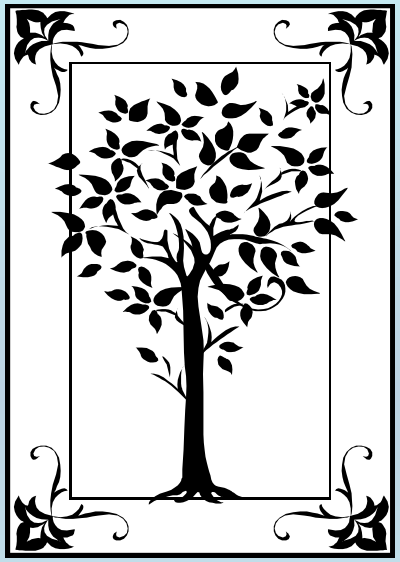
METADATA AND NUMERICAL DATA CAPTURE:
Vapor-Liquid Equilibria: *PTx*
(BUBBLE POINT *T* at constant *p*)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Vapor-Liquid Equilibria (2 components): *PTx* data (Bubble Point *T* at constant *p*)**
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 is from:

J. Chem. Eng. Data 1998, *43*, 555−557

Bubble-Temperature Measurements on *p*-Xylene with Methanol, Propan-1-ol, and Butan-1-ol at 95.1 kPa†

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Properties Group, Chemical Engineering Laboratory, Indian Institute of Chemical Technology, Hyderabad-500 007, India

Bubble temperatures at 95.1 kPa at nine liquid compositions, spaced evenly over the entire composition range, were measured for three binary systems—methanol (1) + *p*-xylene (2), propan-1-ol (1) + *p*-xylene (2), and butan-1-ol (1) + *p*-xylene (2)—using a Swietoslawski-type ebulliometer. The composition (x_1) vs temperature (T) data were found to be well-represented by the Wilson model.

PTx bubble point data for 1-butanol + *p*-xylene

Table 2. Bubble-Temperature Measurements at 95.7 kPa

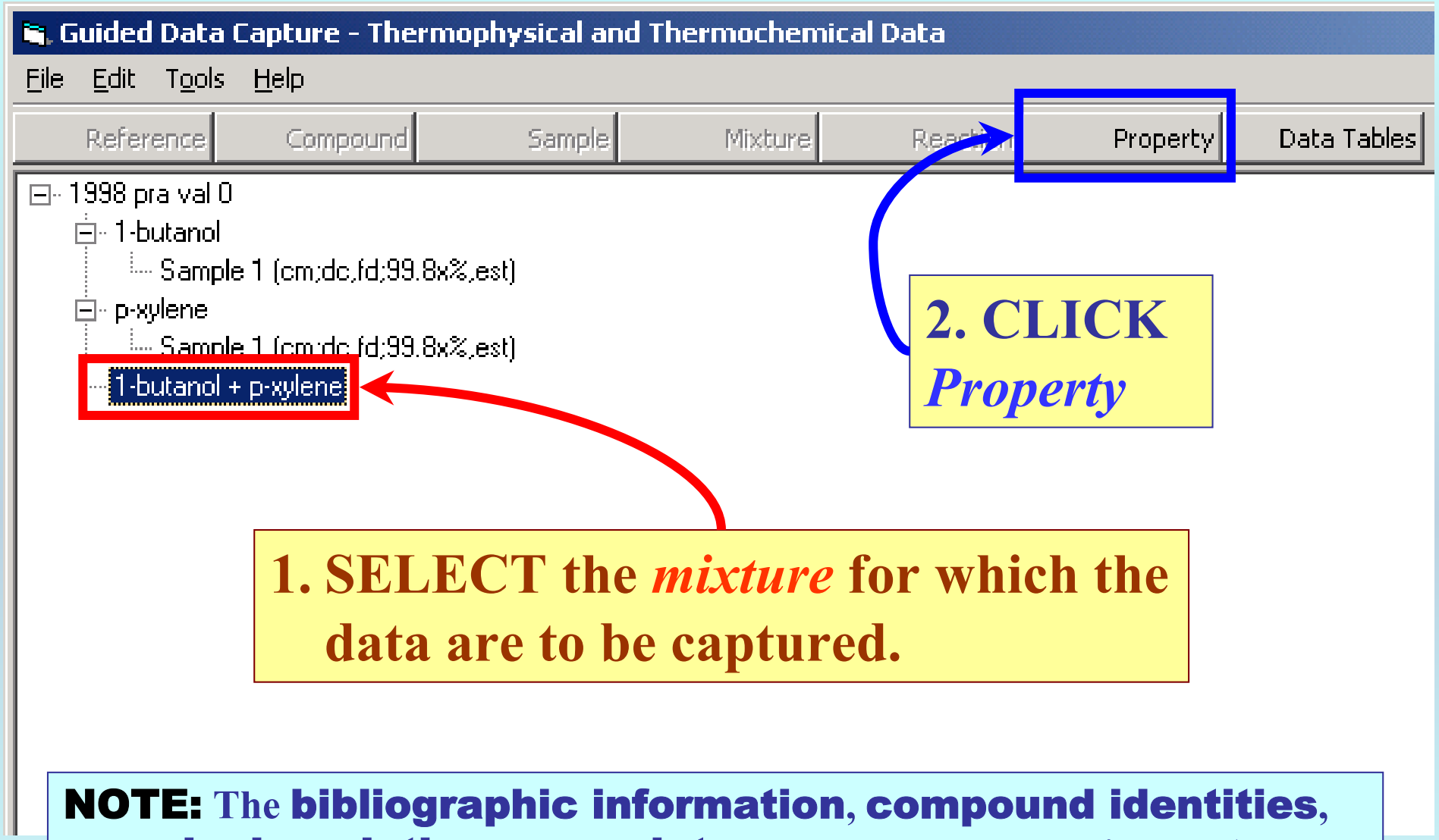
methanol (1) + *p*-xylene (2) system		propan-1-ol (1) + *p*-xylene (2) system		butan-1-ol (1) + *p*-xylene (2) system	
x_1	T/K	x_1	T/K	x_1	T/K
0.0000	409.2	0.0000	409.2	0.0000	409.2
0.1235	346.5	0.0996	380.5	0.1019	396.1
0.2228	340.8	0.1997	374.5	0.2010	391.0
0.3111	338.4	0.2969	372.4	0.2988	388.5
0.4237	337.7	0.3990	371.1	0.3898	387.2
0.5008	337.3	0.4969	370.2	0.5033	386.2
0.5889	337.0	0.5949	369.5	0.6059	385.8
0.6920	336.8	0.6954	368.9	0.7002	385.6
0.8052	336.5	0.7965	368.5	0.8030	385.7
0.8965	336.2	0.9018	368.3	0.9006	386.5
1.0000	336.4	1.0000	368.8	1.0000	389.2

This data set is considered here.

