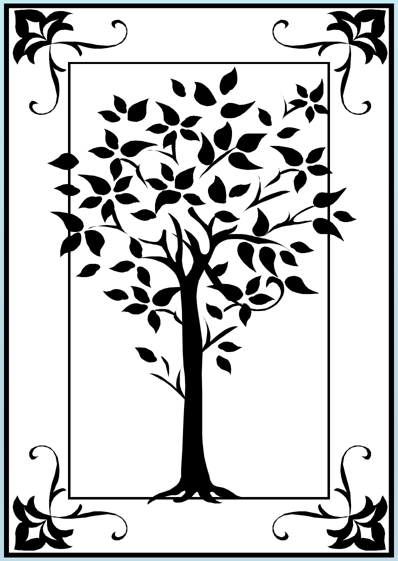
METADATA AND NUMERICAL DATA CAPTURE:
AZEOTROPIC composition, x_i
(2 components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
AZEOTROPIC composition x_i
(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*, 535−540 535

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 Garriga, 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 composition
for 1-chlorobutane + ethanol

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

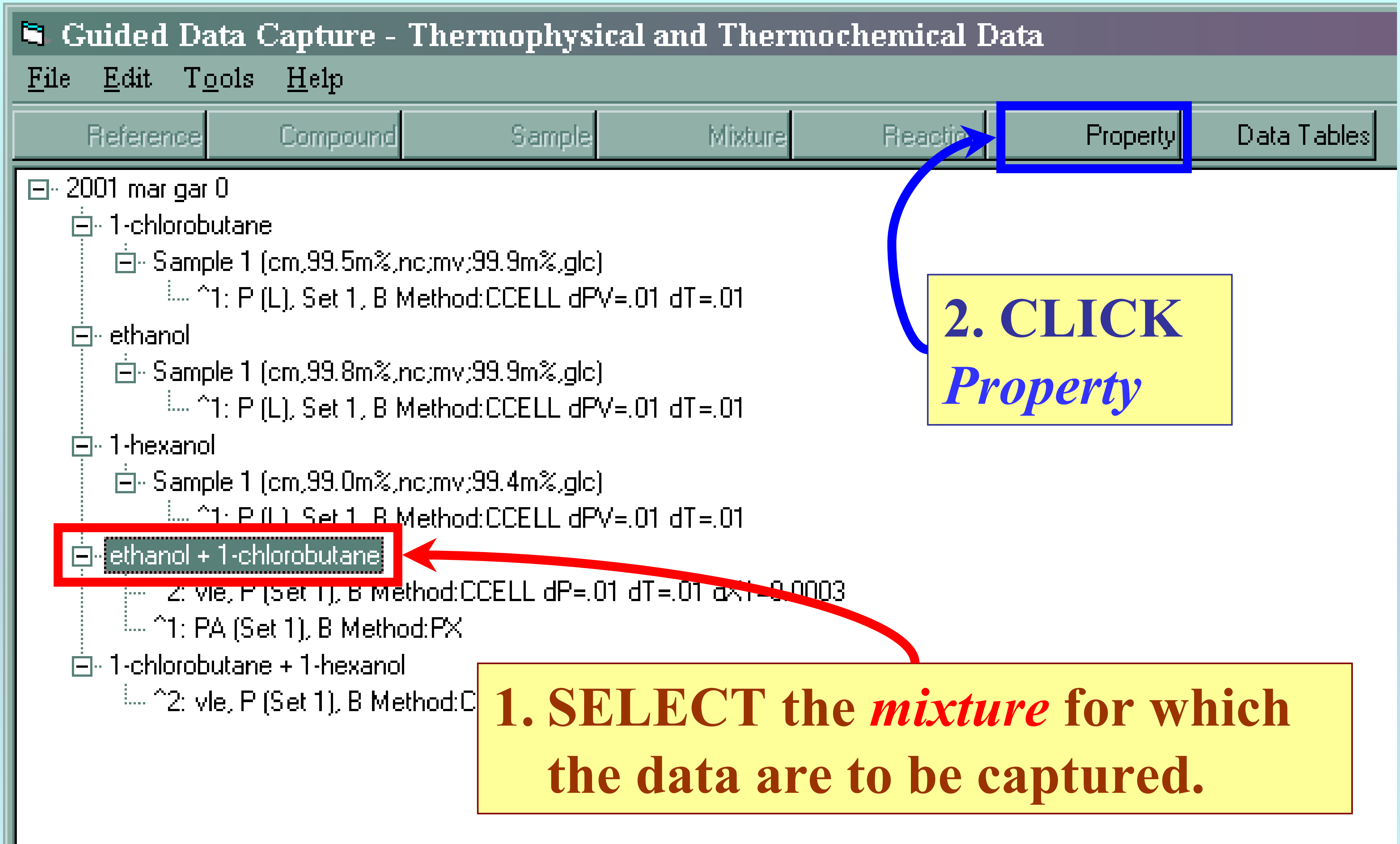
T/K	z(exptl)	P_z(exptl)/kPa	z(calcd from eq 11)	P_z(calcd from eq 13)/kPa
278.15	0.245	6.172	0.244	6.213
283.15	0.259	8.166	0.259	8.167
288.15	0.274	10.640	0.274	10.633
293.15	0.288	13.756	0.289	13.720
298.15	0.304	17.612	0.304	17.553
303.15	0.318	22.383	0.319	22.274
308.15	0.334	28.128	0.334	28.047
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.

