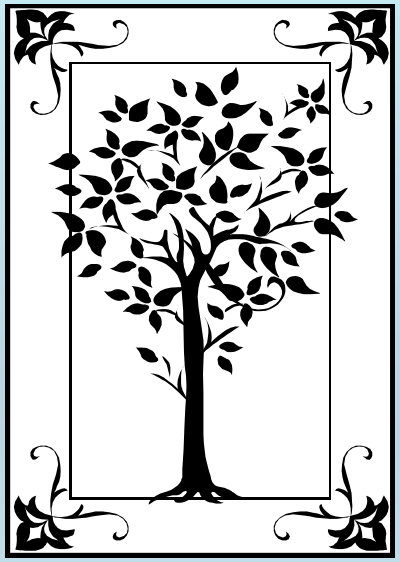
METADATA AND NUMERICAL DATA CAPTURE:
Vapor-Liquid Equilibria: *PTx*
(2 component mixture)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Vapor-Liquid Equilibria (2 components):**
***PTx* data**
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 2001, *46,* 1487−1489

Vapor−Liquid Equilibria and Excess Enthalpy Data for the Binary System Propionic Aldehyde + 2-Methyl-2-butanol at 333.15 K

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Isothermal vapor−liquid equilibrium (VLE) and excess enthalpy (H^E) data are reported for the system propionic aldehyde + 2-methyl-2-butanol at 333.15 K. The data were measured by means of a computer-operated static apparatus and isothermal flow calorimetry, respectively. The experimental data were correlated simultaneously by using linear temperature-dependent UNIQUAC parameters.

PTx data for **(propionic aldehyde + 2-methyl-2butanol)** at $T = 333.15$ K

Table 1. Vapor−Liquid Equilibrium Data for the System Propionic Aldehyde (1) + 2-Methyl-2-butanol (2) at 333.15 K

x_1	P/kPa	x_1	P/kPa	x_1	P/kPa
0.0000	16.87	0.3814	79.17	0.9014	138.73
0.0038	17.75	0.4315	85.29	0.9242	141.46
0.0078	18.62	0.4805	91.14	0.9434	143.81
0.0147	20.11	0.5276	96.62	0.9591	145.73
0.0211	21.49	0.5564	99.72	0.9714	147.27
0.0274	22.83	0.5722	101.71	0.9808	148.47
0.0429	26.11	0.5984	104.46	0.9870	149.24
0.0623	29.99	0.6134	106.38	0.9911	149.78
0.0873	34.72	0.6408	109.21	0.9939	150.14
0.1165	40.07	0.6835	113.96	0.9958	150.40
0.1506	45.91	0.7254	118.62	0.9977	150.65
0.1893	52.15	0.7658	123.14	0.9992	150.89
0.2315	58.60	0.8041	127.46	1.0000	150.93
0.2803	65.67	0.8400	131.56		
0.3308	72.56	0.8724	135.32		

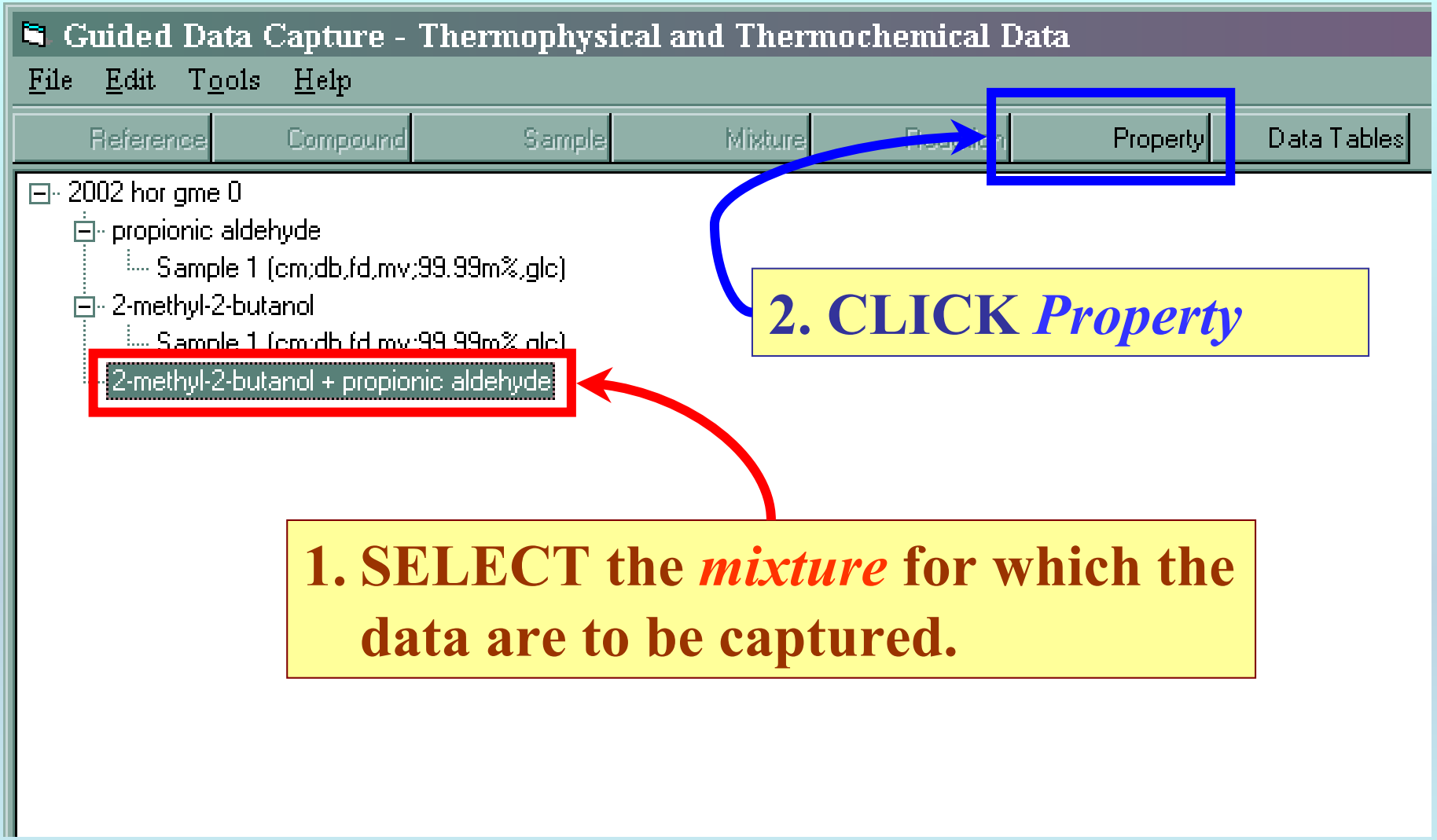
This data set is considered here.

Experimental Method:

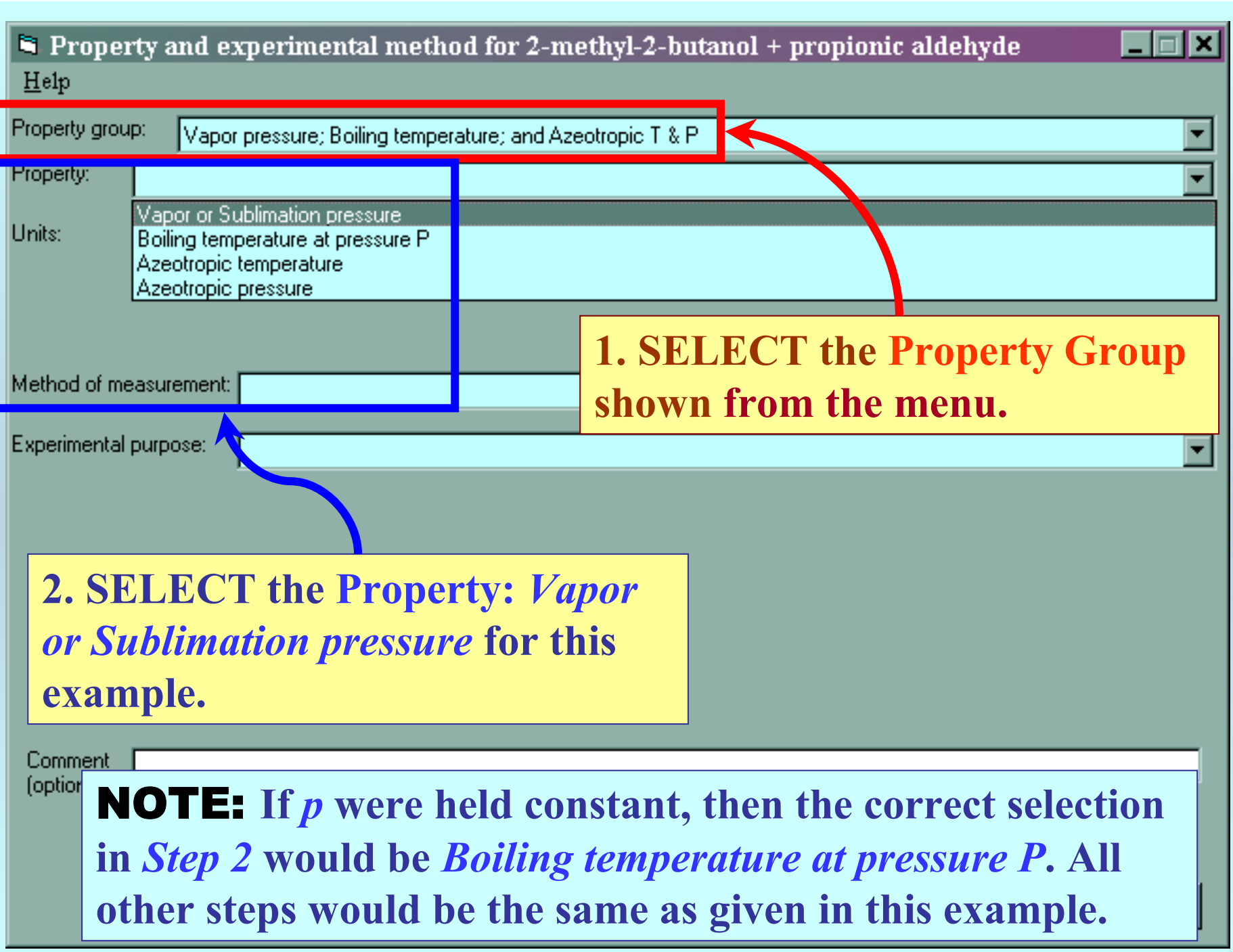
Apparatus and Procedures. The isothermal $P-x$ data were measured with a computer-driven static apparatus.

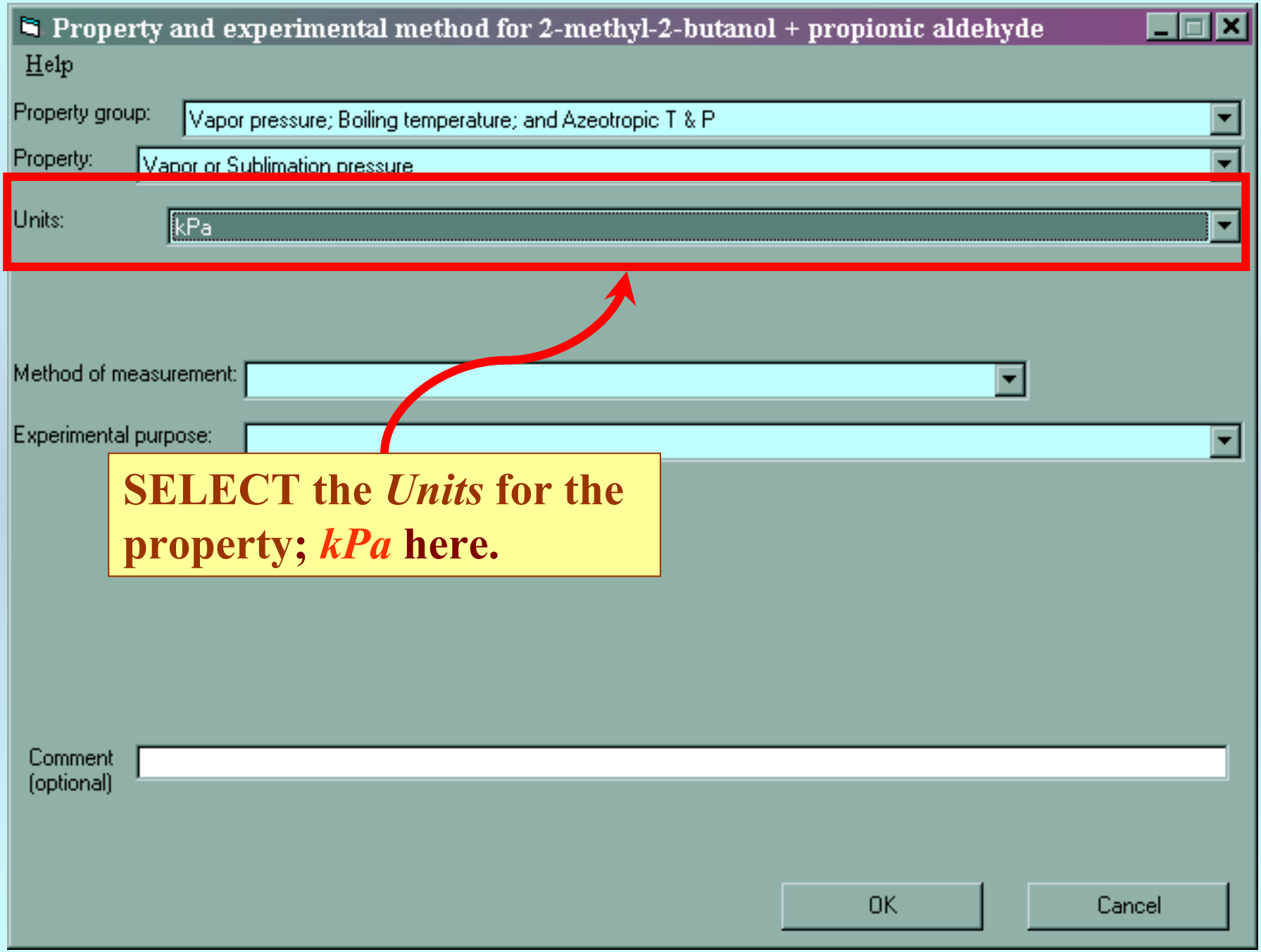
Precision Information:

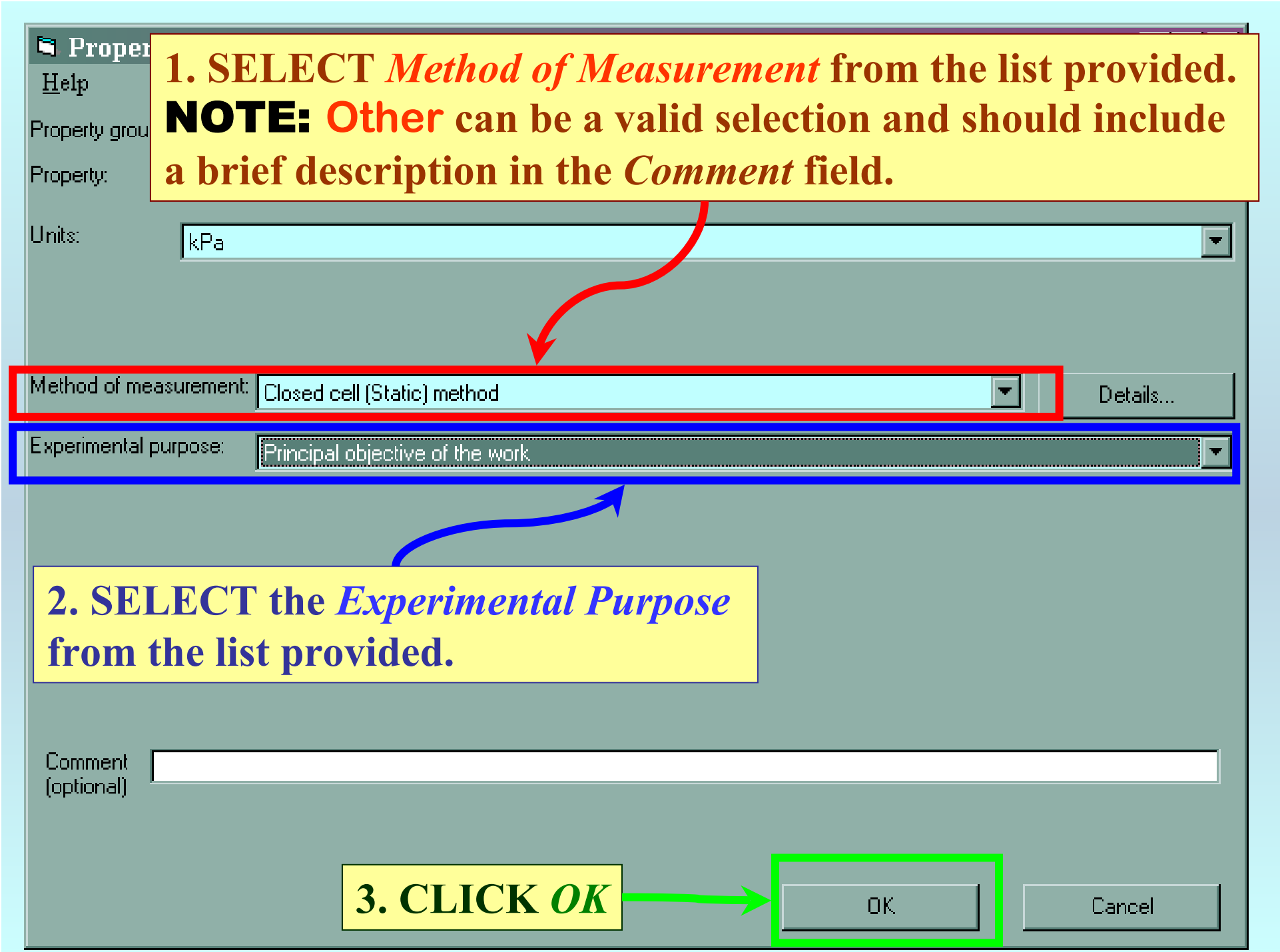
At low system pressure as in this investigation, the calculated liquid phase compositions are identical to the feed compositions within ±0.002. The experimental uncertainties of this apparatus are as follows: $\sigma(T) = 0.03$ K, $\sigma(P) = 20$ Pa + 0.0001 (P/Pa), $\sigma(x_i) = 0.0001$.

