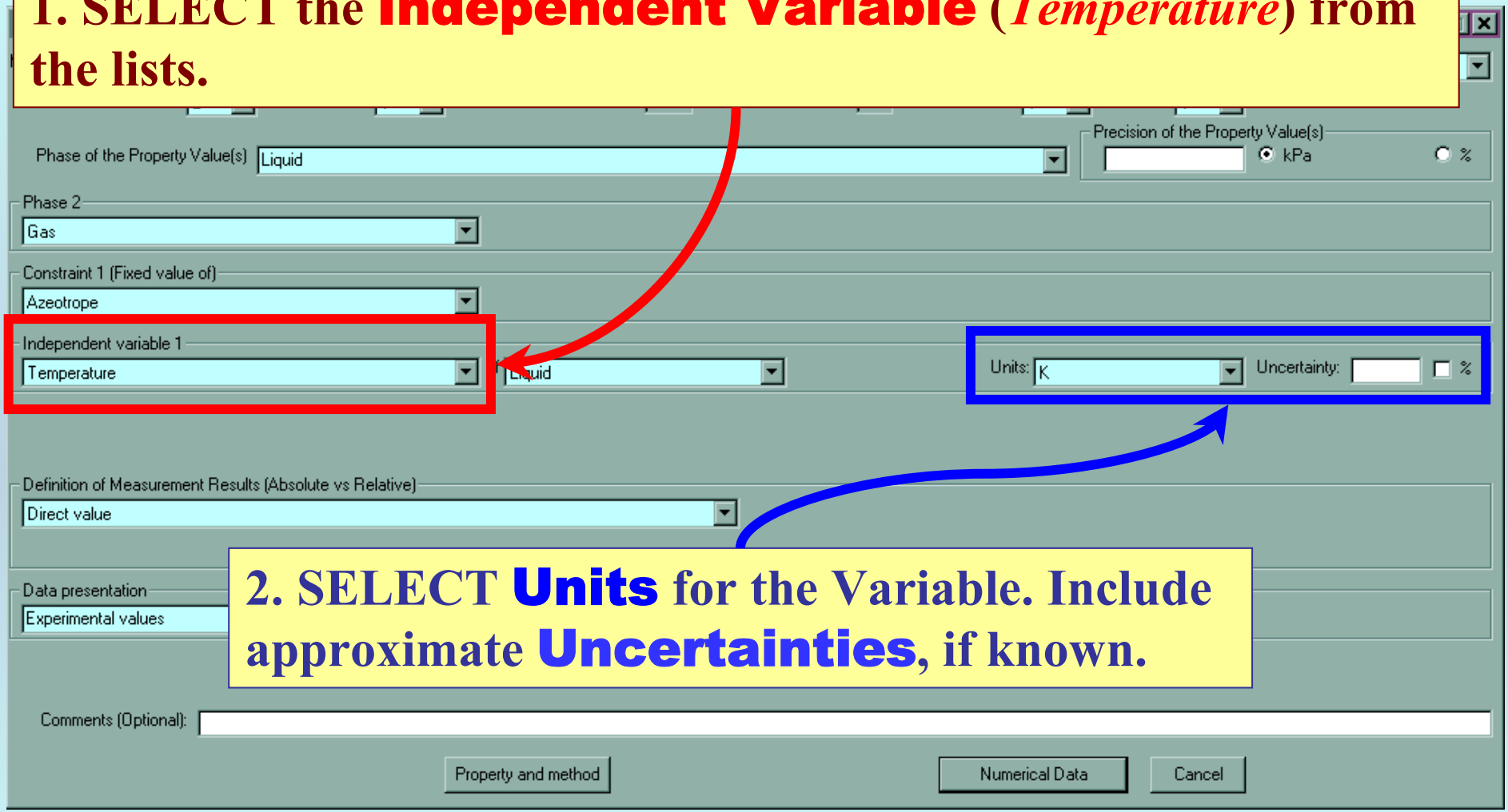




NOTE: Multiple **samples** for a given component can be accommodated, but this is rarely needed.