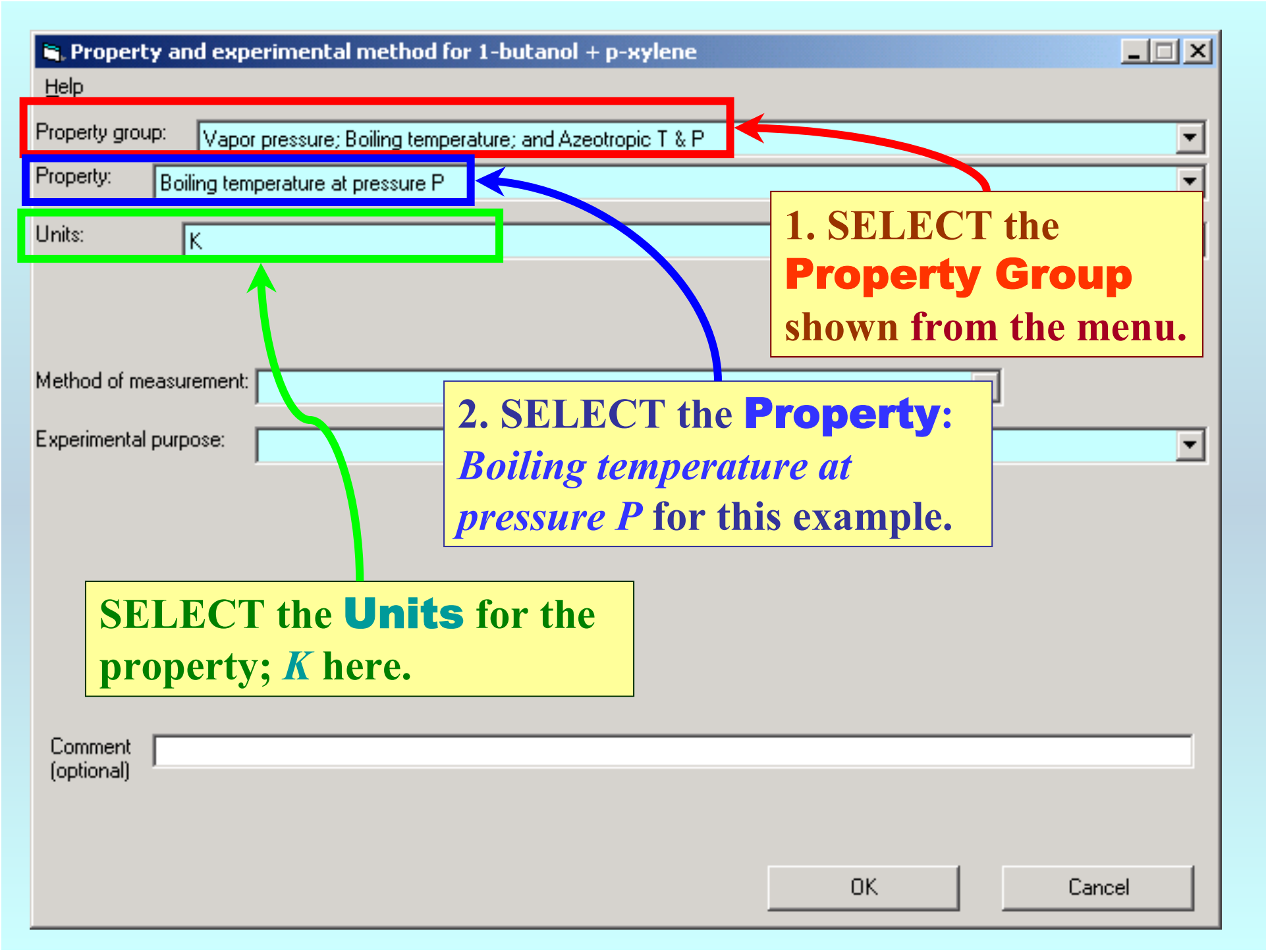
Experimental Method & Precision/Accuracy Information:

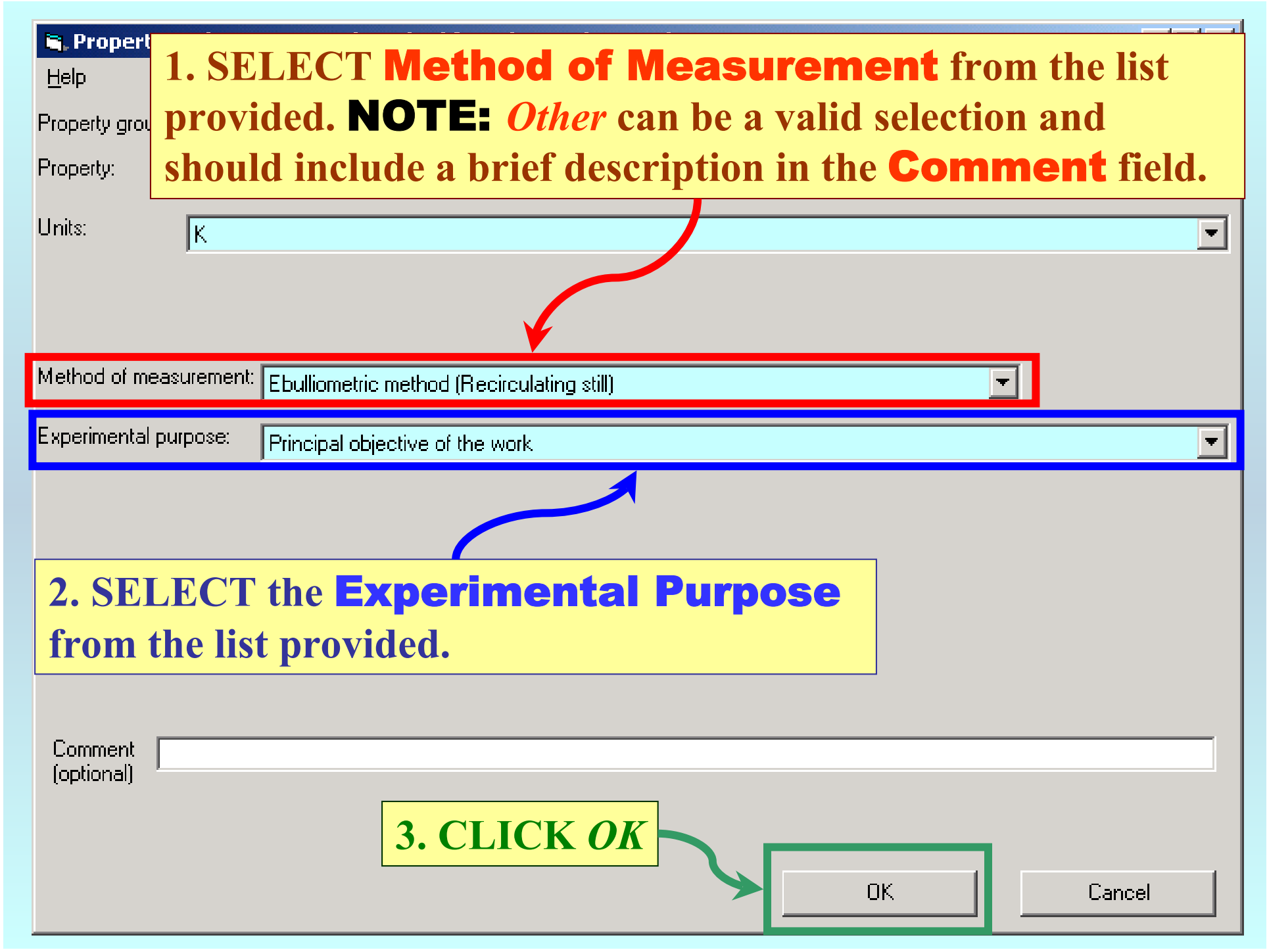
A Swietoslowski-type ebullimeter, very similar to the one described by Hala et al. (1958), was used for the experiments.