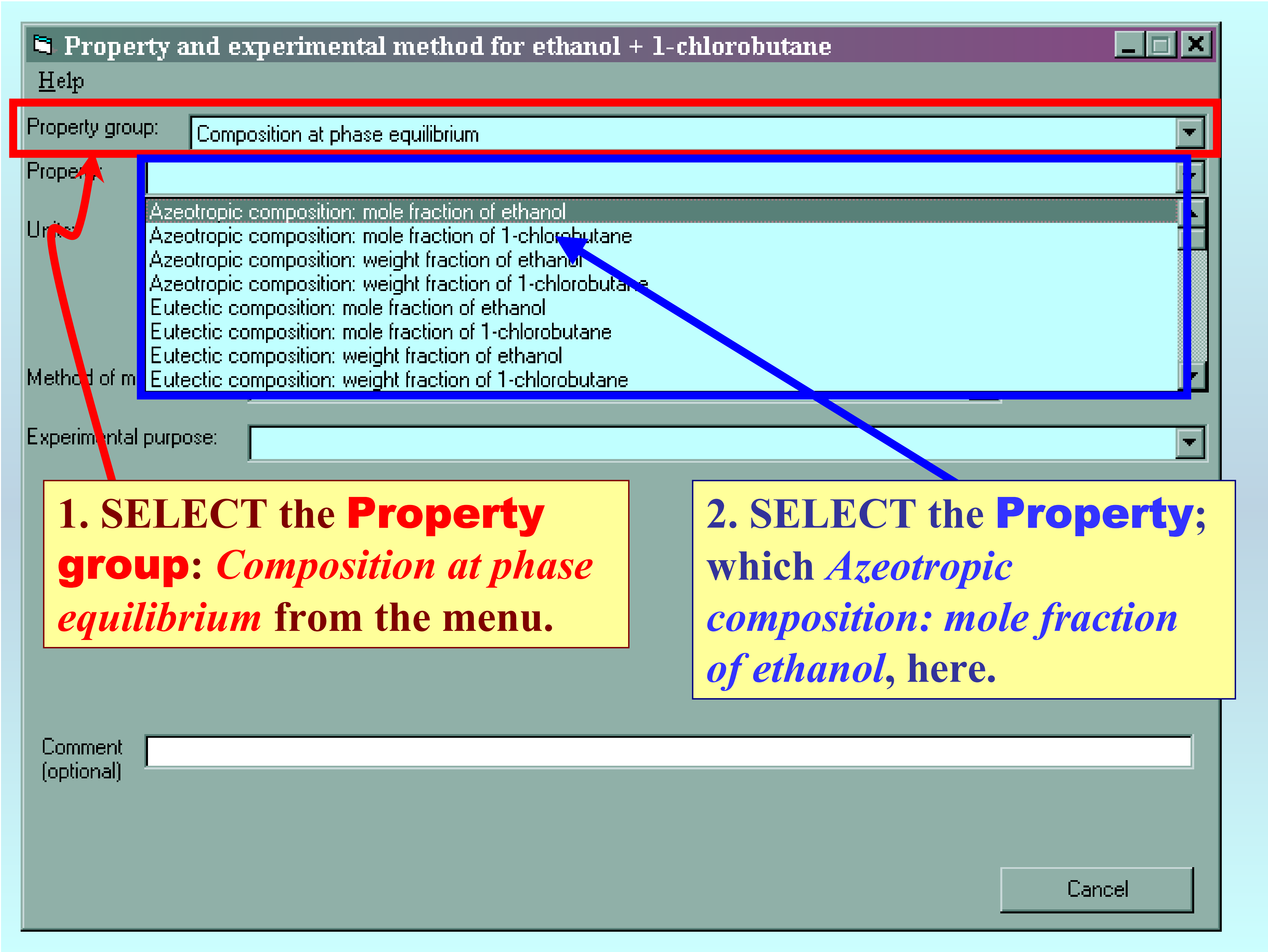
Method Information:

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, $\gamma_1/\gamma_2 = P_2^\circ/P_1^\circ$.

