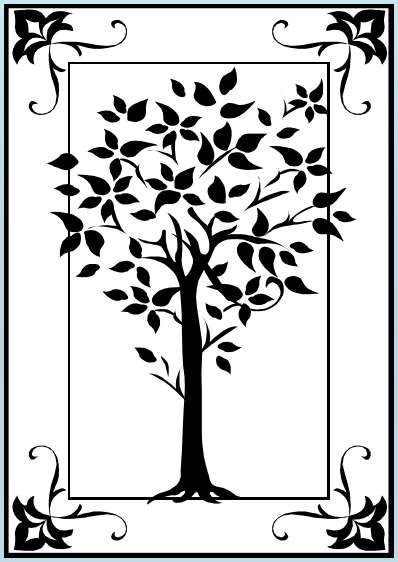
METADATA AND NUMERICAL DATA CAPTURE:
SOLUBILITY (composition)
2 – Components: *Liquid/Liquid* or *Solid/Liquid*

*G*uided *D*ata *C*apture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components: Liquid/Liquid or Solid/Liquid**
SOLUBILITY (composition)
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:

398 *J. Chem. Eng. Data* 2003, *48,* 398−401

Apparatus for the On-line GC Determination of Hydrocarbon Solubility in Water: Benzene and Cyclohexane from 70 °C to 150 °C

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Laboratoire des Sciences et Stratégies Analytiques, Université Claude Bernard-Lyon 1, Bât J. Raulin, 2 ème étage, 43 Boulevard du 11 novembre 1918, 69622 Villeurbanne Cedex, France; and Laboratoire d'Application de la Chimie à l'Environnement, Université Claude Bernard-Lyon 1, Bât J. Raulin, 4 ème étage, 43 Boulevard du 11 novembre 1918, 69622 Villeurbanne Cedex, France

An apparatus has been designed and constructed to measure liquid hydrocarbon solubility in water. On-line analysis coupled with gas chromatography has been applied to the determination of binary mixtures of water with benzene and cyclohexane for the temperature range (70 to 150) °C. Measurements obtained for benzene show good agreement with literature values and allow us to validate this new method. Increasing the temperature from 70 °C to 150 °C increases the mole fraction solubility of cyclohexane in water from $(19.7 \pm 0.02) \times 10^{-6}$ to $(131 \pm 3) \times 10^{-6}$.

SOLUBILITY (composition)

(2 Components)

Benzene in Water

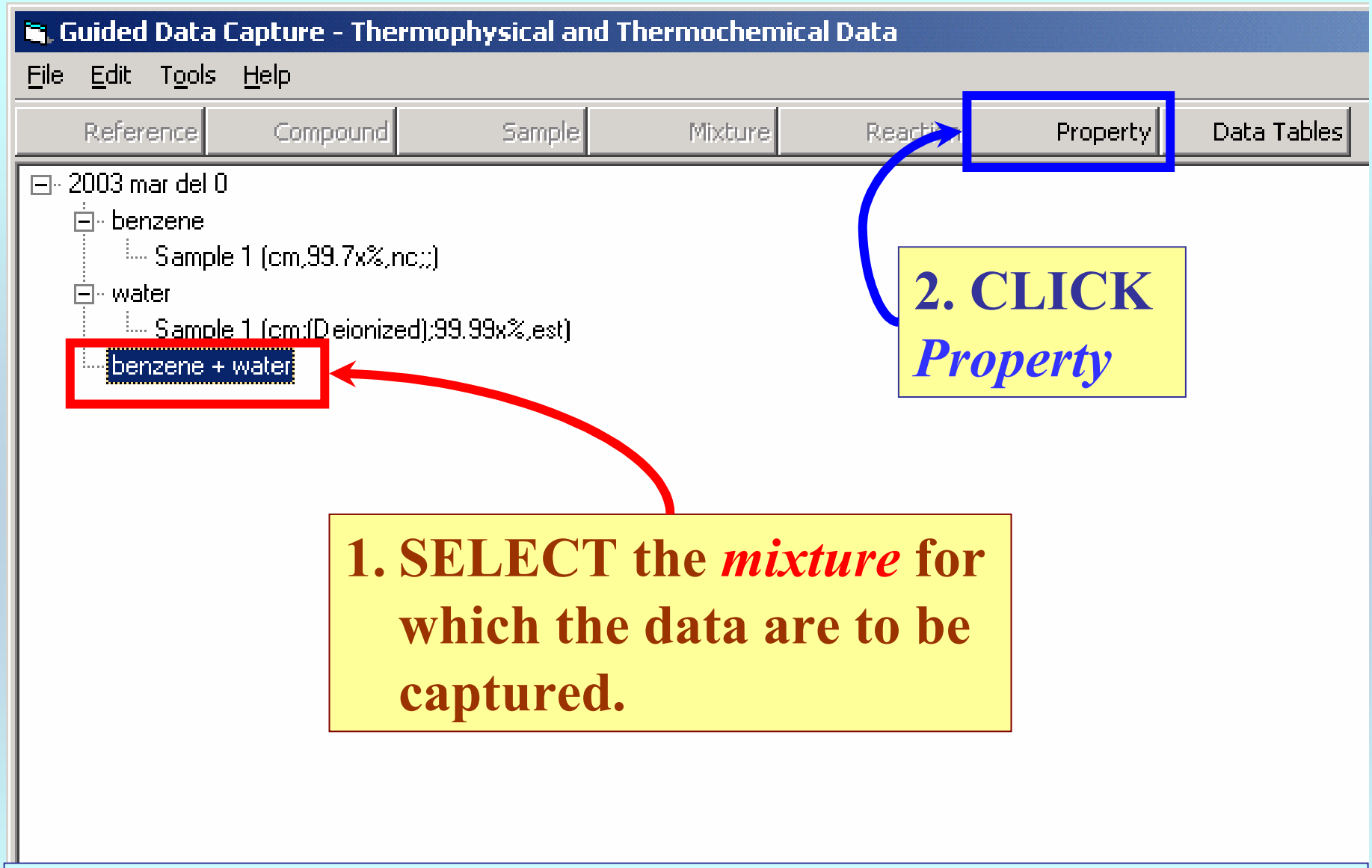
Table 1. Mole Fraction Solubility of Benzene in Water