The total pressure in the present set of experiments was maintained to within ±0.1 kPa, by frequently reading the mercury manometer and carrying out the required corrective adjustment. A mercury-in-glass thermometer, calibrated by means of point-to-point comparison with a platinum resistance thermometer certified by the National Institute of Standards and Technology, Boulder, CO, was used for the measurement of temperature to an accuracy of ±0.1 K.



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

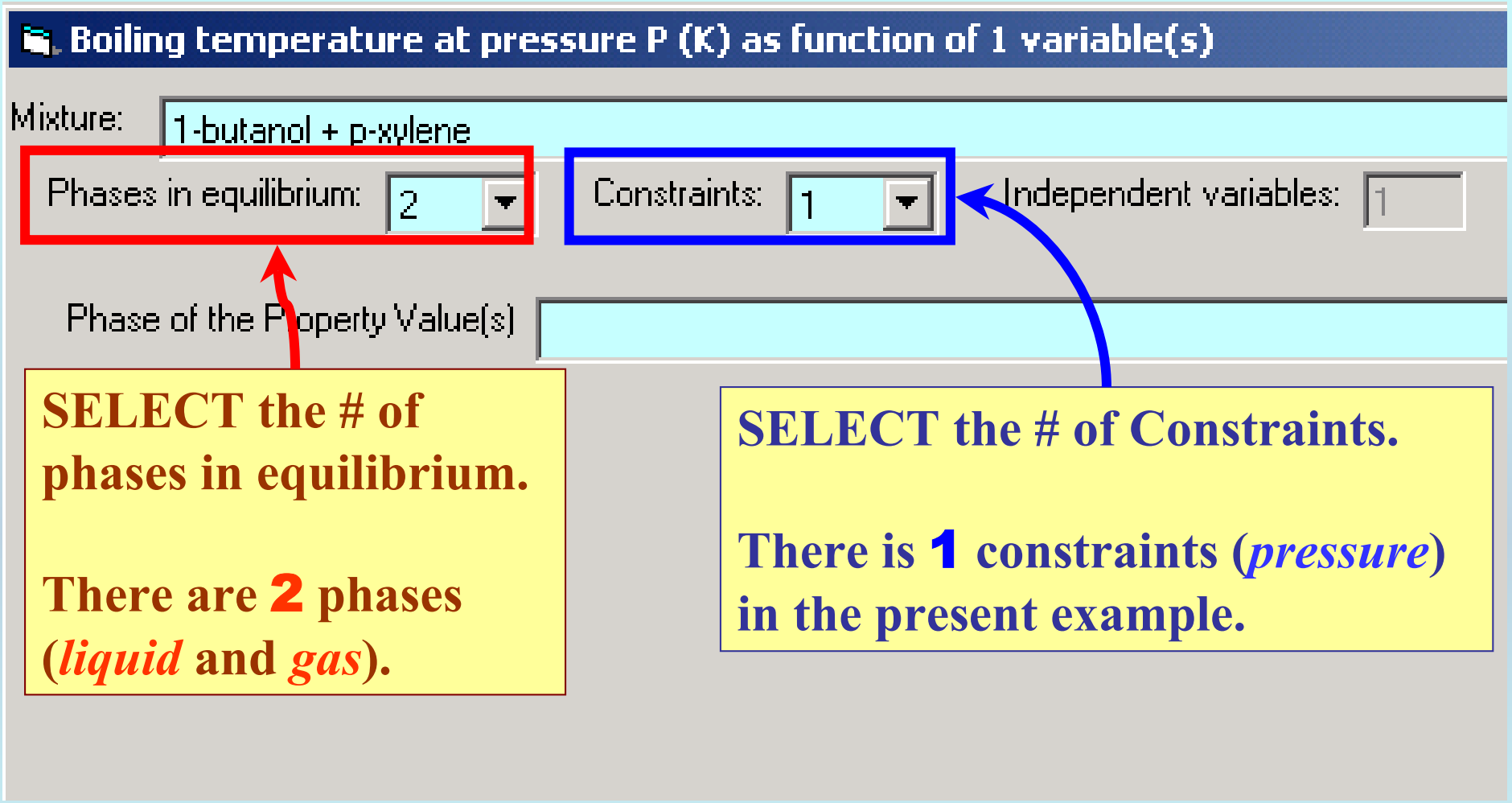

Property and experimental method for 1-butanol + p-xylene
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Boiling temperature at pressure P
Units:
K
1. SELECT the Property Group shown from the menu.
Method of measurement:
Experimental purpose:
2. SELECT the Property: Boiling temperature at pressure P for this example.
SELECT the Units for the property; K here.
Comment (optional)
OK
Cancel