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

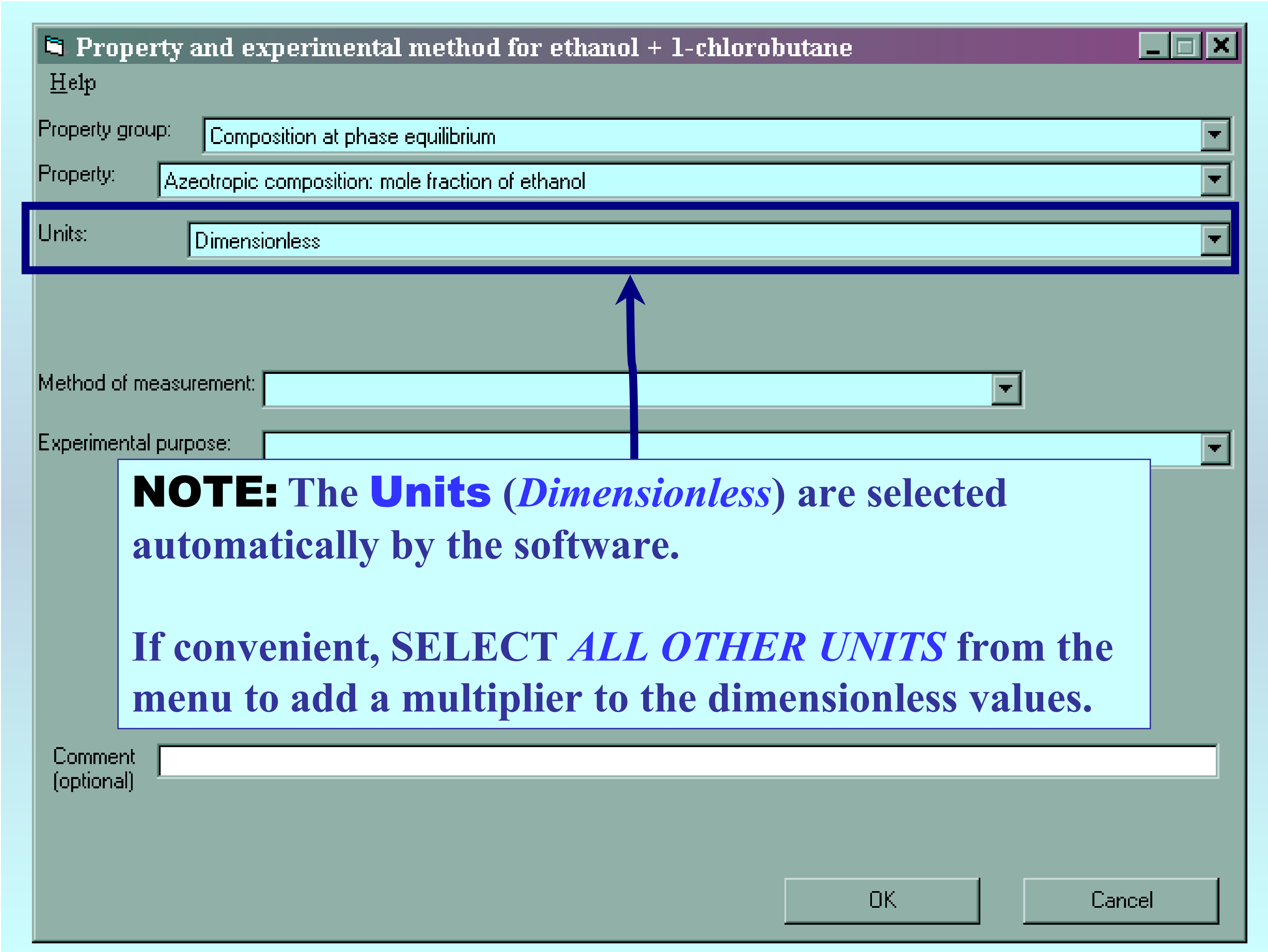


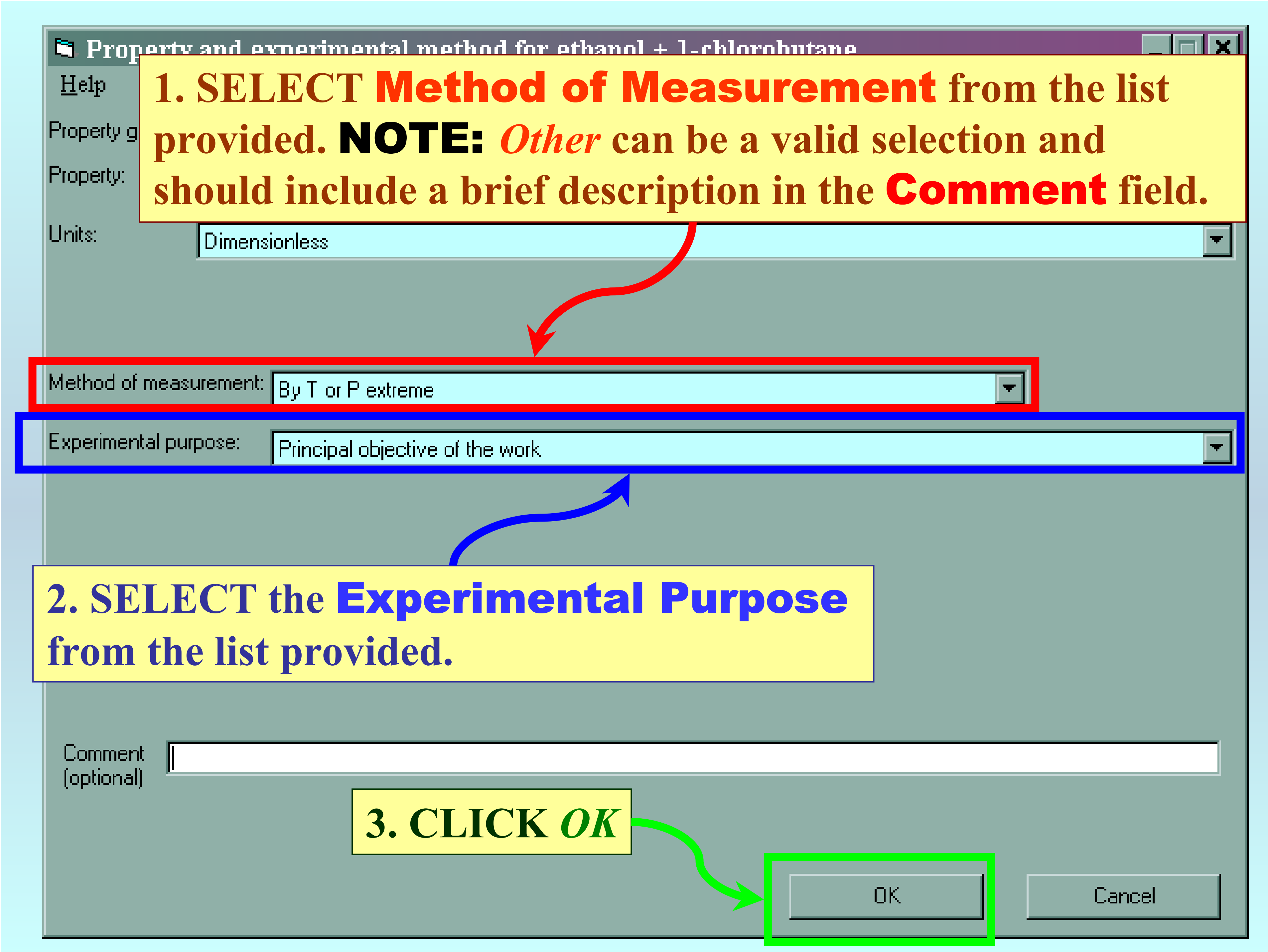
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)



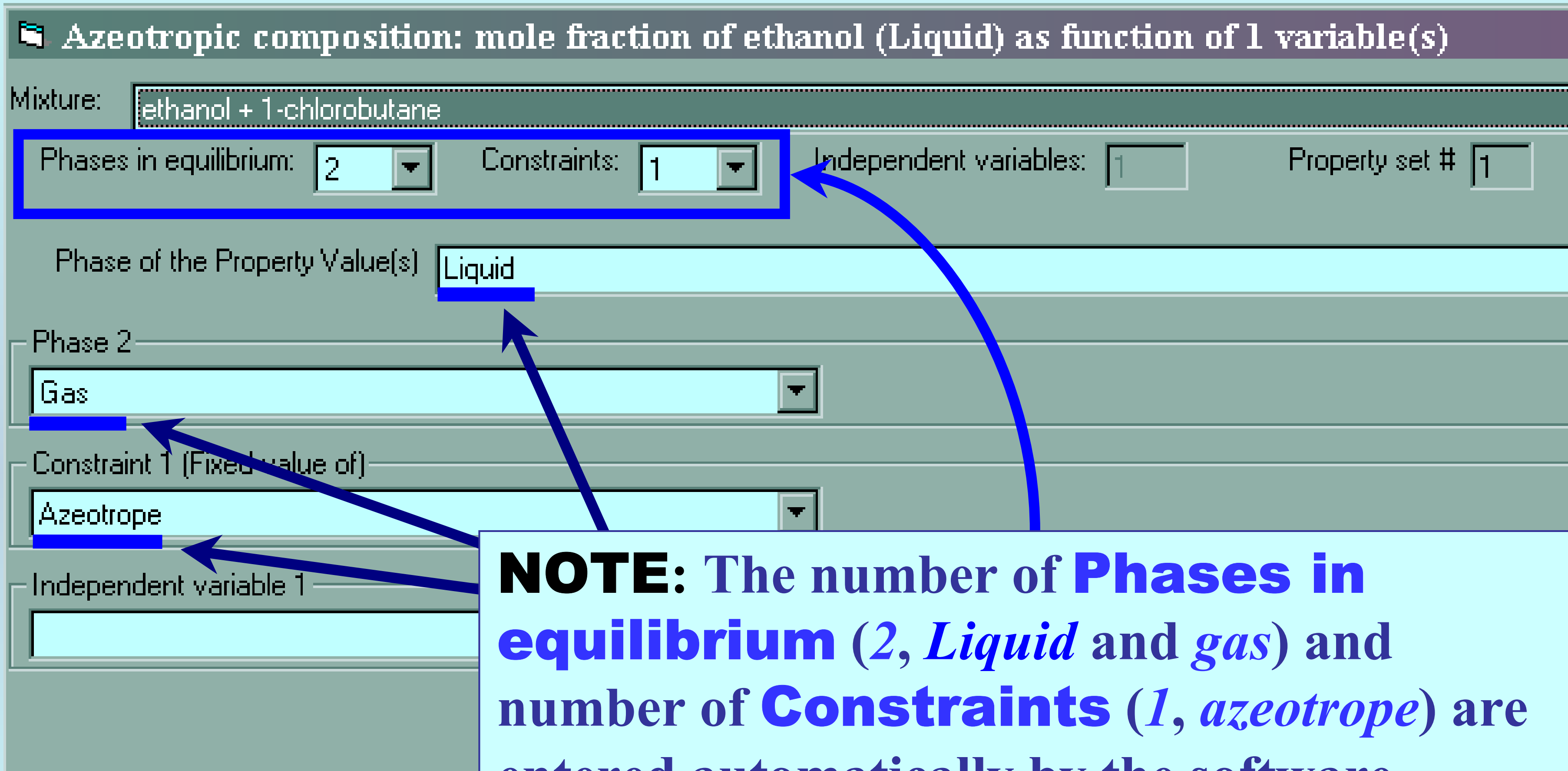
1. SELECT the Property group: *Composition at phase equilibrium* from the menu.