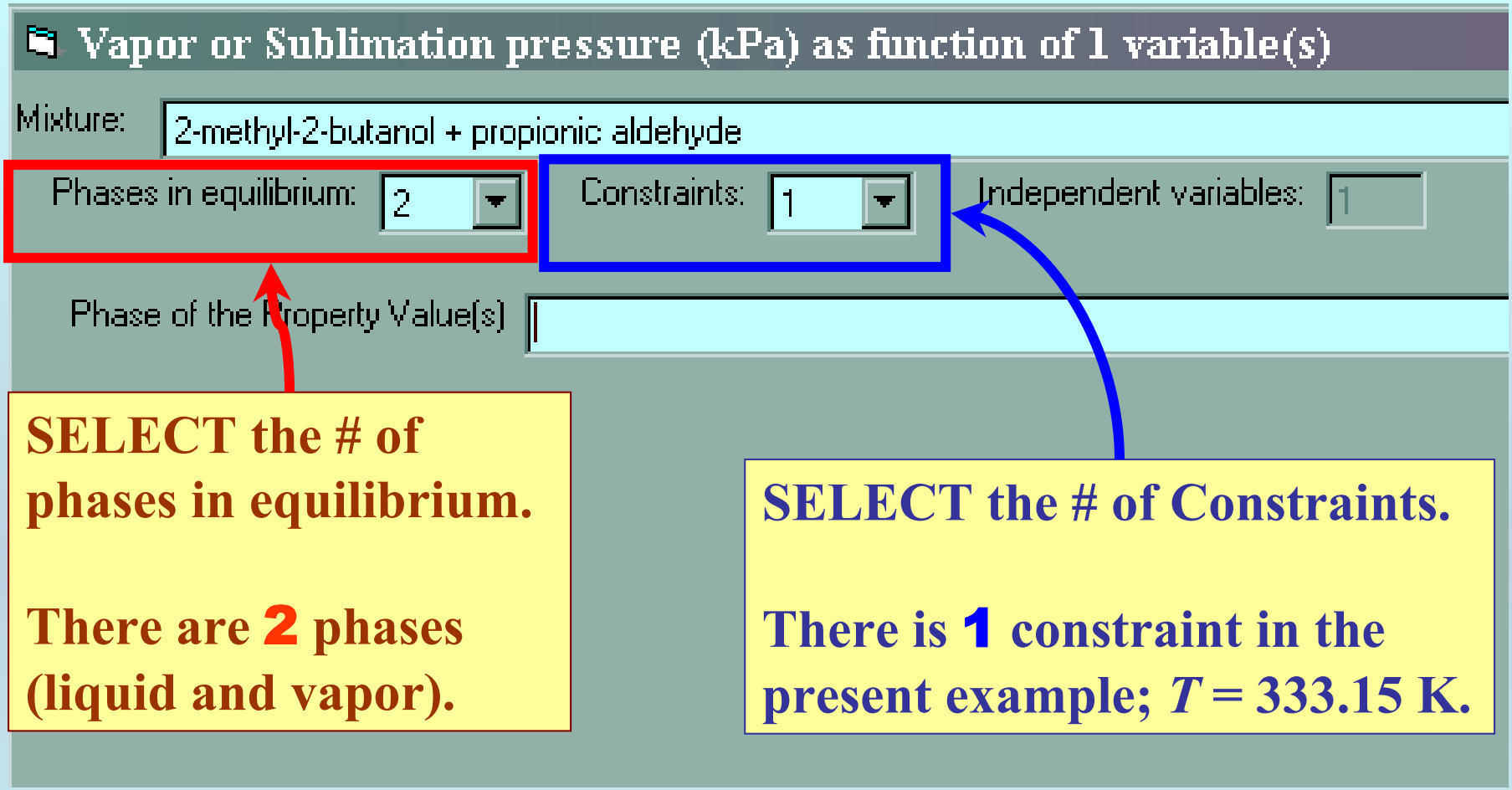


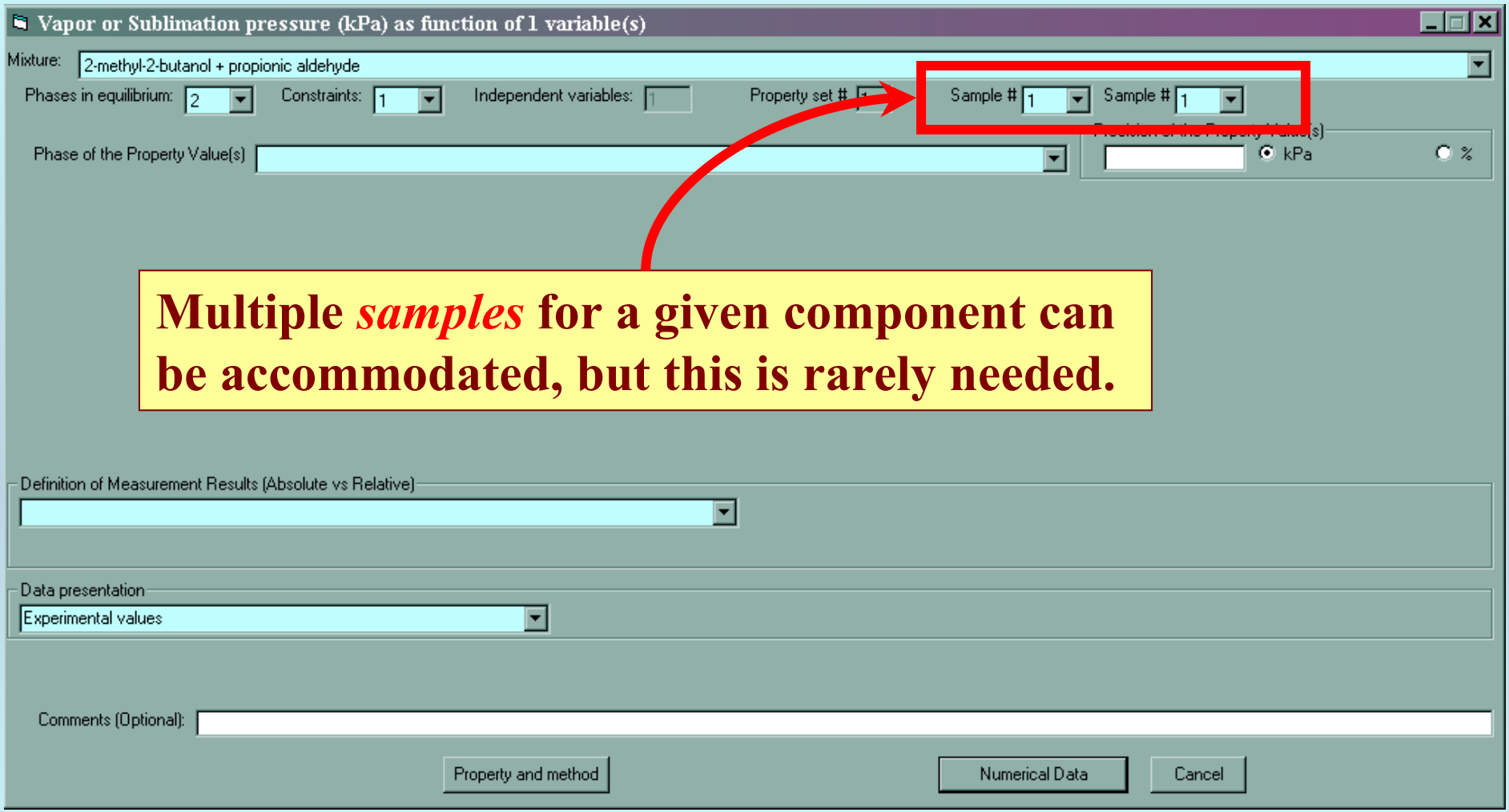
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials related to capture of this information, if needed.)