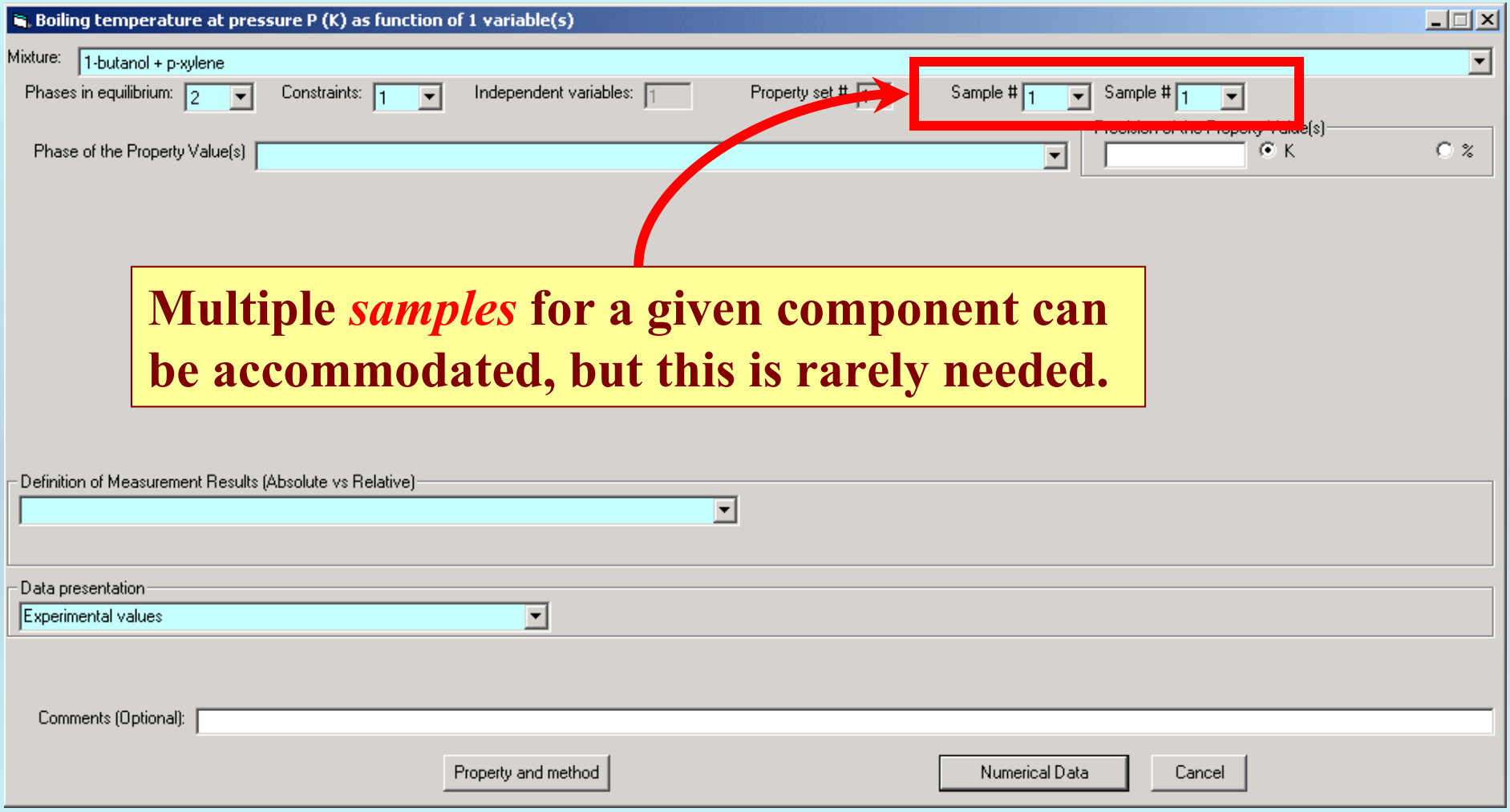


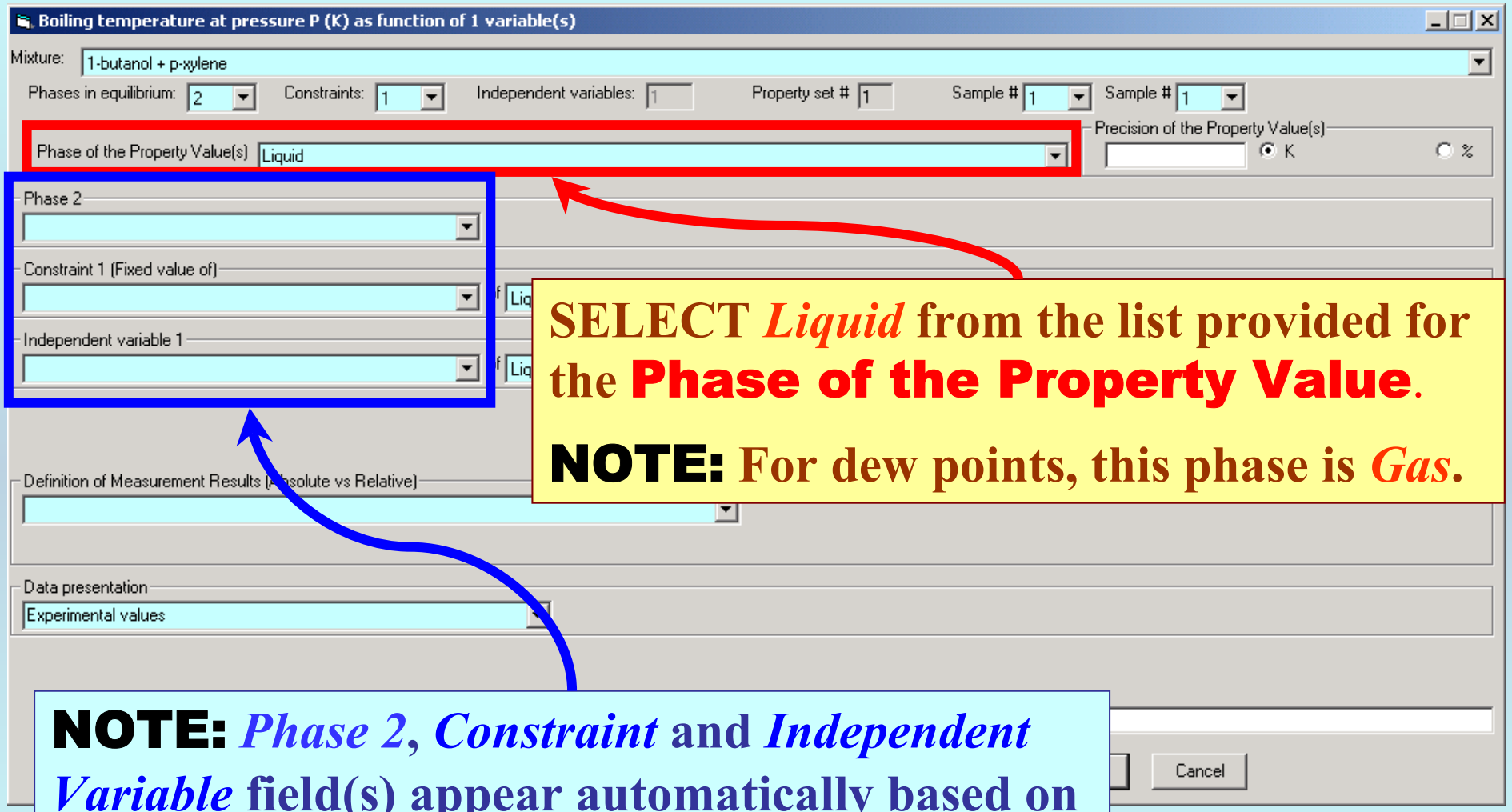
1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