2. SELECT the Property; which *Azeotropic composition: mole fraction of ethanol*, here.

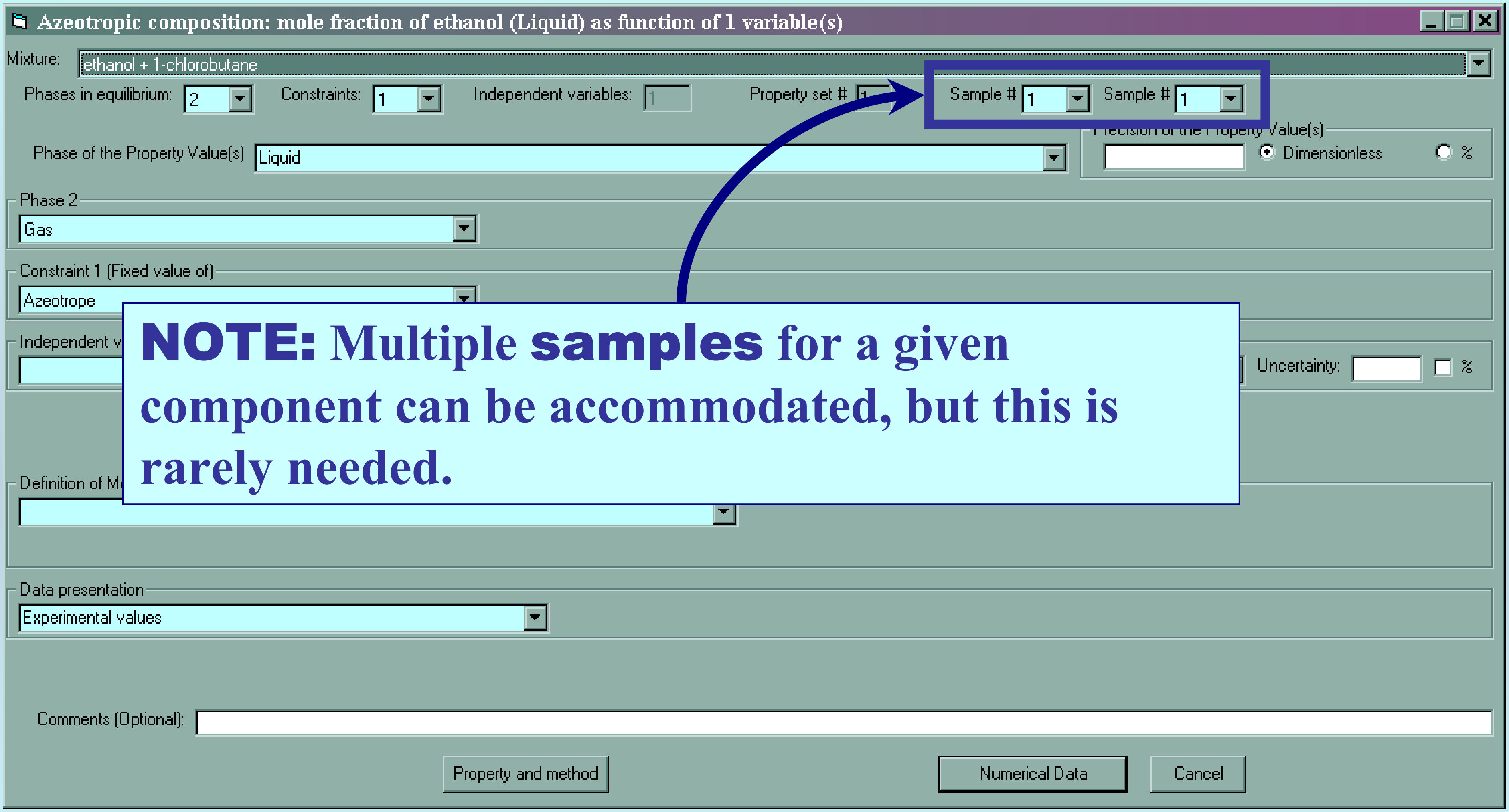

Property and experimental method for ethanol + 1-chlorobutane
Help
Property group:
Composition at phase equilibrium
Property:
Azeotropic composition: mole fraction of ethanol
Units:
Dimensionless
Method of measurement:
Experimental purpose:
NOTE: The Units (Dimensionless) are selected automatically by the software.
If convenient, SELECT ALL OTHER UNITS from the menu to add a multiplier to the dimensionless values.
Comment (optional)
OK
Cancel


Property and experimental method for ethanol + 1-chlorobutane
Help
Property:
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.
Units:
Dimensionless
Method of measurement:
By T or P extreme
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK OK
OK
Cancel