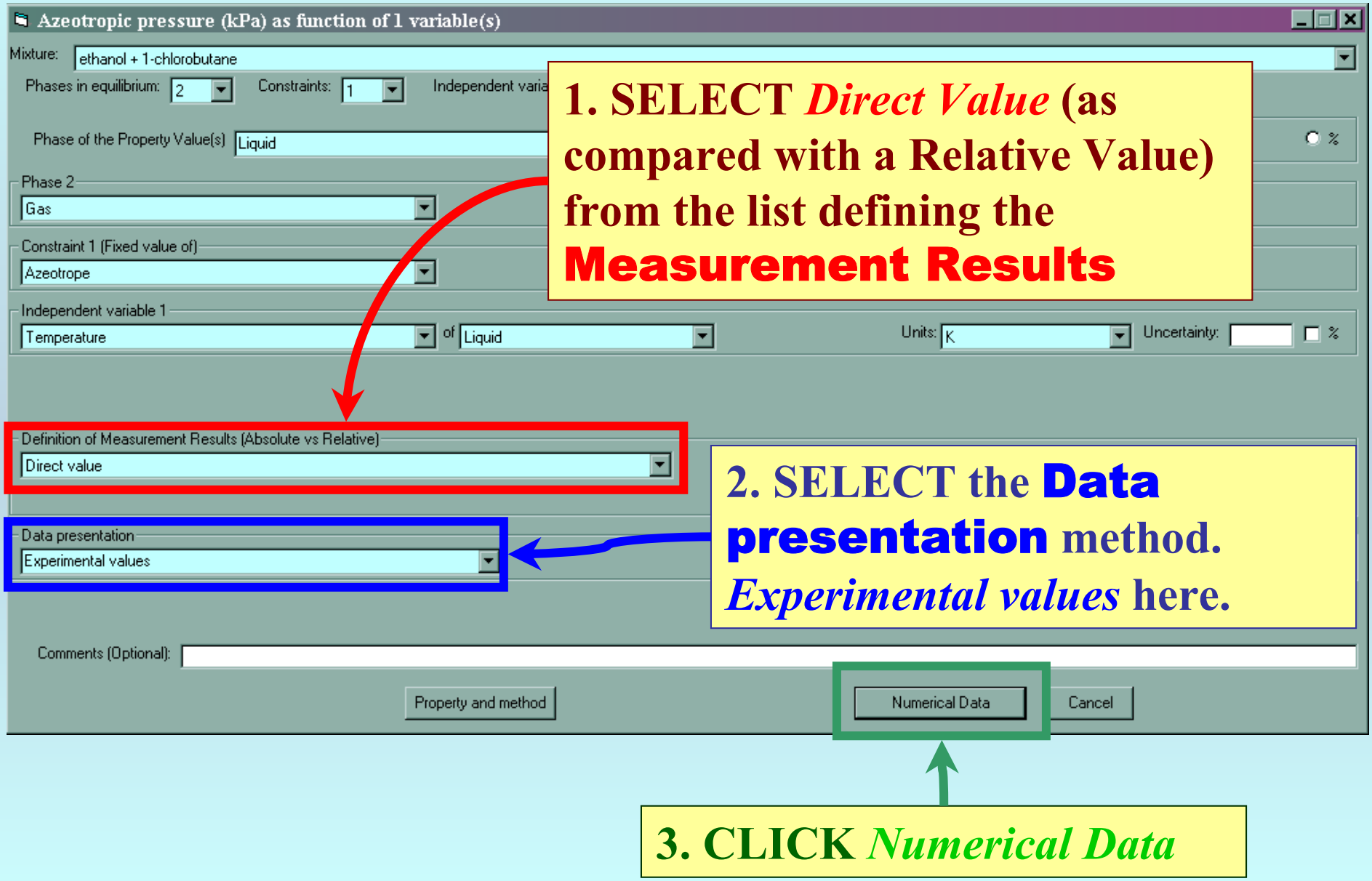
Specification of variables, units

1. SELECT the Independent Variable (*Temperature*) from the lists.



2. SELECT Units for the Variable. Include approximate Uncertainties, if known.

Measurement definition and Data presentation



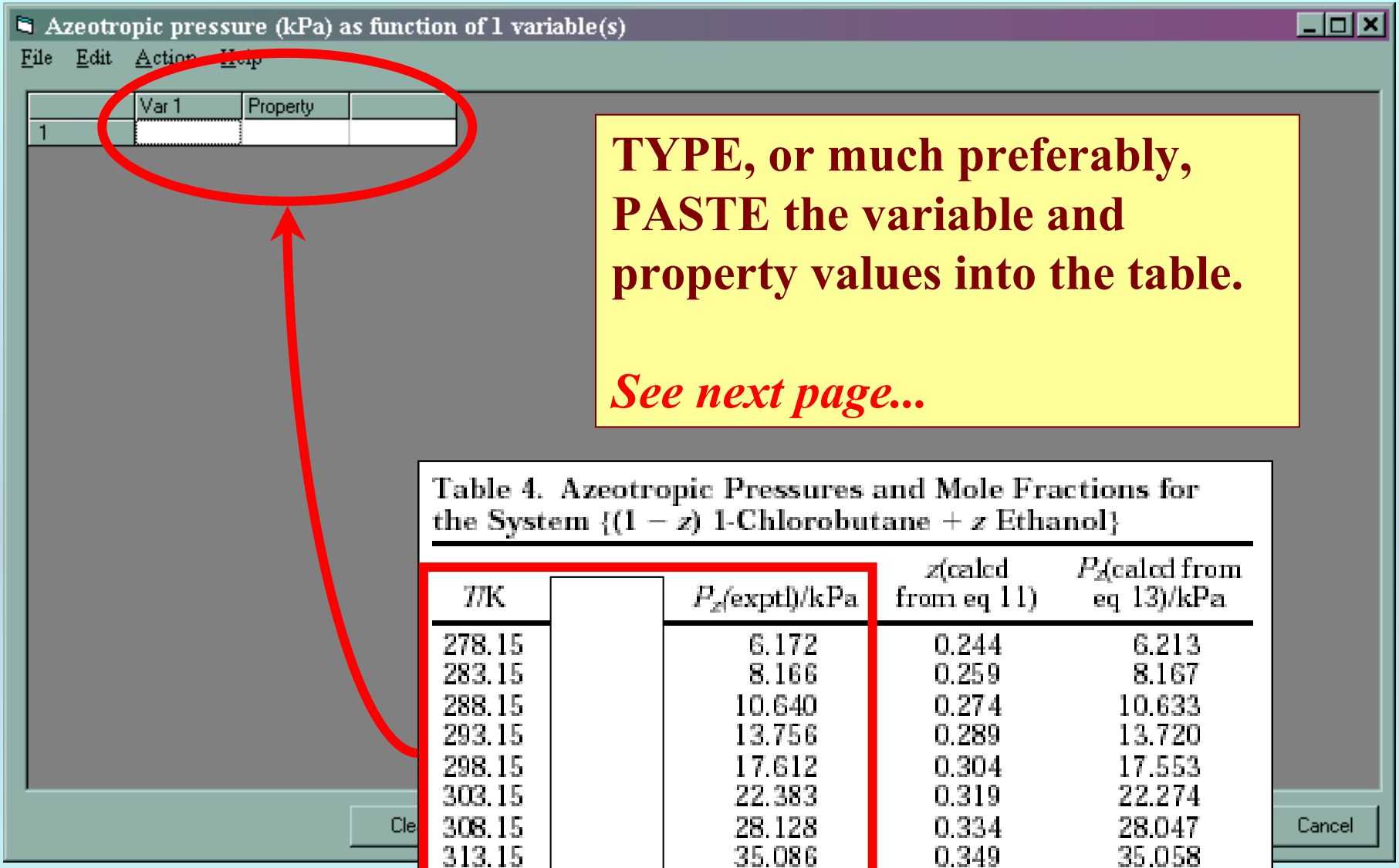


Table 4. Azeotropic Pressures and Mole Fractions for the System {(1 − *z*) 1-Chlorobutane + *z* Ethanol}

T/K		P_z(exptl)/kPa	*z*(calcd from eq 11)	P_z(calcd from eq 13)/kPa
278.15		6.172	0.244	6.213
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323.15		53.328	0.379	53.654

Azeotropic pressure (kPa) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property	
1	278.15	6.172	
2	283.15	8.166	
3	288.15	10.640	
4	293.15	13.756	
5	298.15	17.612	
6	303.15	22.383	
7	308.15	28.128	
8	313.15	35.086	
9	318.15	43.410	
10	323.15	53.328	

Clear the Table

Table 4. Azeotropic Pressures and Mole Fractions for the System {(1 − z) 1-Chlorobutane + z Ethanol}