	$10^{-4}(x \pm \sigma)^a$	$10^{-4}x$	
t/°C	exp	lit.	calc by eq 2
70.0	5.75 ± 0.01	6.17,[7] 6.25[1]	5.97
100.8	9.22 ± 0.03	9.50,[1] 9.49,[2] 10.2[3]	9.23
131.1	16.20 ± 0.07		15.41
151.2	23.2 ± 0.5	24.2 (at 150 °C),[2] 22.8 (at 149.8 °C)[3]	22.37

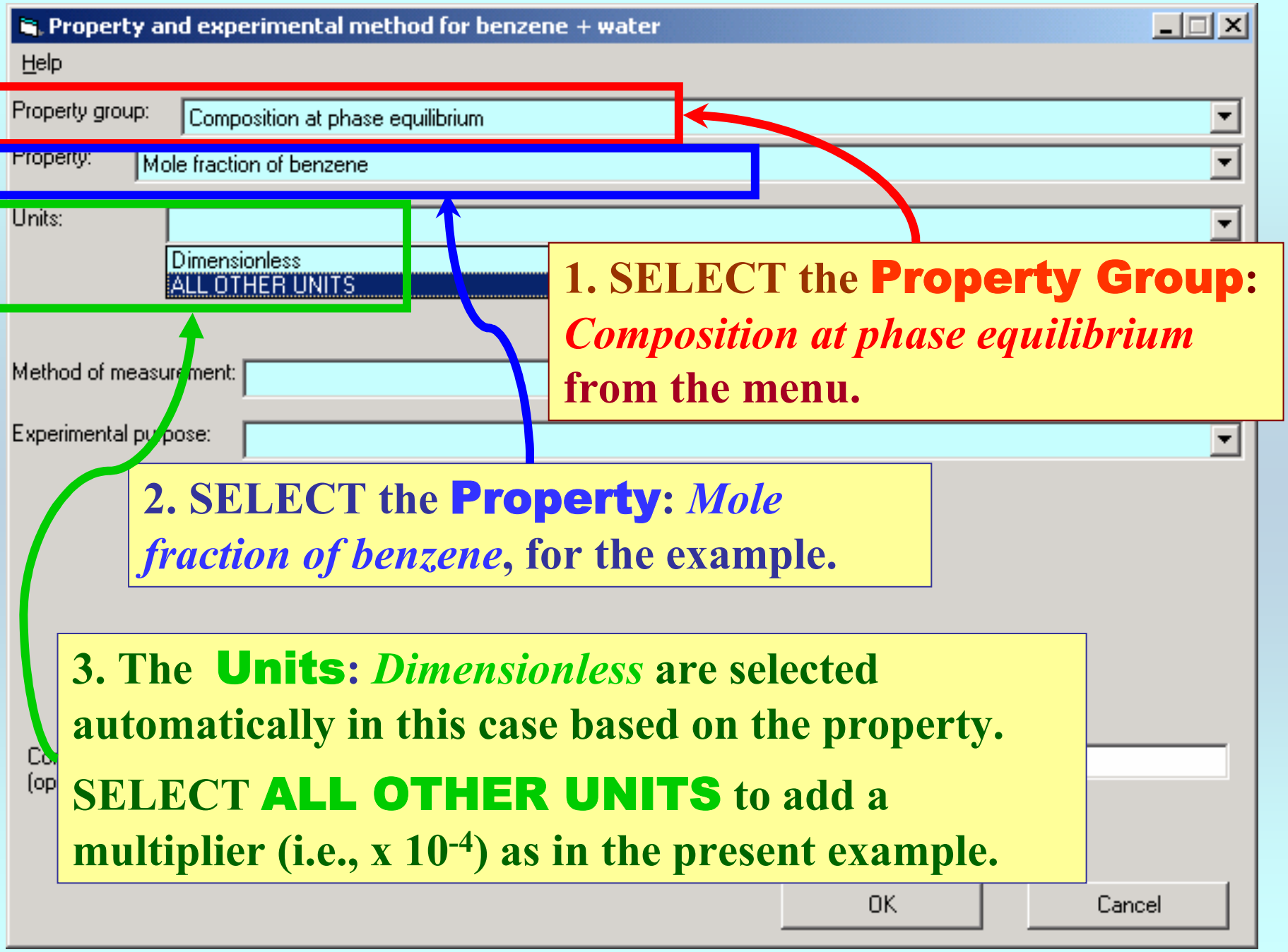
This data set is considered here.