Specification of # of Phases in Equilibrium and # of Constraints



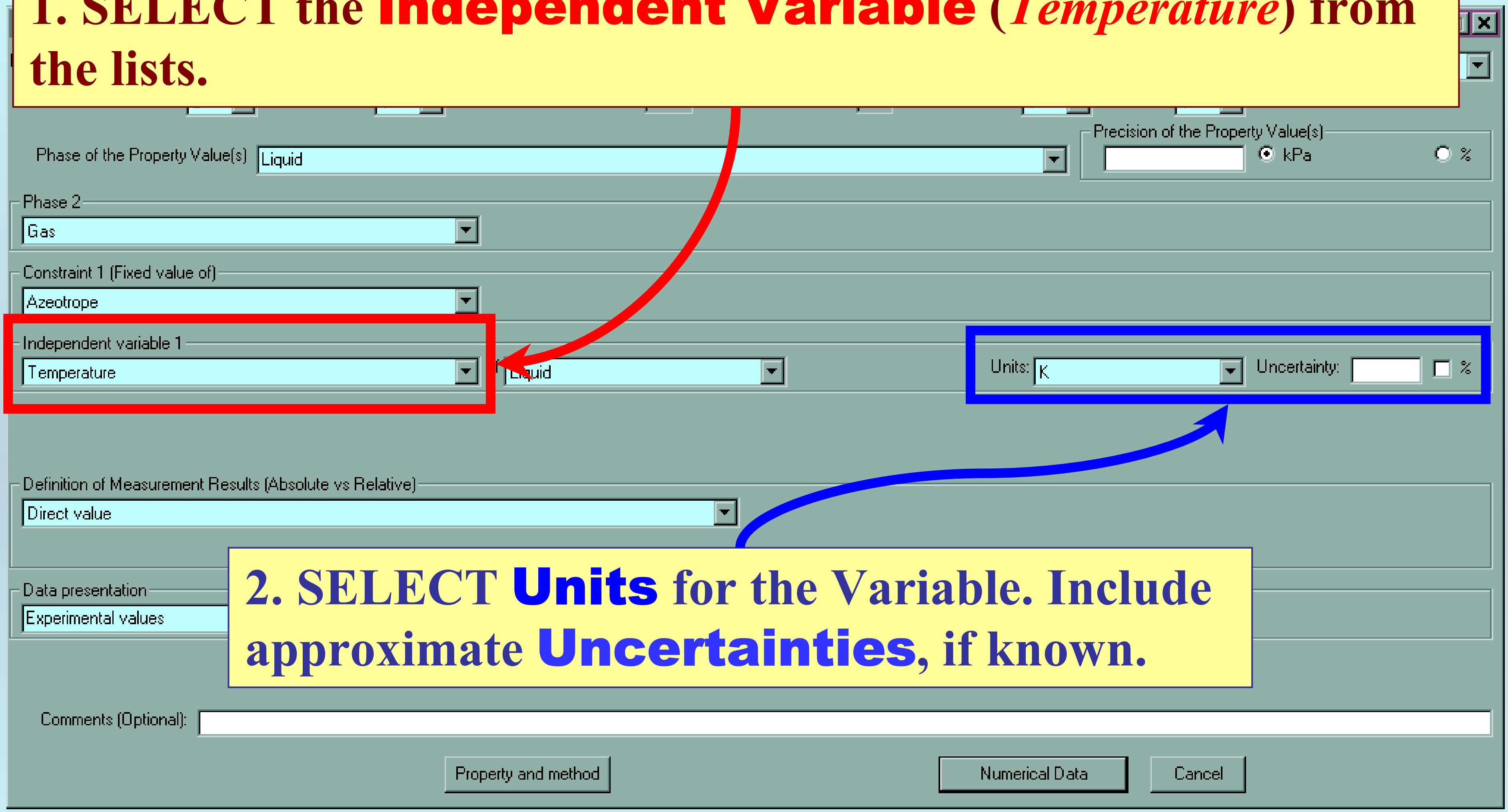
NOTE: The number of **Phases in equilibrium** (*2*, ***Liquid*** and *gas*) and number of **Constraints** (*1*, *azeotrope*) are entered automatically by the software.