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

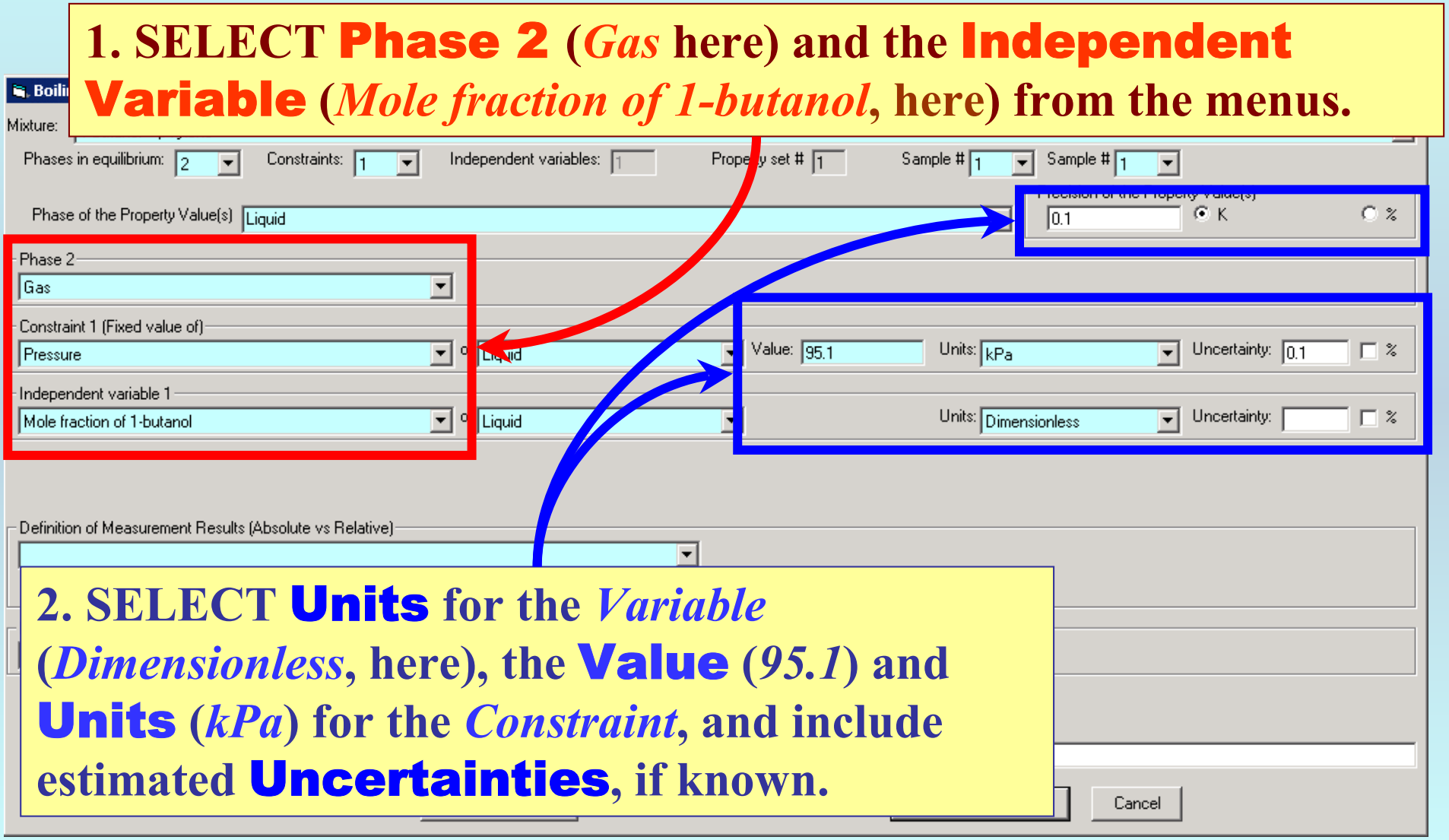
3. CLICK *OK*


Boiling temperature at pressure P (K) as function of 1 variable(s)
Mixture:
1-butanol + p-xylene
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Phase of the Property Value(s)
SELECT the # of phases in equilibrium.
There are 2 phases (liquid and gas).
SELECT the # of Constraints.
There is 1 constraints (pressure) in the present example.

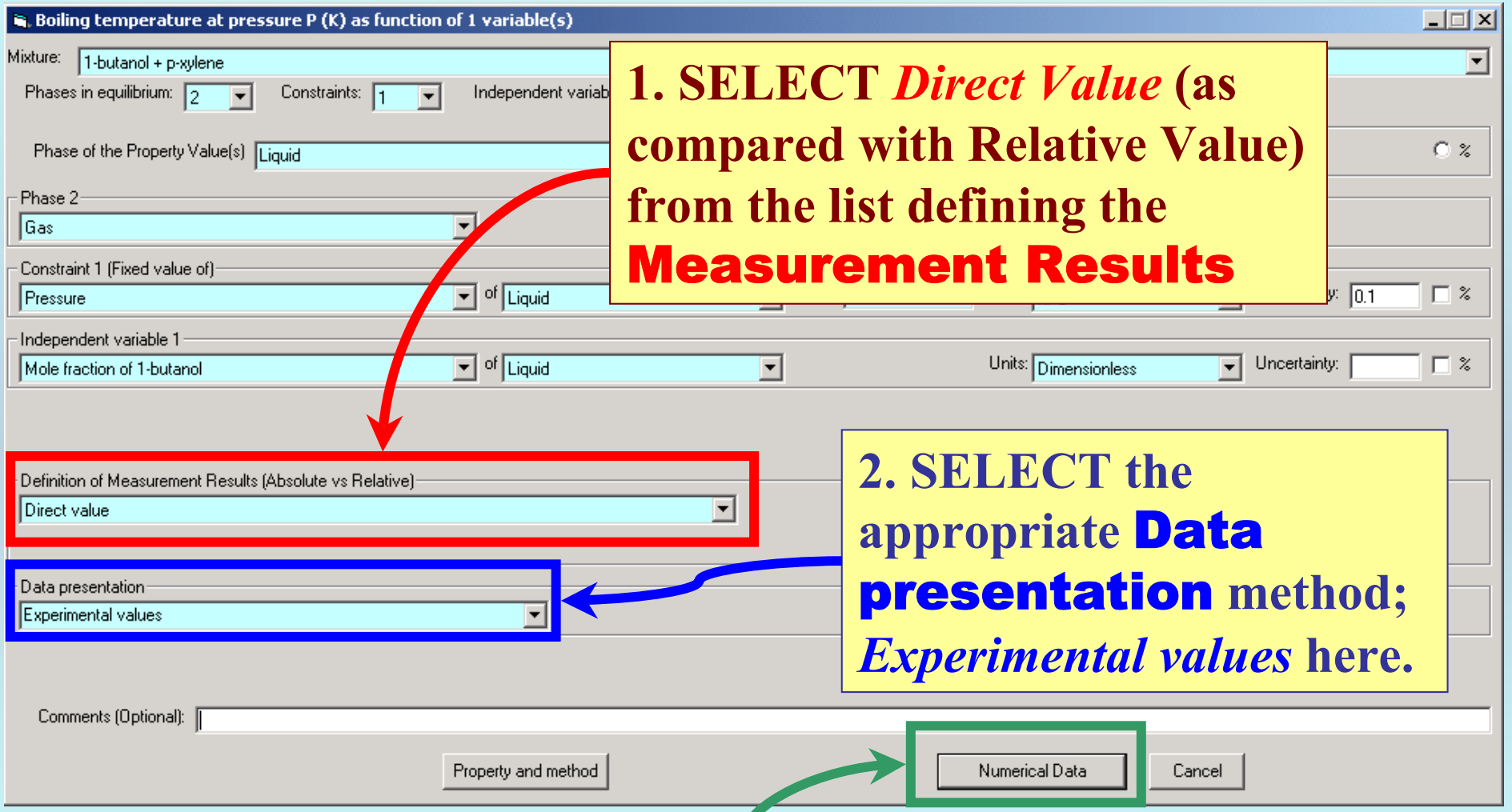

Boiling temperature at pressure P (K) as function of 1 variable(s)
Mixture:
1-butanol + p-xylene
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
K
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel

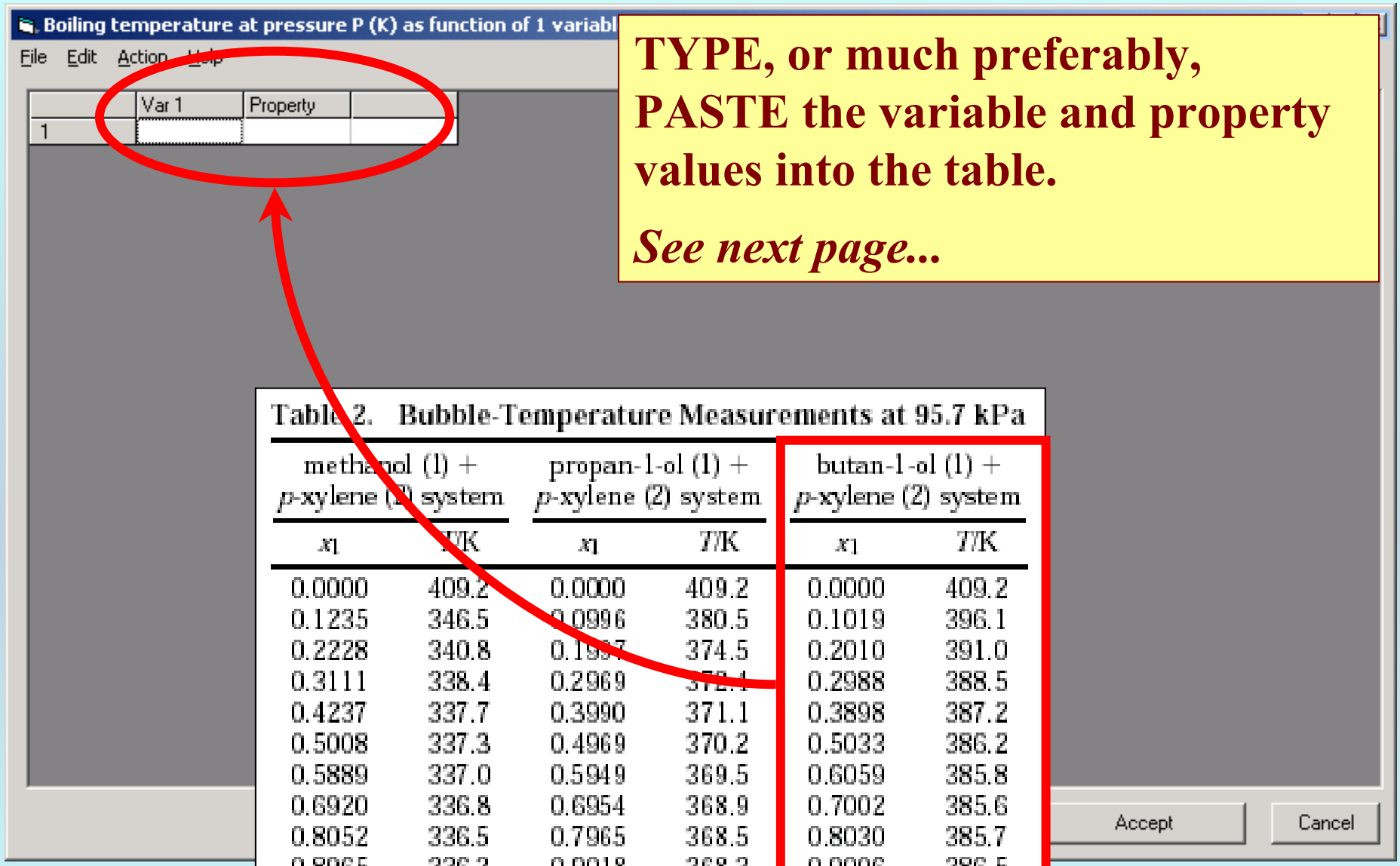

Boiling temperature at pressure P (K) as function of 1 variable(s)
Mixture:
1-butanol + p-xylene
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
K
%
Phase 2
Constraint 1 (Fixed value of)
Independent variable 1
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Cancel
SELECT Liquid from the list provided for the Phase of the Property Value.
NOTE: For dew points, this phase is Gas.
NOTE: Phase 2, Constraint and Independent Variable field(s) appear automatically based on the Gibbs Phase Rule.

Specification of 2nd phase, constraint and independent variable



Measurement definition and Data presentation





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

See next page...

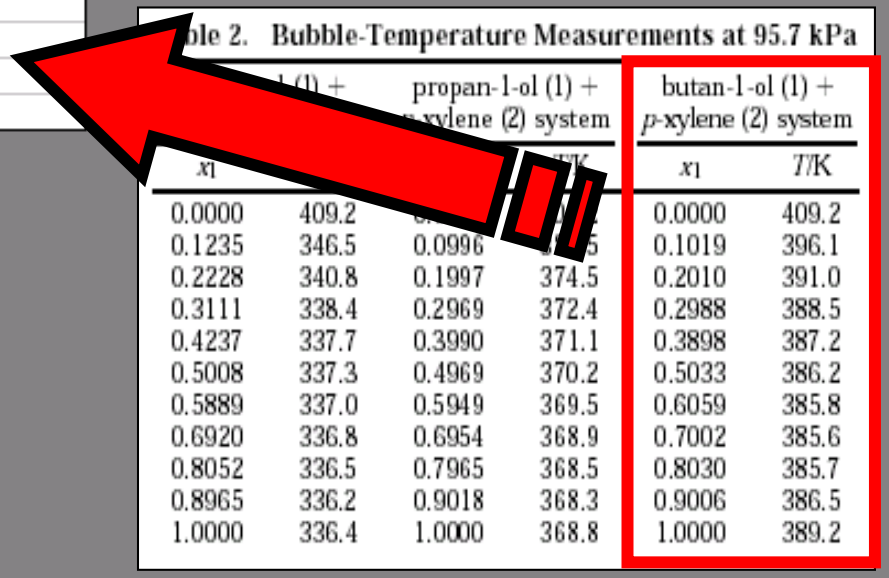
Table 2. Bubble-Temperature Measurements at 95.7 kPa

methanol (1) + *p*-xylene (2) system		propan-1-ol (1) + *p*-xylene (2) system		butan-1-ol (1) + *p*-xylene (2) system	
x_1	T/K	x_1	T/K	x_1	T/K
0.0000	409.2	0.0000	409.2	0.0000	409.2
0.1235	346.5	0.0996	380.5	0.1019	396.1
0.2228	340.8	0.1997	374.5	0.2010	391.0
0.3111	338.4	0.2969	372.4	0.2988	388.5
0.4237	337.7	0.3990	371.1	0.3898	387.2
0.5008	337.3	0.4969	370.2	0.5033	386.2
0.5889	337.0	0.5949	369.5	0.6059	385.8
0.6920	336.8	0.6954	368.9	0.7002	385.6
0.8052	336.5	0.7965	368.5	0.8030	385.7
0.8965	336.2	0.9018	368.3	0.9006	386.5
1.0000	336.4	1.0000	368.8	1.0000	389.2