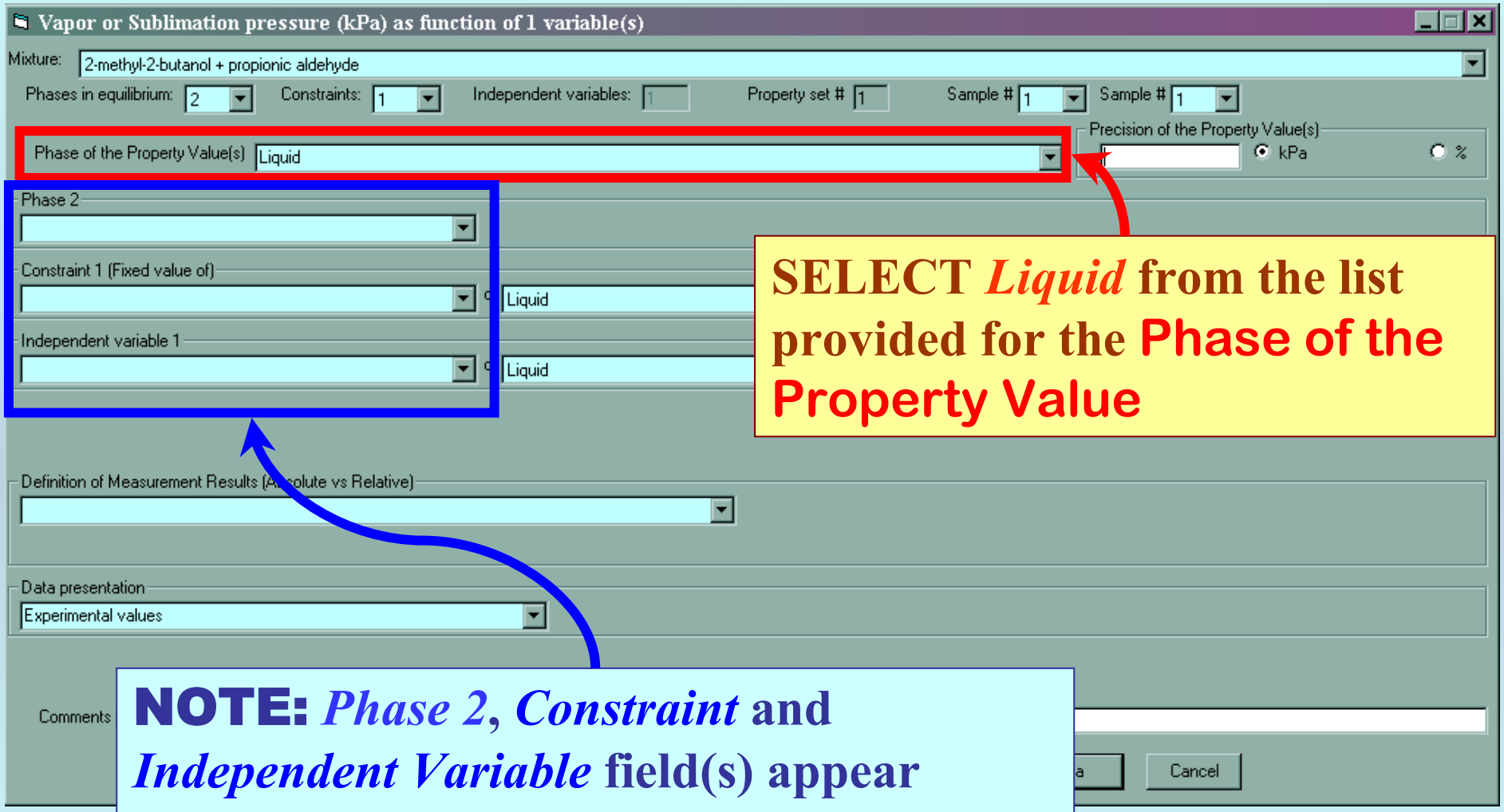

Property and experimental method for 2-methyl-2-butanol + propionic aldehyde
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Units:
Vapor or Sublimation pressure
Boiling temperature at pressure P
Azeotropic temperature
Azeotropic pressure
Method of measurement:
Experimental purpose:
1. SELECT the Property Group shown from the menu.
2. SELECT the Property: Vapor or Sublimation pressure for this example.
Comment
NOTE: If p were held constant, then the correct selection in Step 2 would be Boiling temperature at pressure P. All other steps would be the same as given in this example.


Property and experimental method for 2-methyl-2-butanol + propionic aldehyde
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Vapor or Sublimation pressure
Units:
kPa
Method of measurement:
Experimental purpose:
SELECT the Units for the property; kPa here.
Comment (optional)
OK
Cancel


Help
Property grou
Property:
Units:
kPa
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.
Method of measurement:
Closed cell (Static) method
Details...
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK OK
OK
Cancel