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

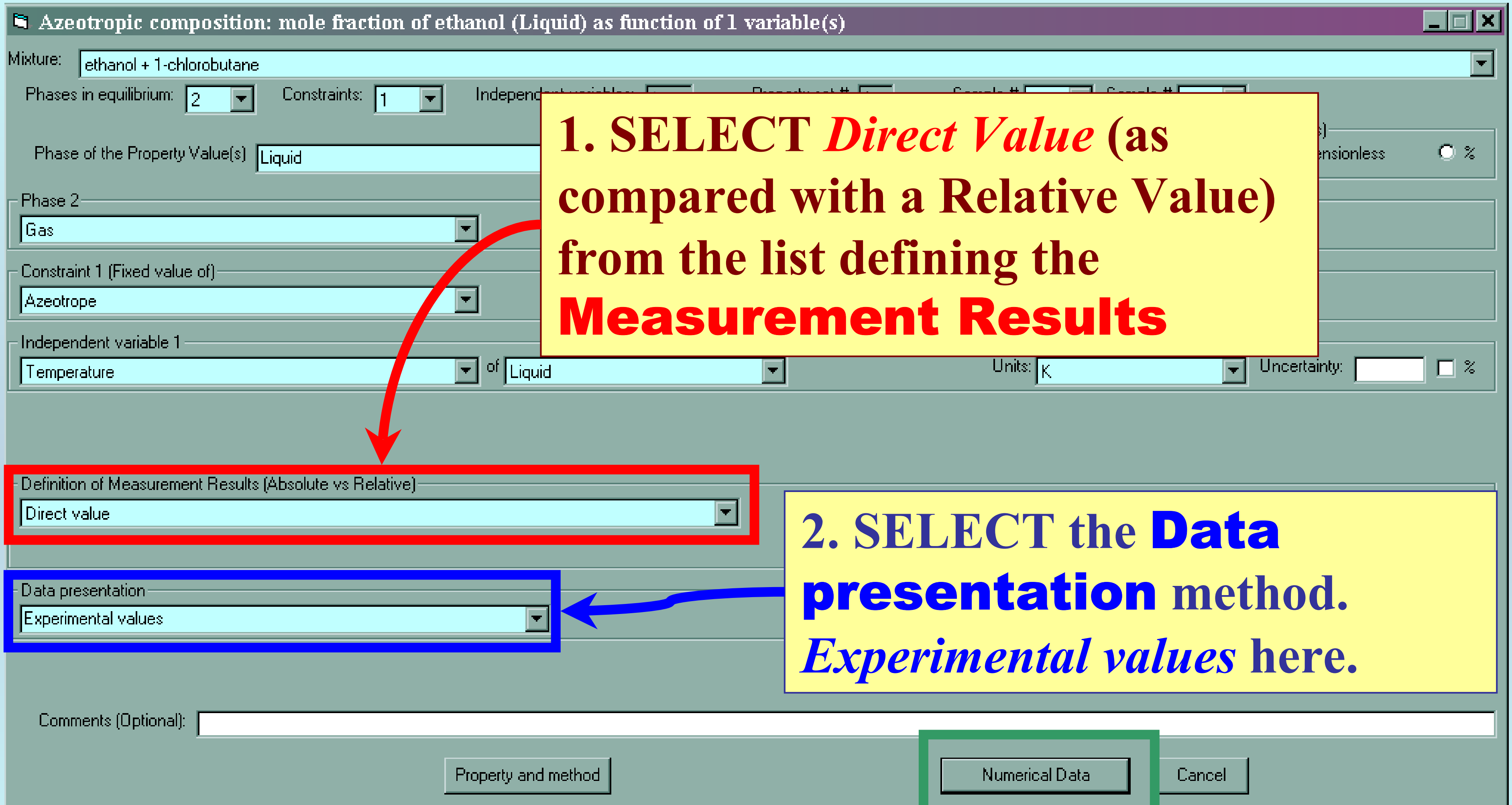
Specification of variables, units

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



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

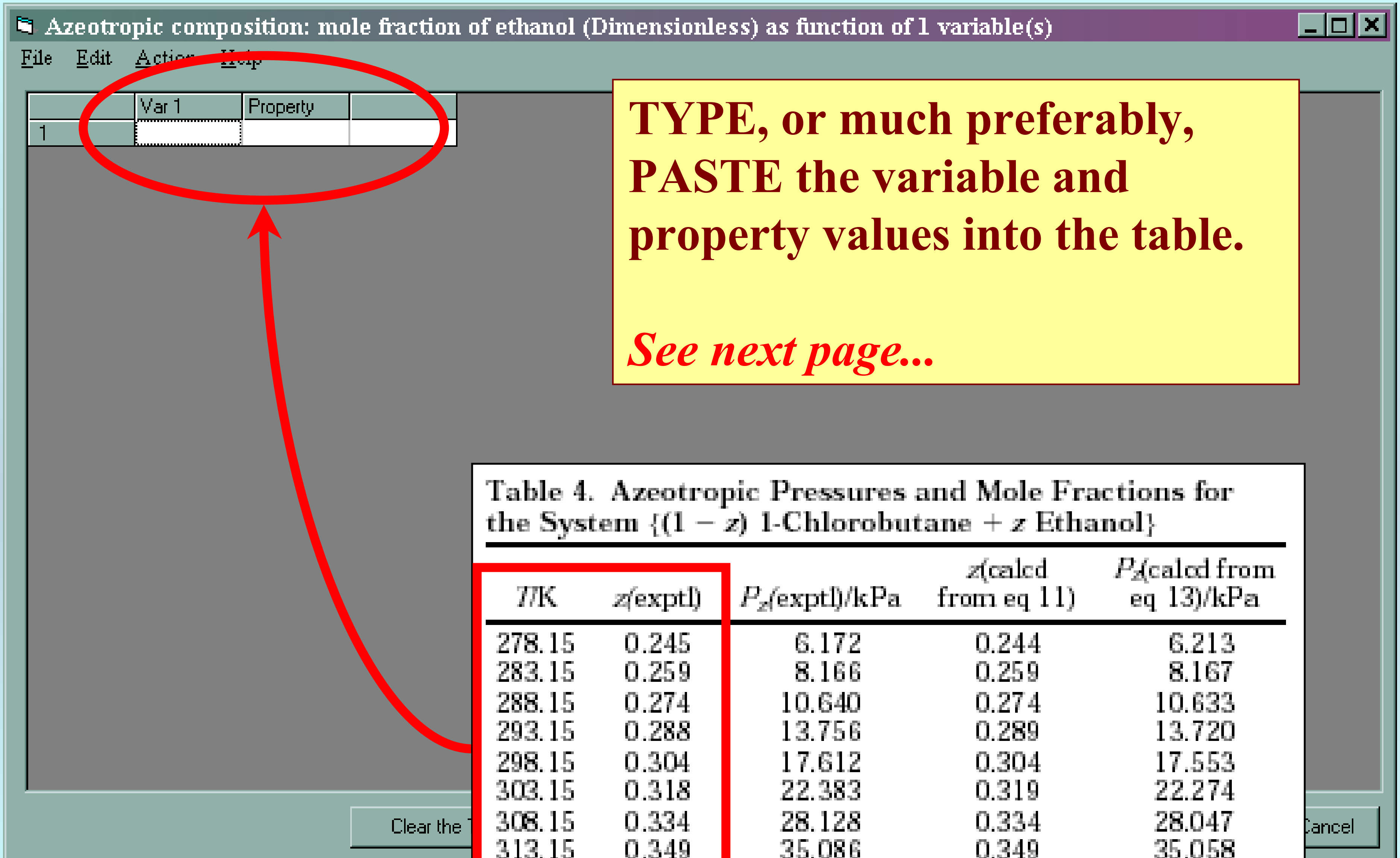
Measurement definition and Data presentation



1. SELECT *Direct Value* (as compared with a Relative Value) from the list defining the **Measurement Results**

2. SELECT the **Data presentation** method. *Experimental values* here.

3. CLICK *Numerical Data*

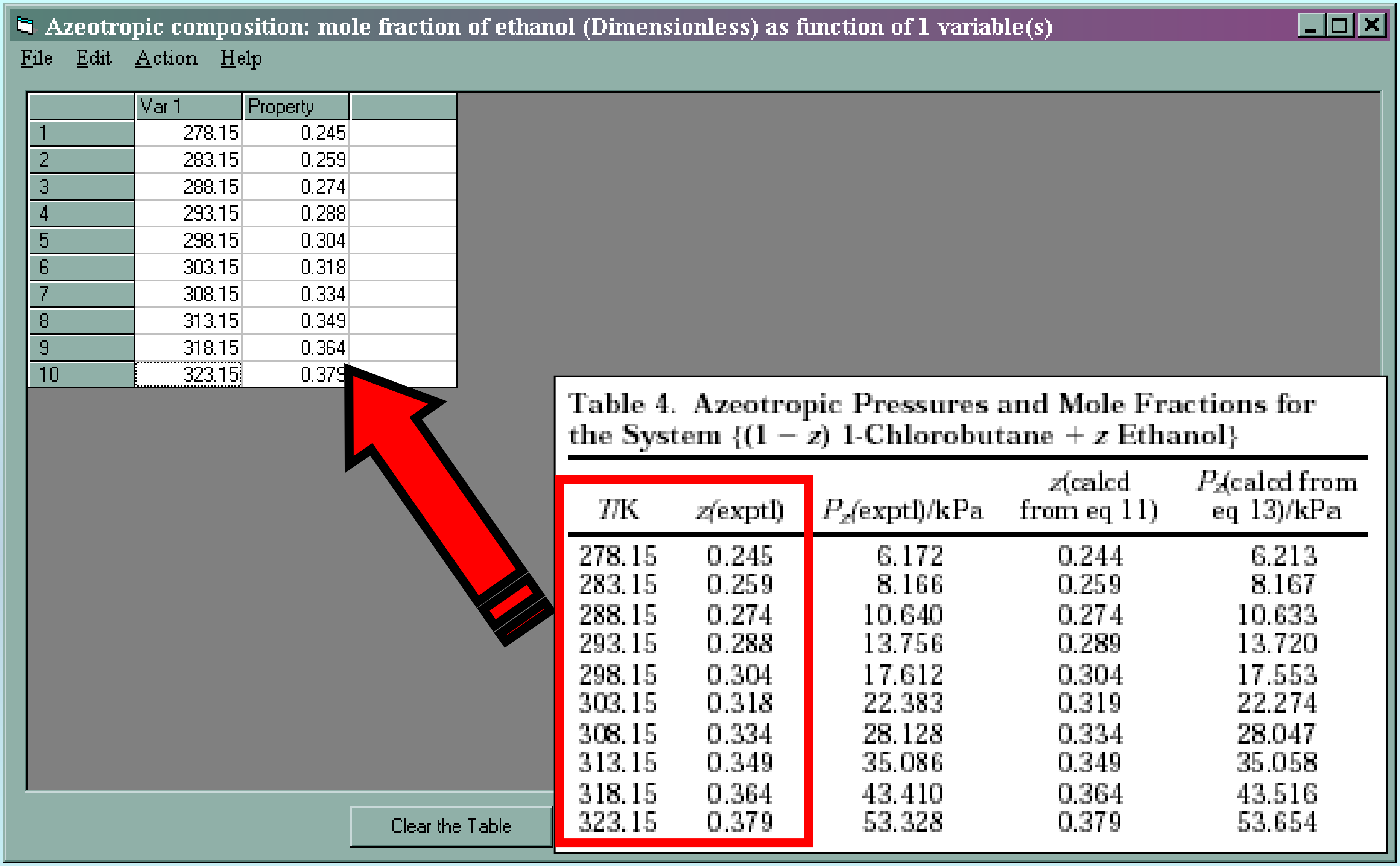


TYPE, or much preferably, PASTE the variable and property values into the table.