Boiling temperature at pressure P (K) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	0.0000	409.2
2	0.1019	396.1
3	0.2010	391.0
4	0.2988	388.5
5	0.3898	387.2
6	0.5033	386.2
7	0.6059	385.8
8	0.7002	385.6
9	0.8030	385.7
10	0.9006	386.5
11	1.0000	389.2



ble 2. Bubble-Temperature Measurements at 95.7 kPa

		propan-1-ol (1) + xylene (2) system		butan-1-ol (1) + *p*-xylene (2) system	
x_1			T/K	x_1	T/K
0.0000	409.2			0.0000	409.2
0.1235	346.5	0.0996	5	0.1019	396.1
0.2228	340.8	0.1997	374.5	0.2010	391.0
0.3111	338.4	0.2969	372.4	0.2988	388.5
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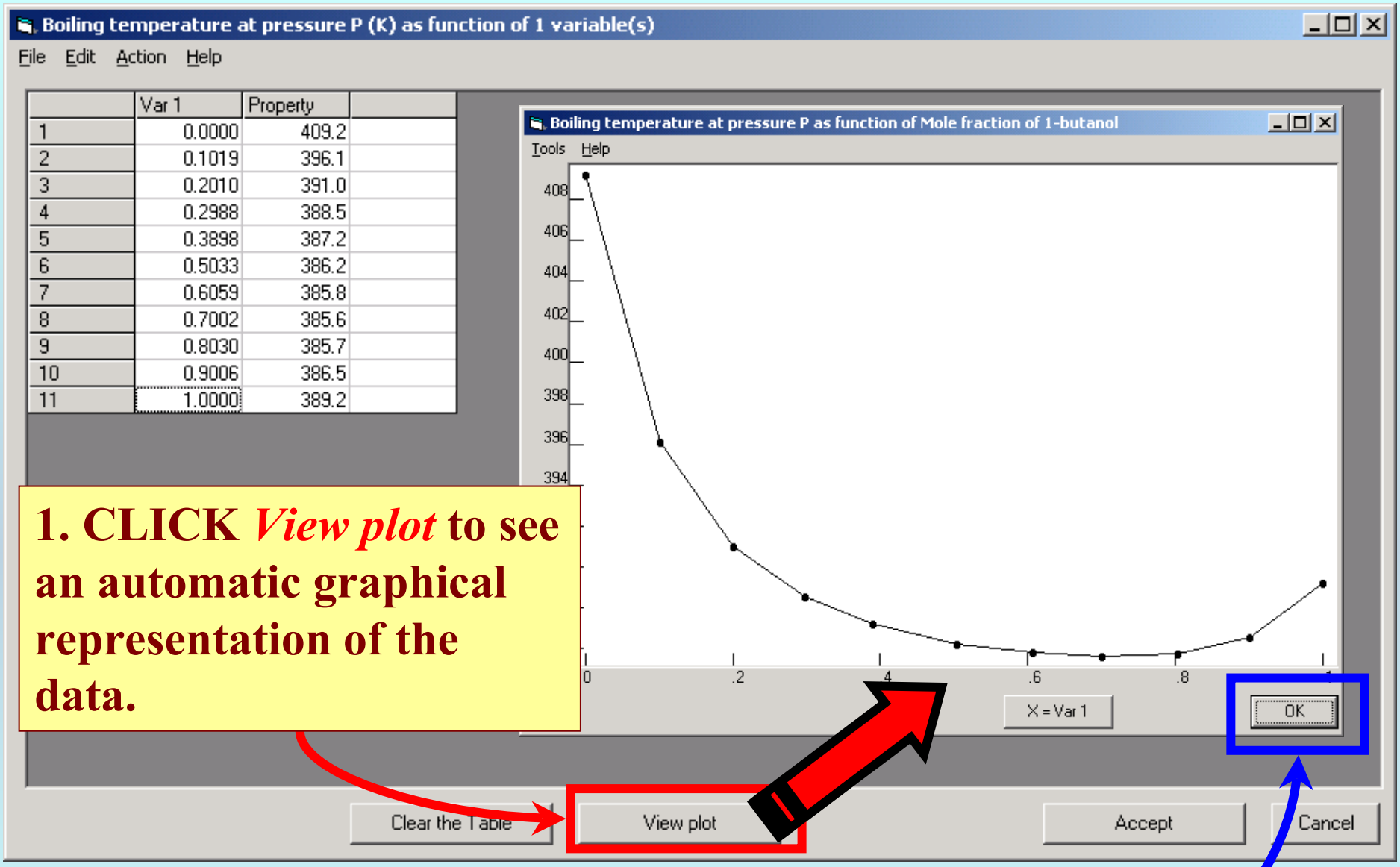
0.8965	336.2	0.9018	368.3	0.9006	386.5
1.0000	336.4	1.0000	368.8	1.0000	389.2