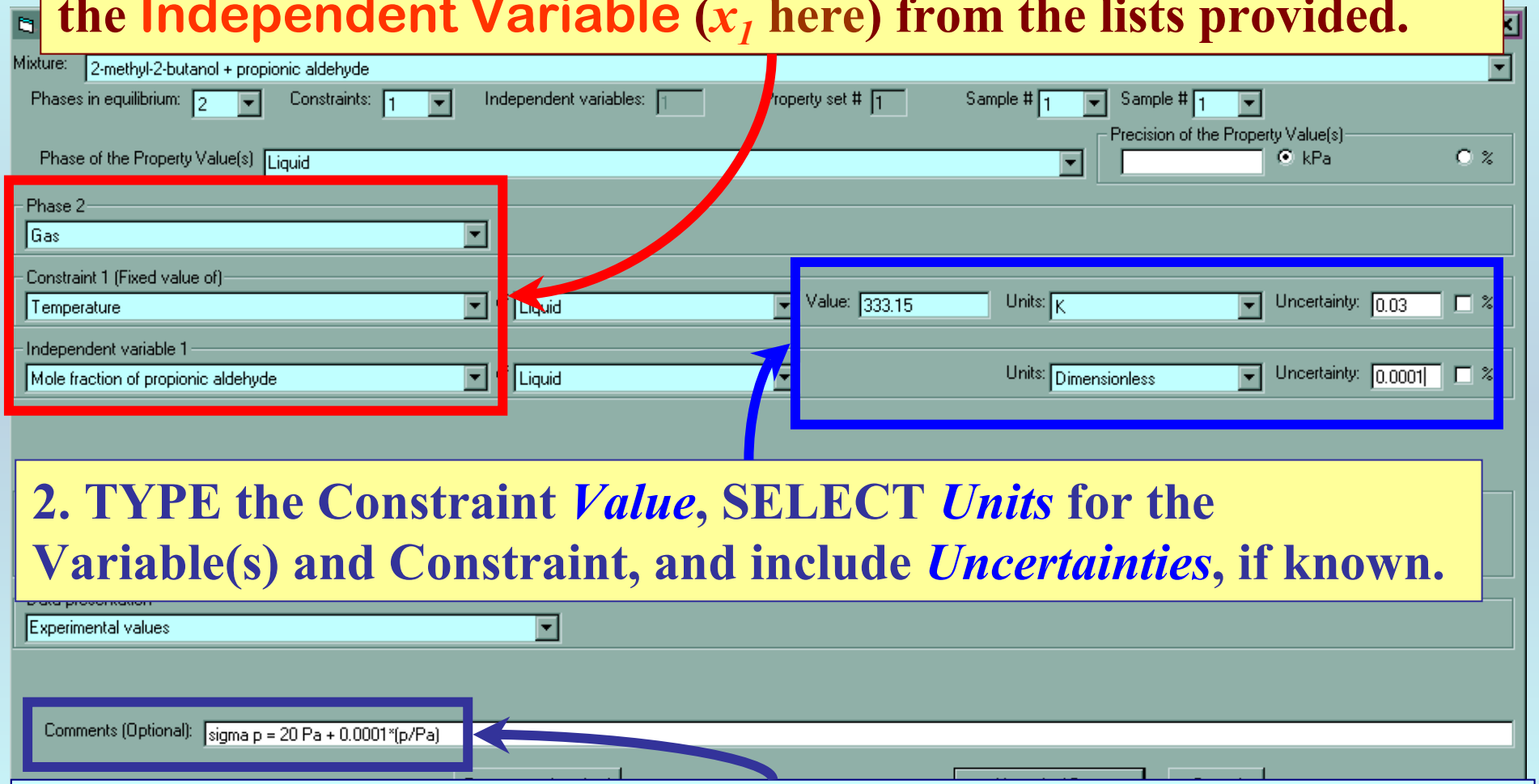

Vapor or Sublimation pressure (kPa) as function of 1 variable(s)
Mixture:
2-methyl-2-butanol + propionic aldehyde
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Phase of the Property Value(s)
SELECT the # of phases in equilibrium.
There are 2 phases (liquid and vapor).
SELECT the # of Constraints.
There is 1 constraint in the present example; T = 333.15 K.


Vapor or Sublimation pressure (kPa) as function of 1 variable(s)
Mixture:
2-methyl-2-butanol + propionic aldehyde
Phases in equilibrium:
2
Constraints:
1
Independent variables:
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
kPa
%
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


Vapor or Sublimation pressure (kPa) as function of 1 variable(s)
Mixture:
2-methyl-2-butanol + propionic aldehyde
Phases in equilibrium:
2
Constraints:
1
Independent variables:
Property set #
Sample #
Sample #
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
kPa
%
Phase 2
Constraint 1 (Fixed value of)
Liquid
Independent variable 1
Liquid
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments
Cancel
SELECT Liquid from the list provided for the Phase of the Property Value
NOTE: Phase 2, Constraint and Independent Variable field(s) appear automatically based on the Gibbs Phase Rule.

Specification of 2nd phase, constraint(s), and independent variable(s)

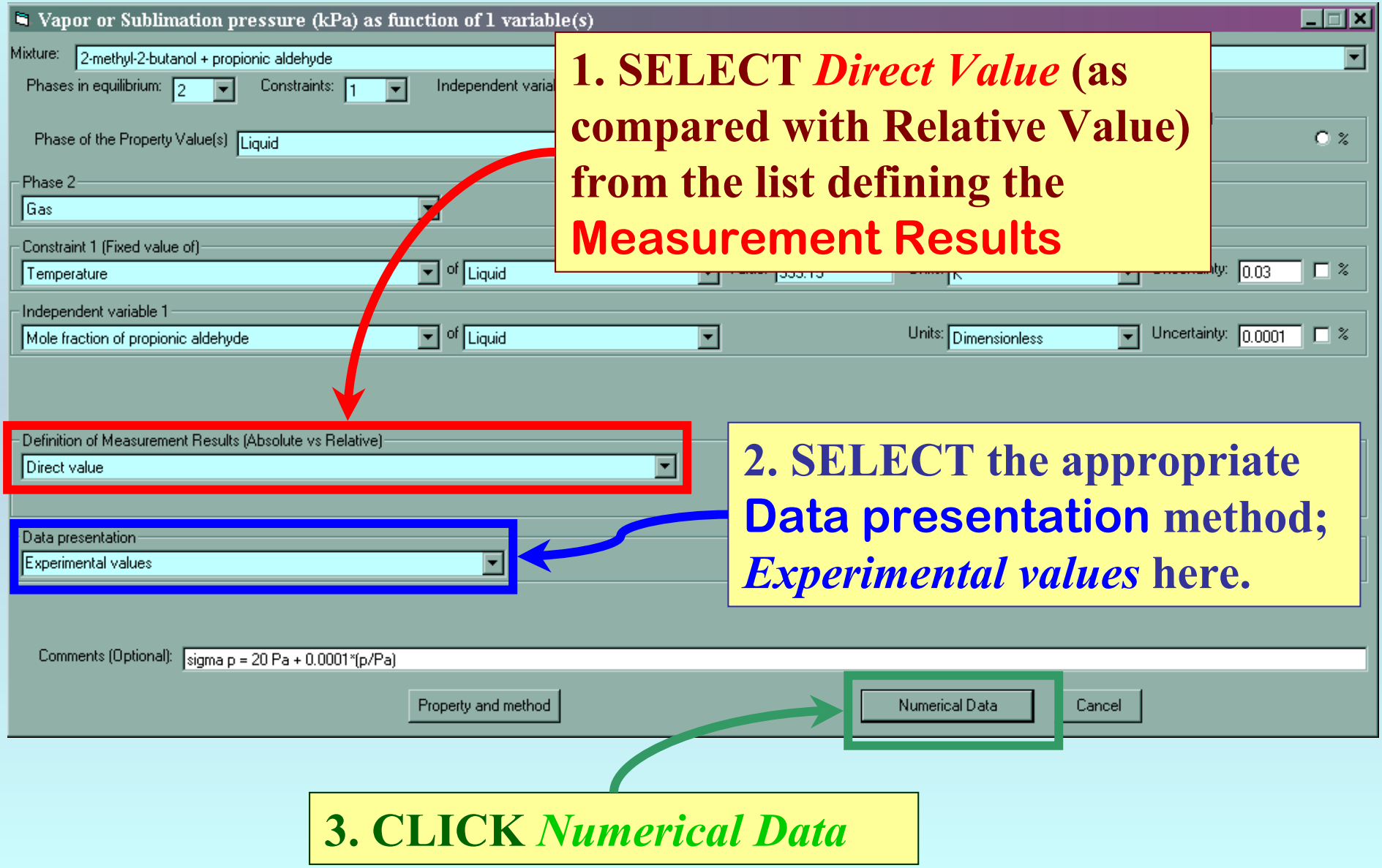
1. SELECT the 2nd Phase (*Gas* here) Constraint (*T* here) and the Independent Variable (x_1 here) from the lists provided.