See next page...

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

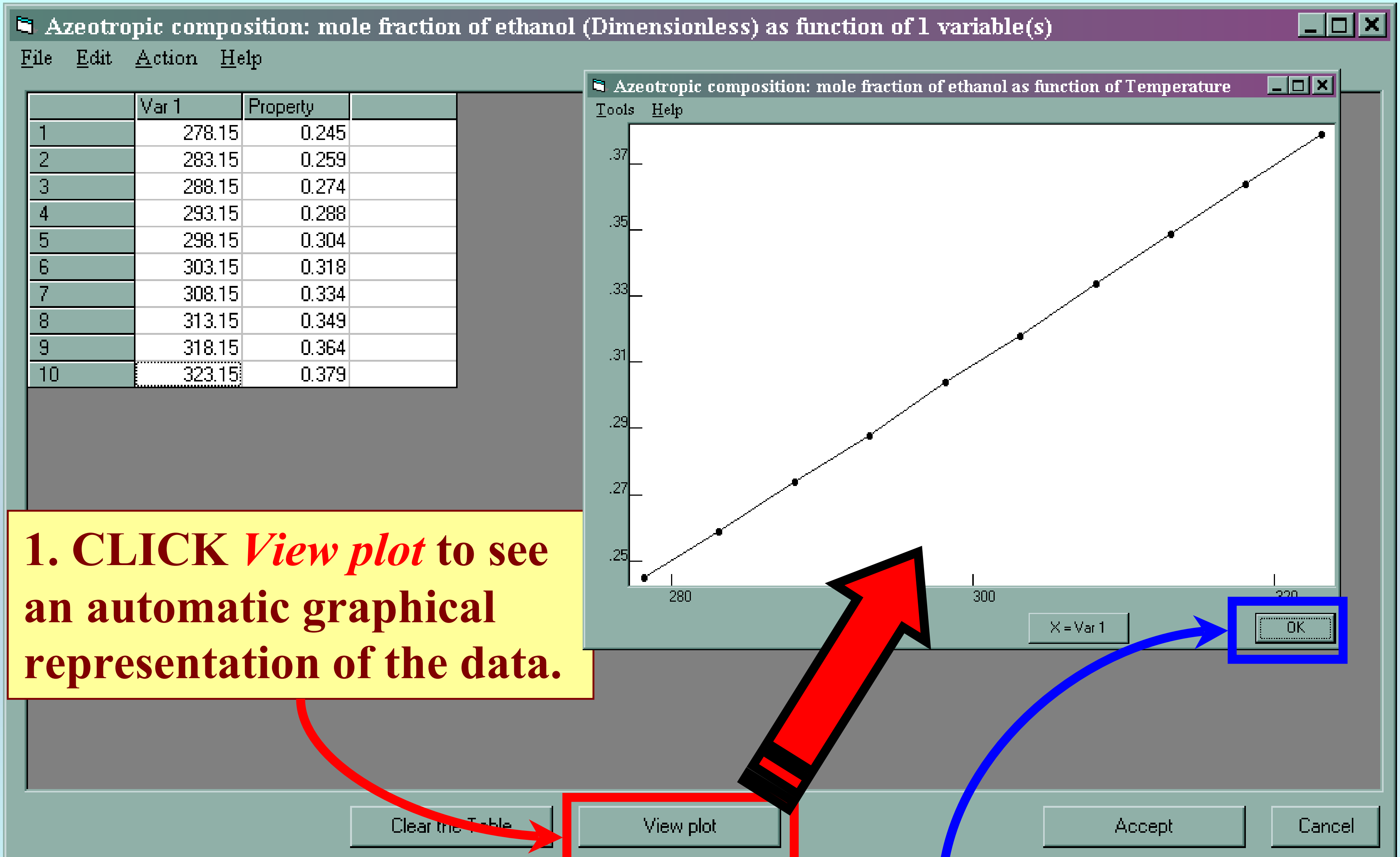


	Var 1	Property
1	278.15	0.245
2	283.15	0.259
3	288.15	0.274
4	293.15	0.288
5	298.15	0.304
6	303.15	0.318
7	308.15	0.334
8	313.15	0.349
9	318.15	0.364
10	323.15	0.379

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

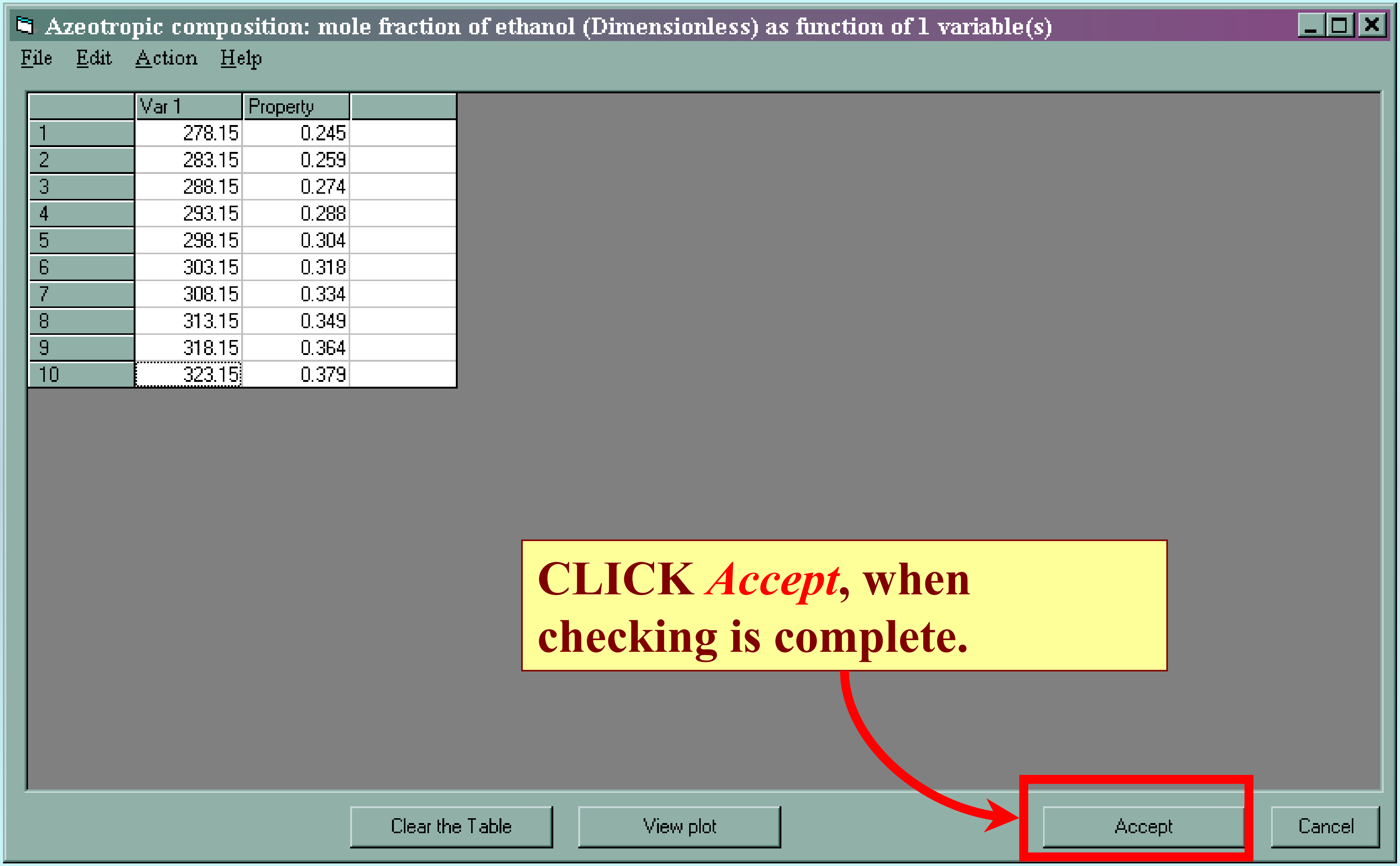
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns.
(This can also be done externally in spreadsheet software, e.g., EXCEL.)