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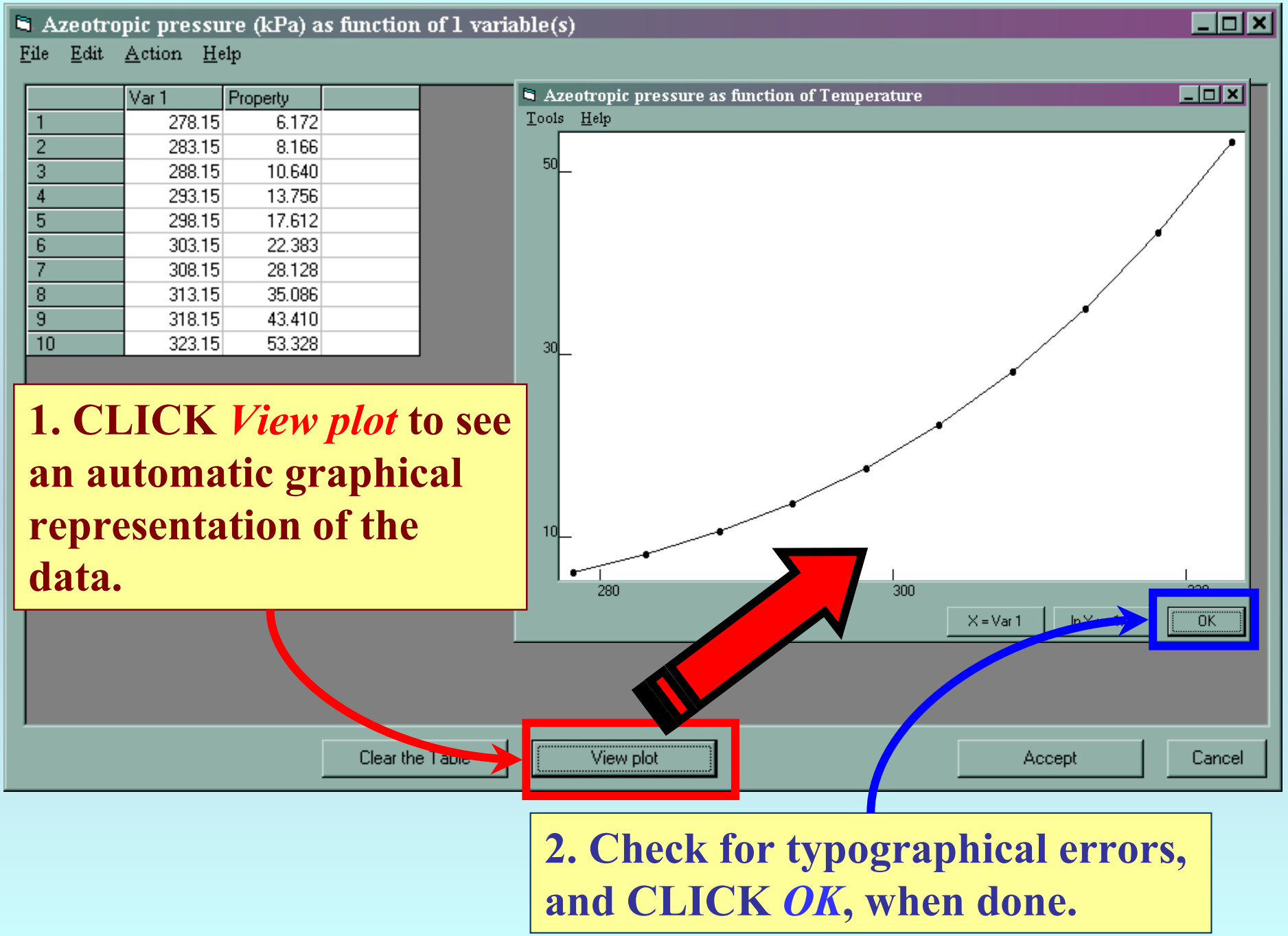
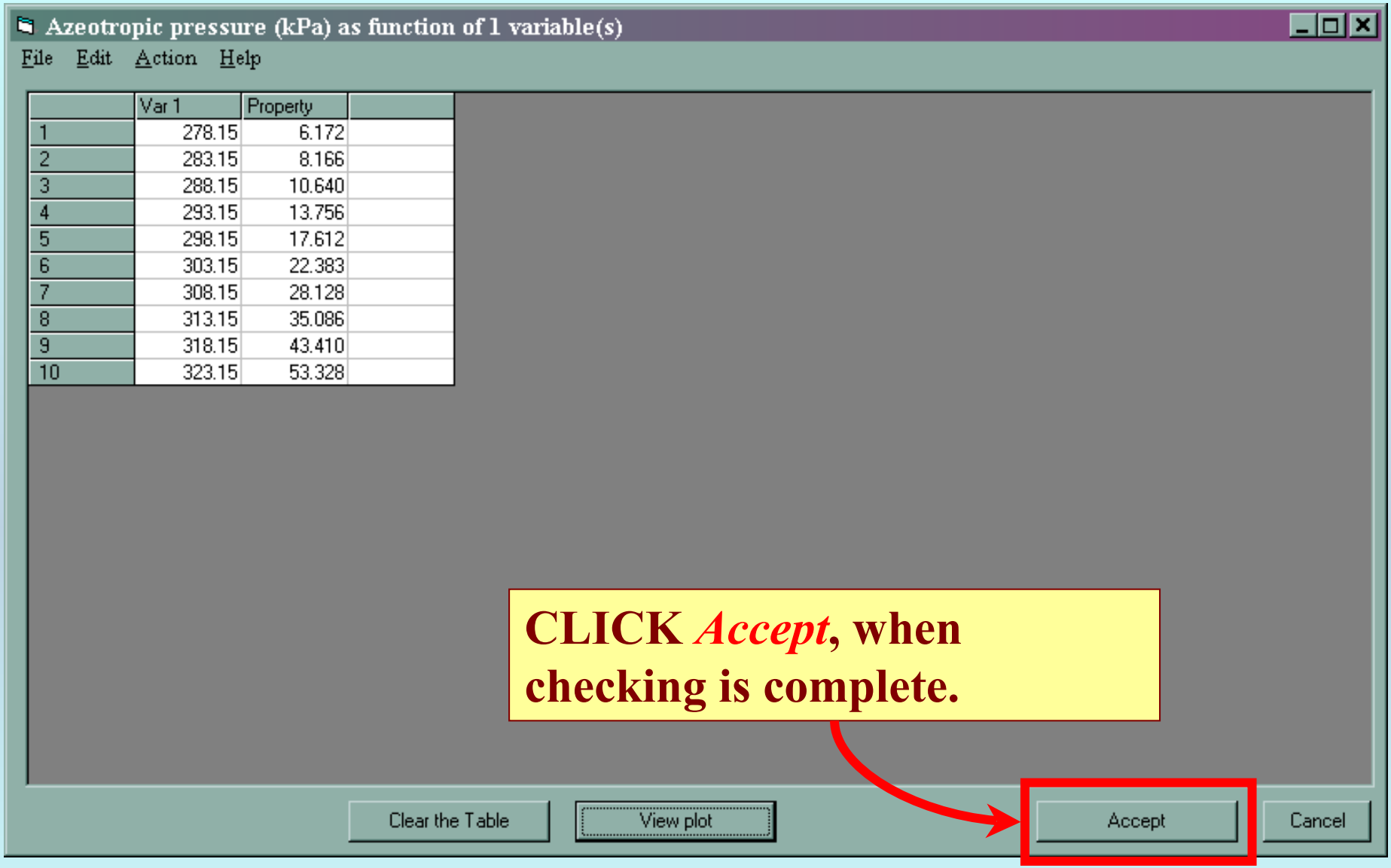