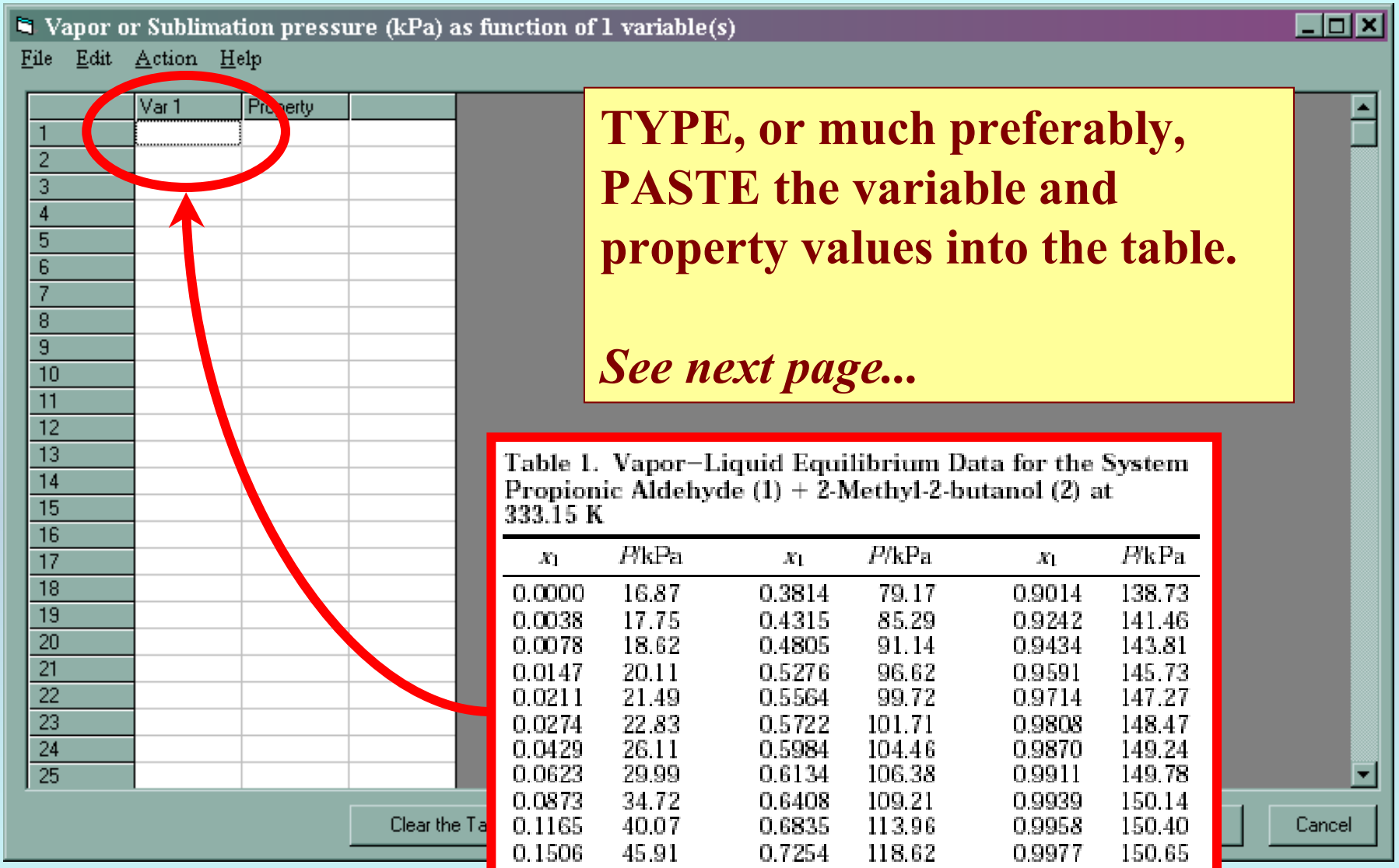


2. TYPE the Constraint *Value*, SELECT *Units* for the Variable(s) and Constraint, and include *Uncertainties*, if known.

NOTE: If a precision cannot be expressed in terms of a constant or percentage (as in this example), it can be included as a *Comment*.

Measurement definition and Data presentation





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

See next page...

Table 1. Vapor−Liquid Equilibrium Data for the System Propionic Aldehyde (1) + 2-Methyl-2-butanol (2) at 333.15 K

x_1	P/kPa	x_1	P/kPa	x_1	P/kPa
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0.0078	18.62	0.4805	91.14	0.9434	143.81
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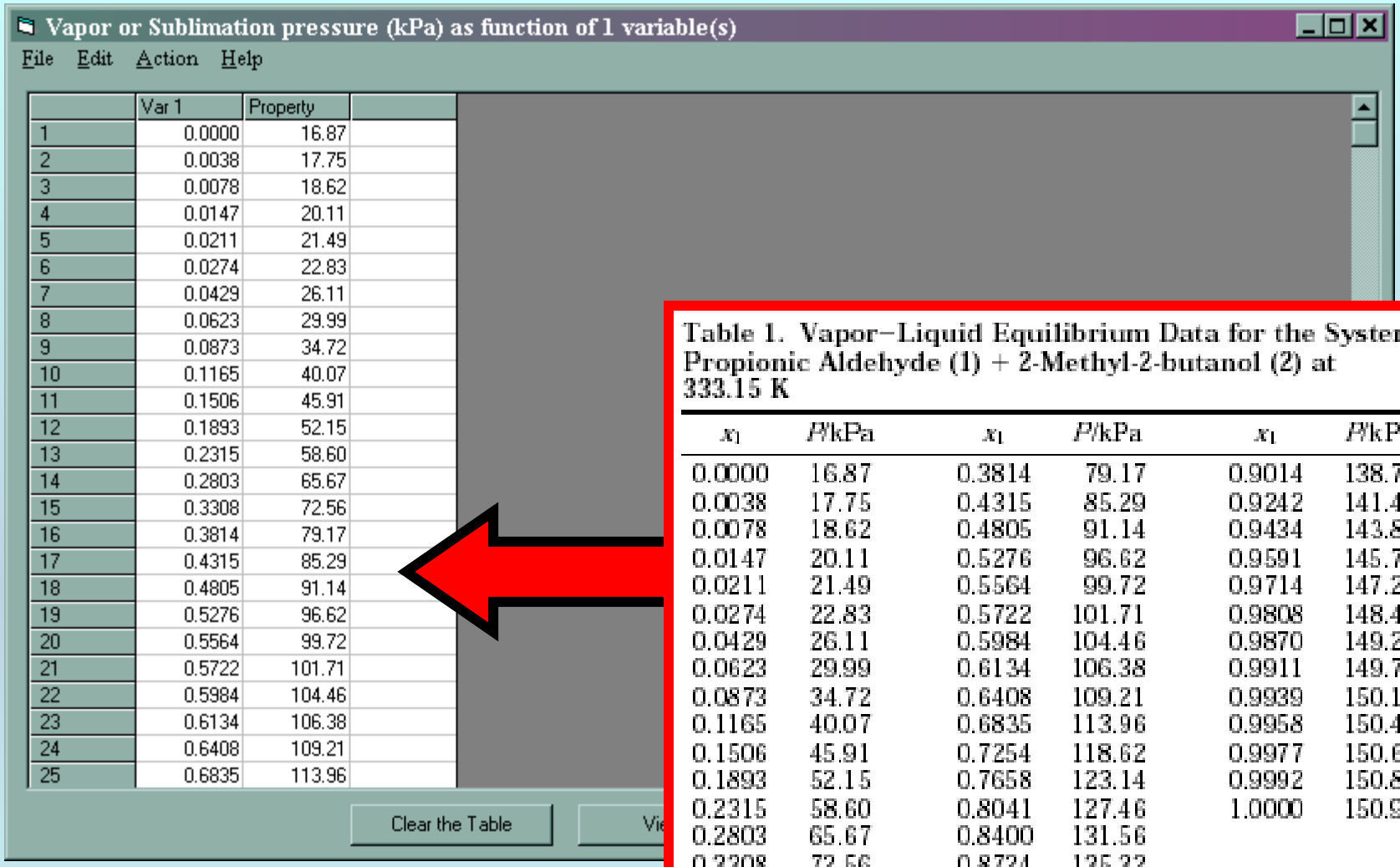
0.0429	26.11	0.5984	104.46	0.9870	149.24
0.0623	29.99	0.6134	106.38	0.9911	149.78
0.0873	34.72	0.6408	109.21	0.9939	150.14
0.1165	40.07	0.6835	113.96	0.9958	150.40
0.1506	45.91	0.7254	118.62	0.9977	150.65
0.1893	52.15	0.7658	123.14	0.9992	150.89
0.2315	58.60	0.8041	127.46	1.0000	150.93
0.2803	65.67	0.8400	131.56		
0.3308	72.56	0.8724	135.32		



	Var 1	Property
1	0.0000	16.87
2	0.0038	17.75
3	0.0078	18.62
4	0.0147	20.11
5	0.0211	21.49
6	0.0274	22.83
7	0.0429	26.11
8	0.0623	29.99
9	0.0873	34.72
10	0.1165	40.07
11	0.1506	45.91
12	0.1893	52.15
13	0.2315	58.60
14	0.2803	65.67
15	0.3308	72.56
16	0.3814	79.17
17	0.4315	85.29
18	0.4805	91.14
19	0.5276	96.62
20	0.5564	99.72
21	0.5722	101.71
22	0.5984	104.46
23	0.6134	106.38
24	0.6408	109.21
25	0.6835	113.96

Table 1. Vapor−Liquid Equilibrium Data for the System Propionic Aldehyde (1) + 2-Methyl-2-butanol (2) at 333.15 K