	Var 1	Property
1	278.15	0.245
2	283.15	0.259
3	288.15	0.274
4	293.15	0.288
5	298.15	0.304
6	303.15	0.318
7	308.15	0.334
8	313.15	0.349
9	318.15	0.364
10	323.15	0.379

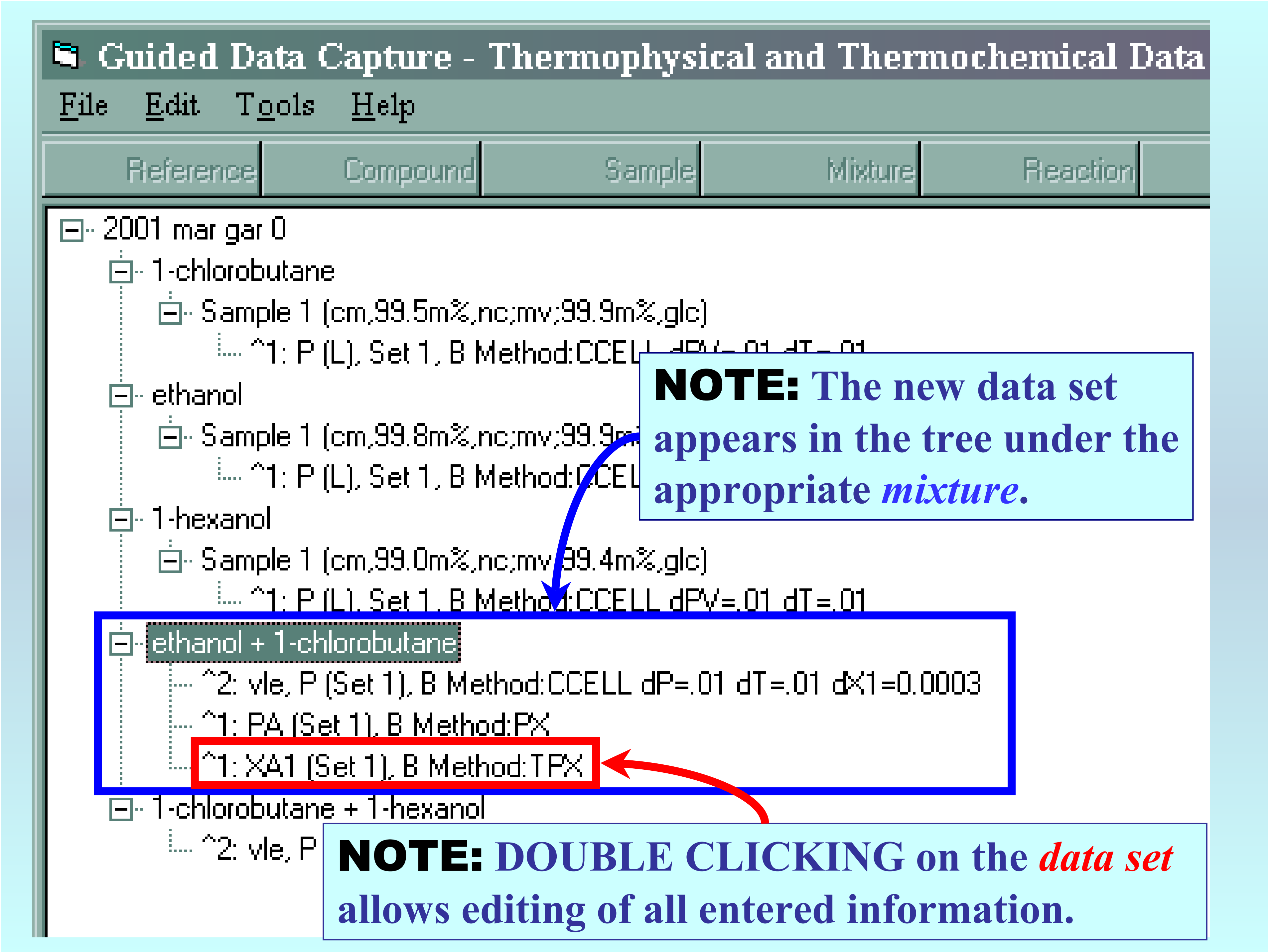
1. CLICK *View plot* to see an automatic graphical representation of the data.

2. Check for typographical errors, and CLICK *OK*, when done.



	Var 1	Property	
1	278.15	0.245	
2	283.15	0.259	
3	288.15	0.274	
4	293.15	0.288	
5	298.15	0.304	
6	303.15	0.318	
7	308.15	0.334	
8	313.15	0.349	
9	318.15	0.364	
10	323.15	0.379	

CLICK *Accept*, when checking is complete.



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;99.9m
^1: P (L), Set 1, B Method:CCEL
1-hexanol
Sample 1 (cm,99.0m%,nc;mv;99.4m%,glc)
^1: P (L), Set 1, B Method:CCELL dPV=.01 dT=.01
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: XA1 (Set 1), B Method:TPX
1-chlorobutane + 1-hexanol
^2: vle, P
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.**