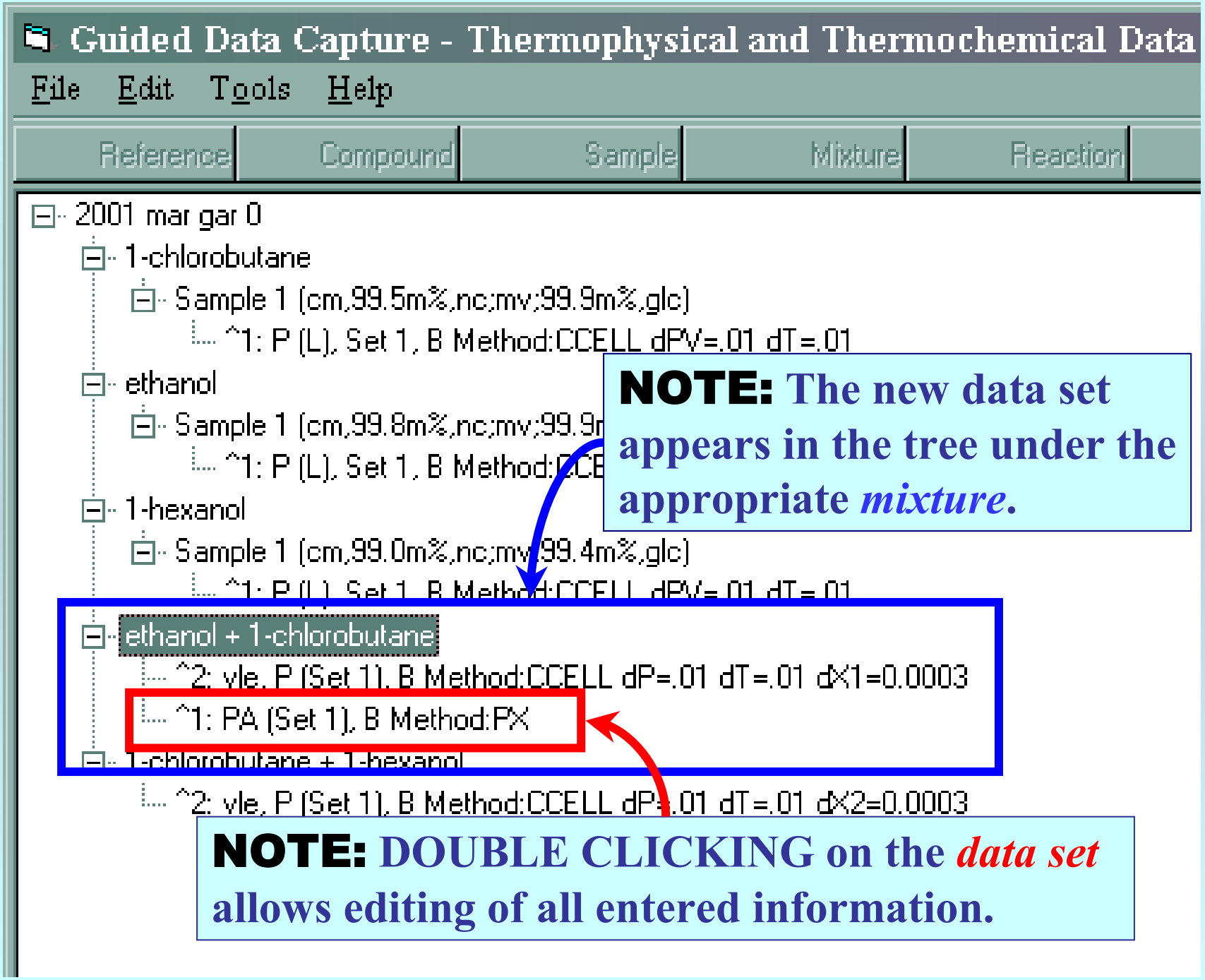
318.15		43.410	0.364	43.516
323.15		53.328	0.379	53.654

NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)


Azeotropic pressure (kPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 278.15 6.172
2 283.15 8.166
3 288.15 10.640
4 293.15 13.756
5 298.15 17.612
6 303.15 22.383
7 308.15 28.128
8 313.15 35.086
9 318.15 43.410
10 323.15 53.328
Azeotropic pressure as function of Temperature
Tools Help
50
30
10
280
300
X = Var 1
OK
1. CLICK View plot to see an automatic graphical representation of the data.
Clear the Table
View plot
Accept
Cancel
2. Check for typographical errors, and CLICK OK, when done.


Azeotropic pressure (kPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 278.15 6.172
2 283.15 8.166
3 288.15 10.640
4 293.15 13.756
5 298.15 17.612
6 303.15 22.383
7 308.15 28.128
8 313.15 35.086
9 318.15 43.410
10 323.15 53.328
CLICK Accept, when checking is complete.
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction
2001 mar gar 0
1-chlorobutane
Sample 1 (cm,99.5m%,nc;mv;99.9m%,glc)
^1: P (L), Set 1, B Method:CCELL dPV=.01 dT=.01
ethanol
Sample 1 (cm,99.8m%,nc;mv;99.9r
^1: P (L), Set 1, B Method:CCE
1-hexanol
Sample 1 (cm,99.0m%,nc;mv;99.4m%,glc)
ethanol + 1-chlorobutane
^2: vle, P (Set 1), B Method:CCELL dP=.01 dT=.01 dX1=0.0003
^1: PA (Set 1), B Method:PX
1-chlorobutane + 1-hexanol
^2: vle, P (Set 1), B Method:CCELL dP=.01 dT=.01 dX2=0.0003
NOTE: The new data set appears in the tree under the appropriate mixture.
NOTE: DOUBLE CLICKING on the data set allows editing of all entered information.

END

Continue with other compounds, samples, properties, reactions, etc...

***or* save your file and exit the program.**