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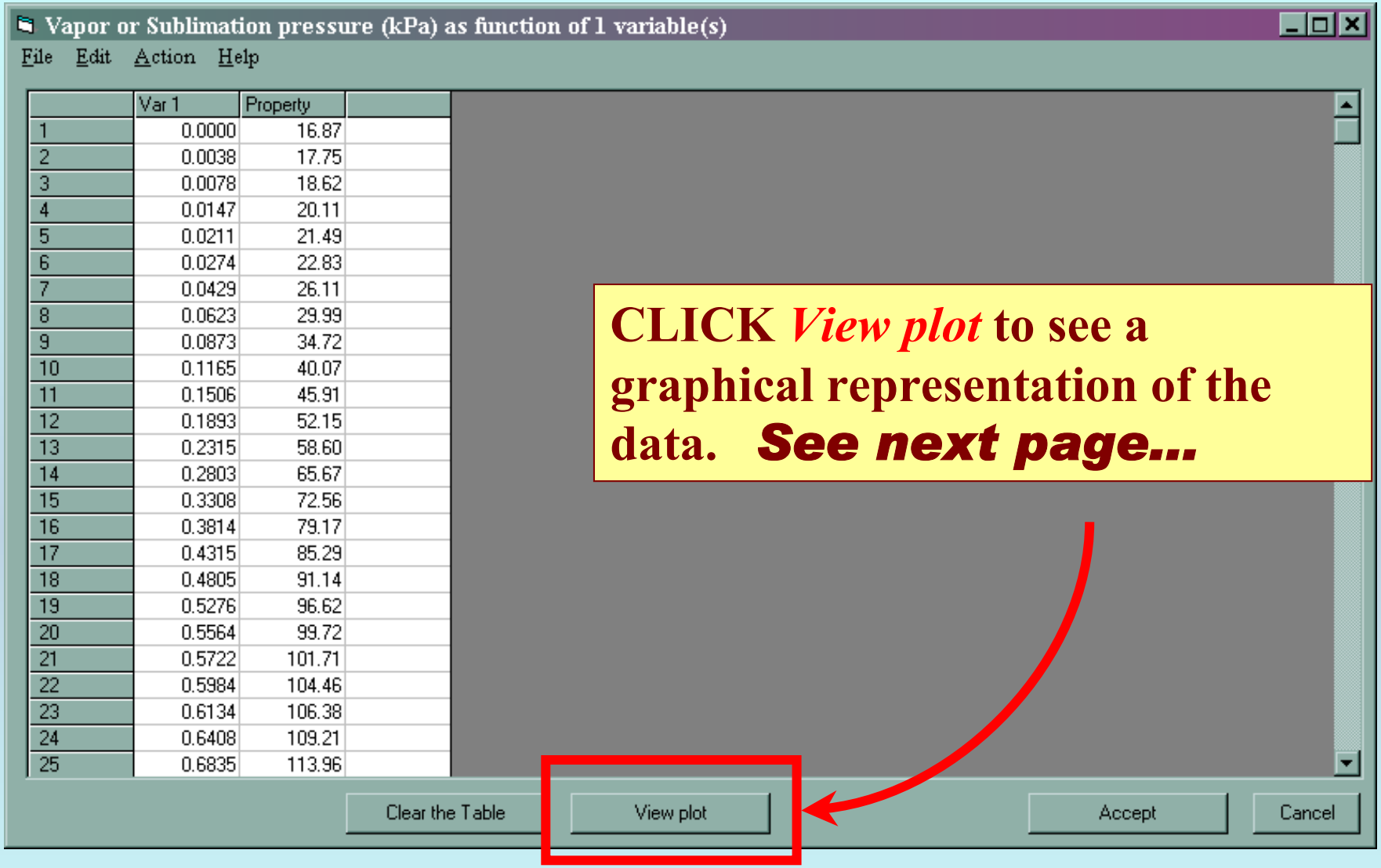
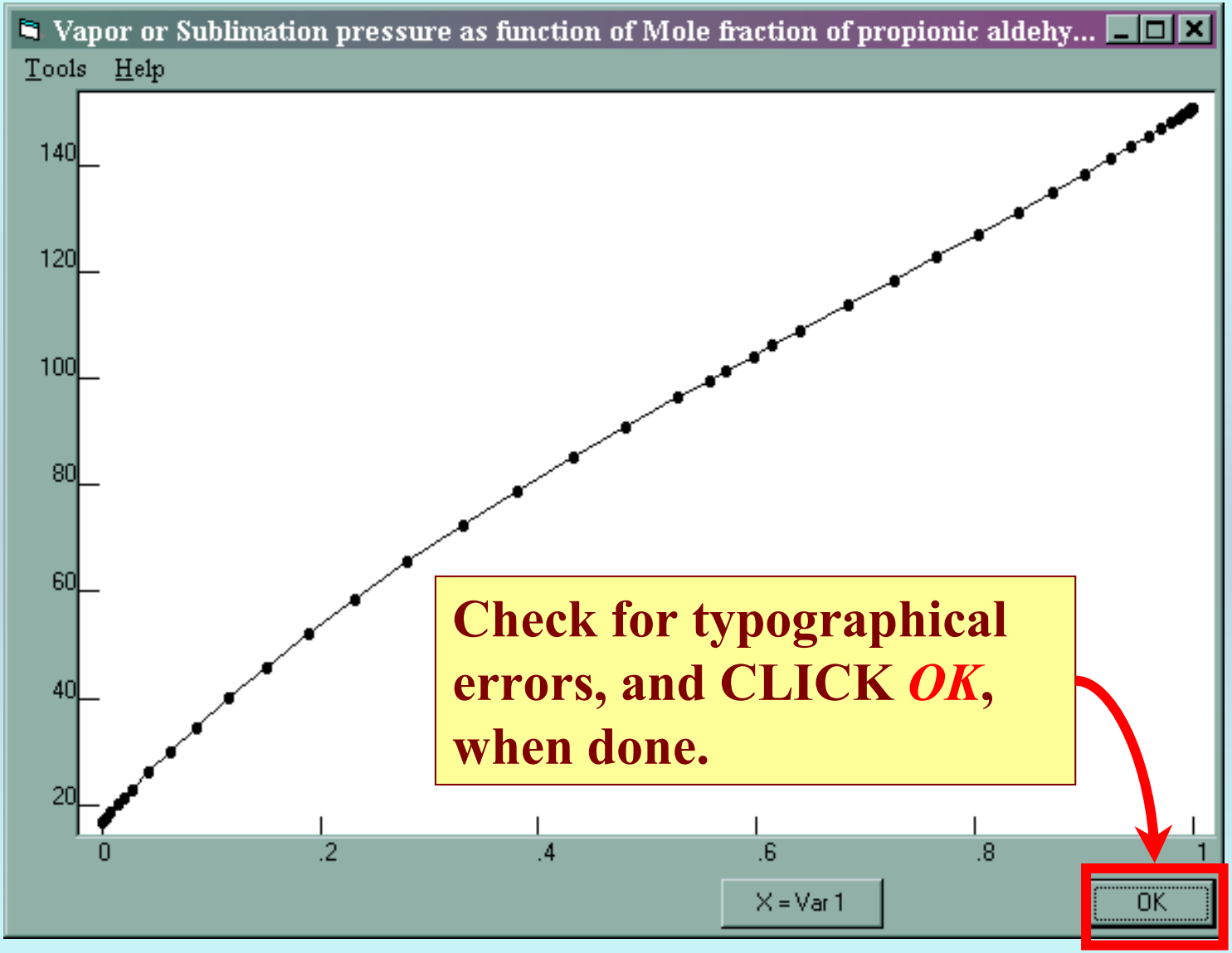
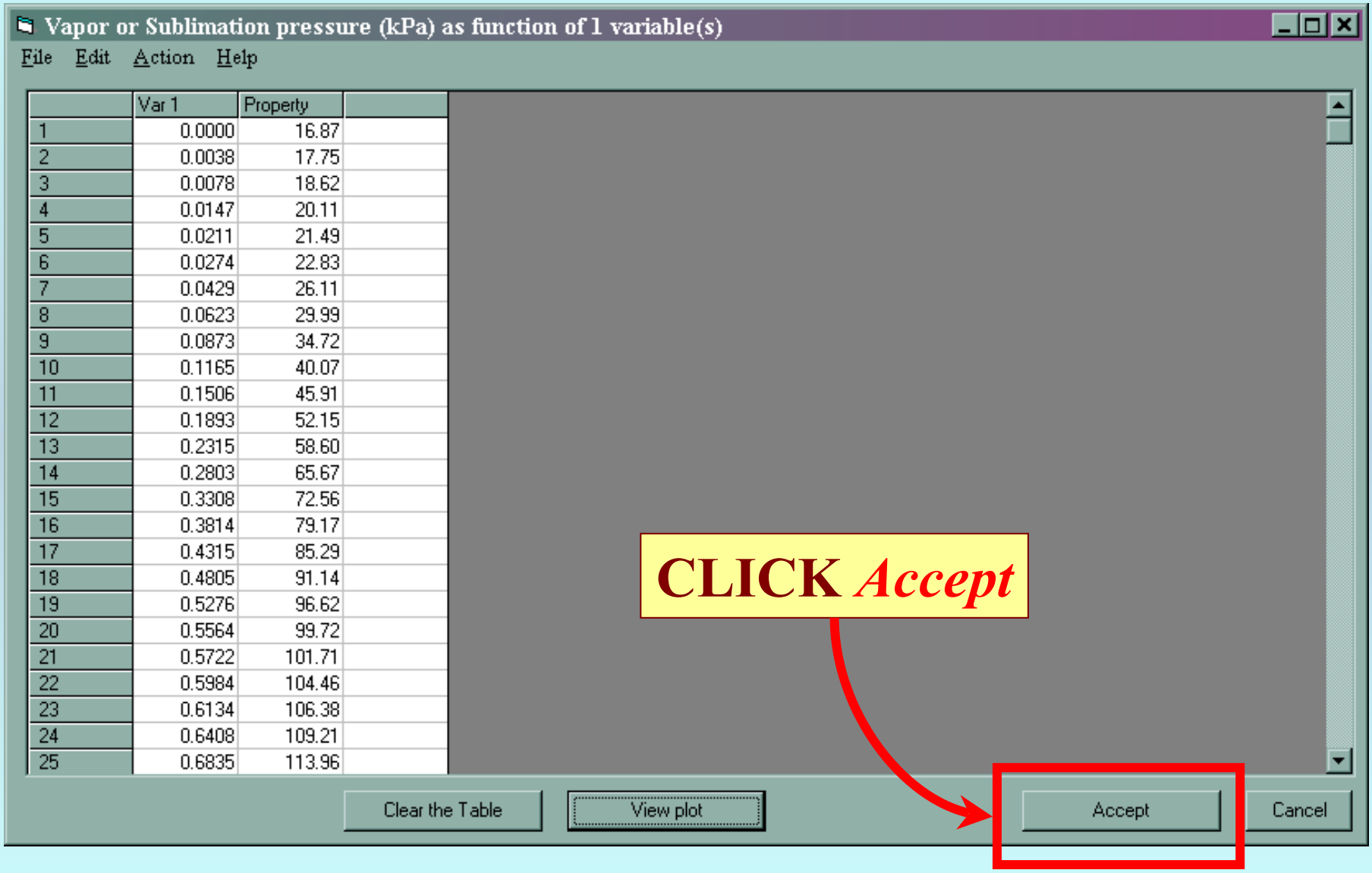
0.0623	29.99	0.6134	106.38	0.9911	149.78
0.0873	34.72	0.6408	109.21	0.9939	150.14
0.1165	40.07	0.6835	113.96	0.9958	150.40
0.1506	45.91	0.7254	118.62	0.9977	150.65
0.1893	52.15	0.7658	123.14	0.9992	150.89
0.2315	58.60	0.8041	127.46	1.0000	150.93
0.2803	65.67	0.8400	131.56		
0.3308	72.56	0.8724	135.32		