Clear the Table | View plot | Accept | Cancel

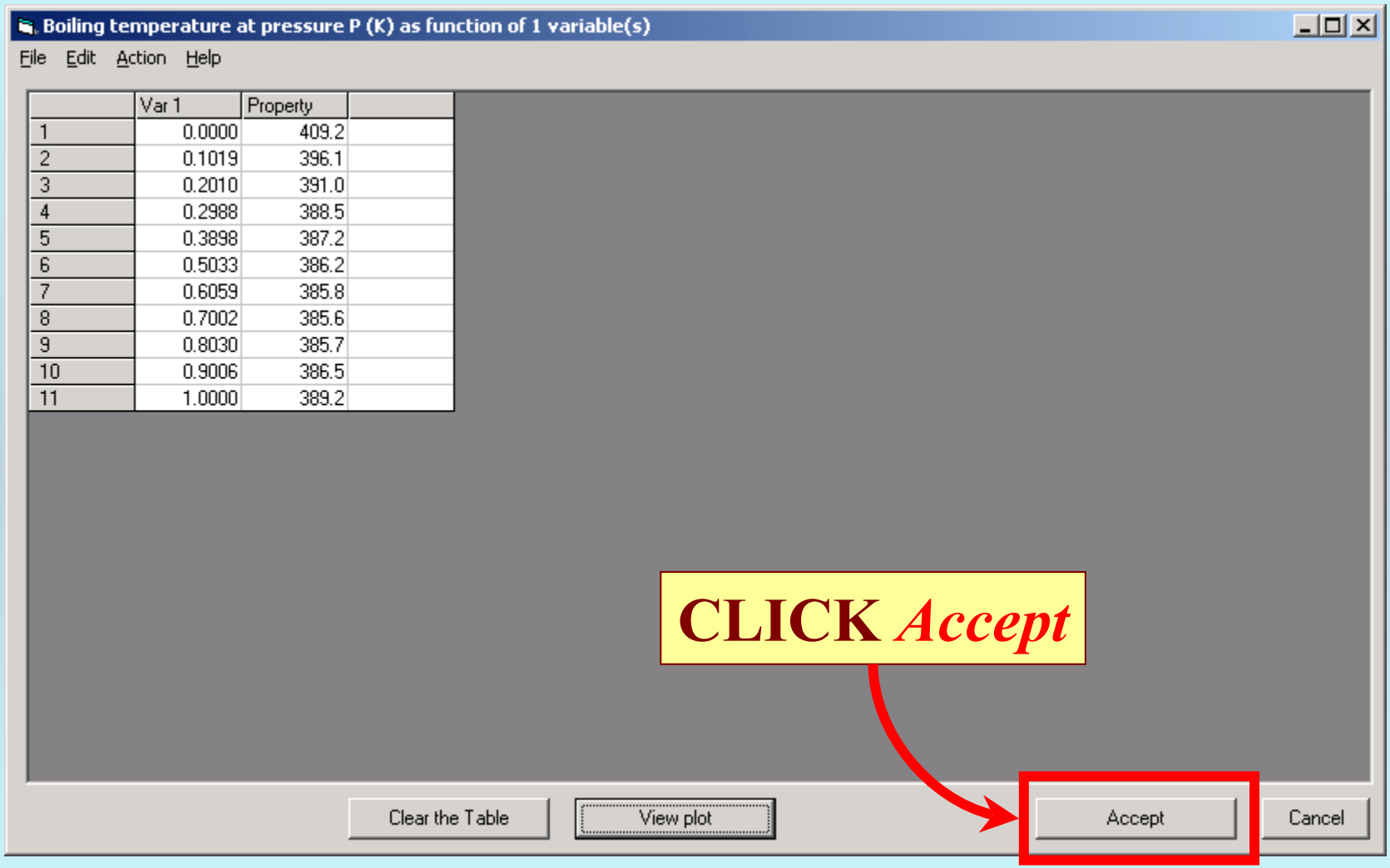
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software; e.g., EXCEL.)

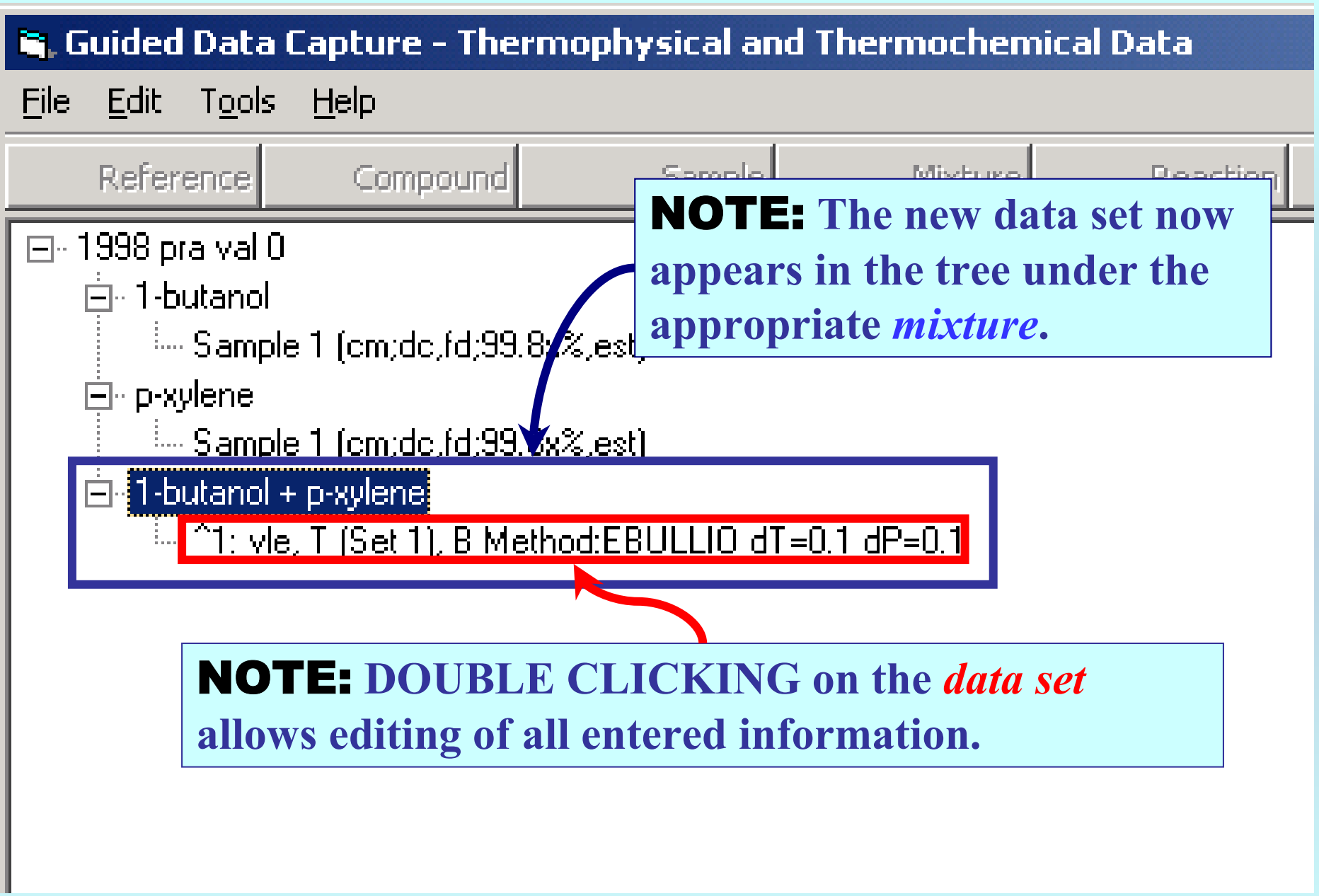


1. CLICK *View plot* to see an automatic graphical representation of the data.

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

You are returned to the previous screen...




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
1998 pra val 0
1-butanol
Sample 1 (cm;dc,fd;99.8x%,est)
p-xylene
Sample 1 (cm;dc,fd;99.8x%,est)
1-butanol + p-xylene
^1: vle, T (Set 1), B Method:EBULLIO dT=0.1 dP=0.1
NOTE: The new data set now 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.**