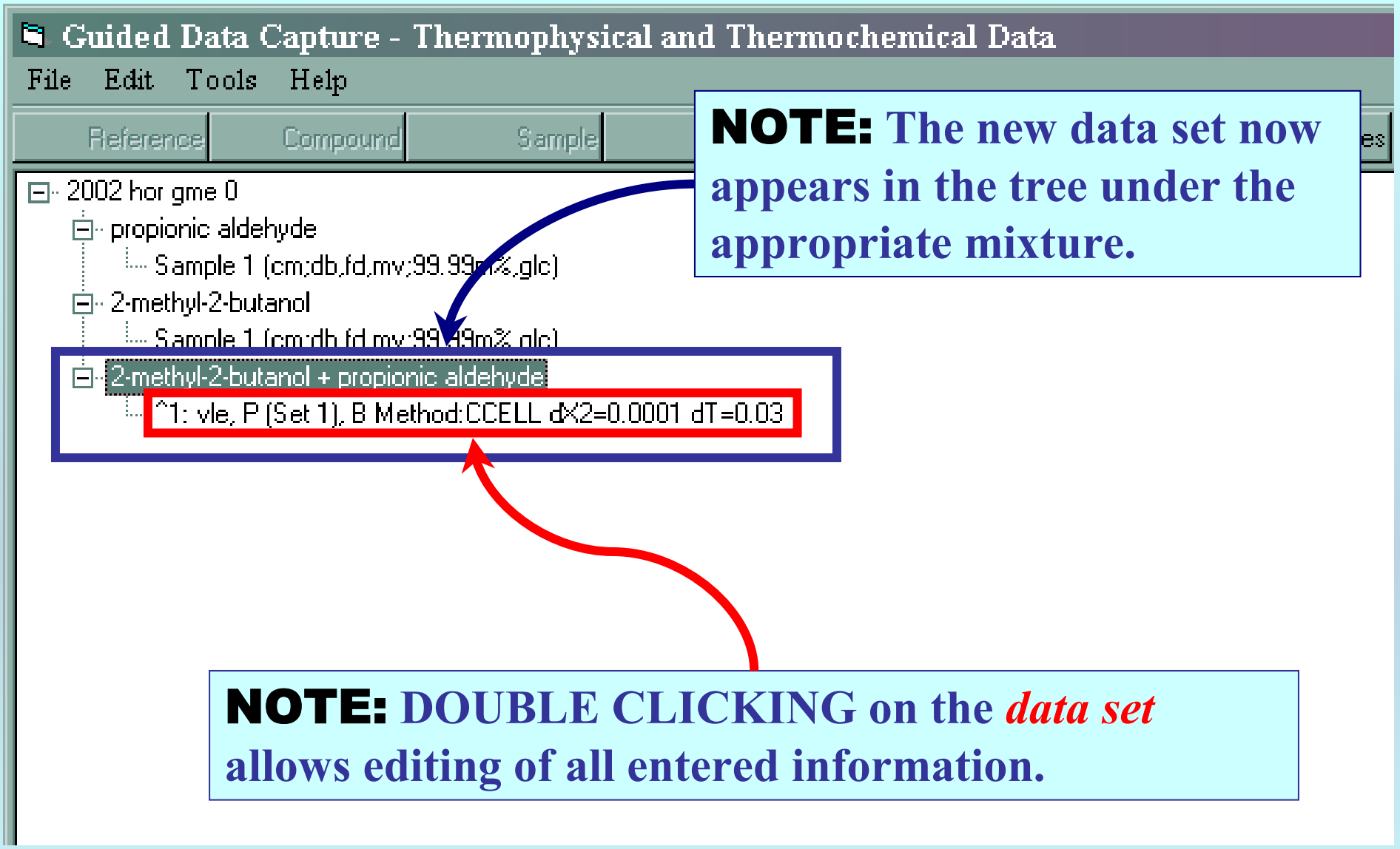
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software; e.g., EXCEL.)


Vapor or Sublimation pressure (kPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 0.0000 16.87
2 0.0038 17.75
3 0.0078 18.62
4 0.0147 20.11
5 0.0211 21.49
6 0.0274 22.83
7 0.0429 26.11
8 0.0623 29.99
9 0.0873 34.72
10 0.1165 40.07
11 0.1506 45.91
12 0.1893 52.15
13 0.2315 58.60
14 0.2803 65.67
15 0.3308 72.56
16 0.3814 79.17
17 0.4315 85.29
18 0.4805 91.14
19 0.5276 96.62
20 0.5564 99.72
21 0.5722 101.71
22 0.5984 104.46
23 0.6134 106.38
24 0.6408 109.21
25 0.6835 113.96
CLICK View plot to see a graphical representation of the data. See next page...
Clear the Table
View plot
Accept
Cancel


Vapor or Sublimation pressure as function of Mole fraction of propionic aldehy...
Tools
Help
140
120
100
80
60
40
20
0
.2
.4
.6
.8
1
X = Var 1
OK
Check for typographical errors, and CLICK OK, when done.

You are returned to the previous screen...




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample
2002 hor gme 0
propionic aldehyde
Sample 1 (cm;db,fd,mv;99.99m%,glc)
2-methyl-2-butanol
Sample 1 (cm;db,fd,mv;99.99m%,glc)
2-methyl-2-butanol + propionic aldehyde
^1: vle, P (Set 1), B Method:CCELL dX2=0.0001 dT=0.03
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.**