Experimental Method Info:

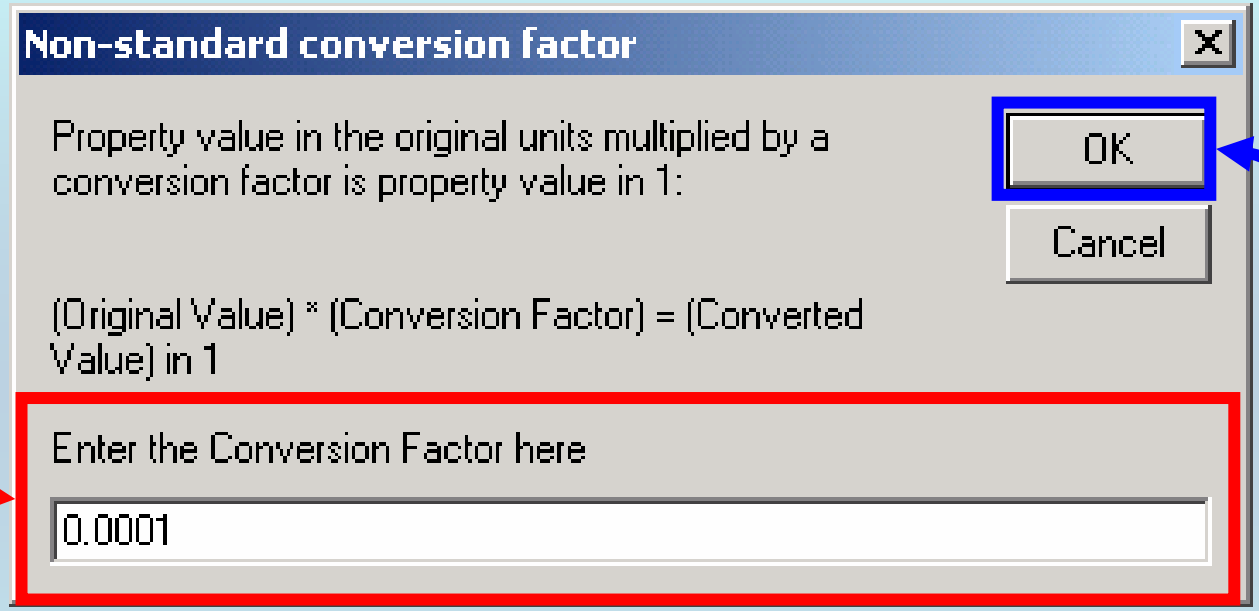
Gas Chromatography



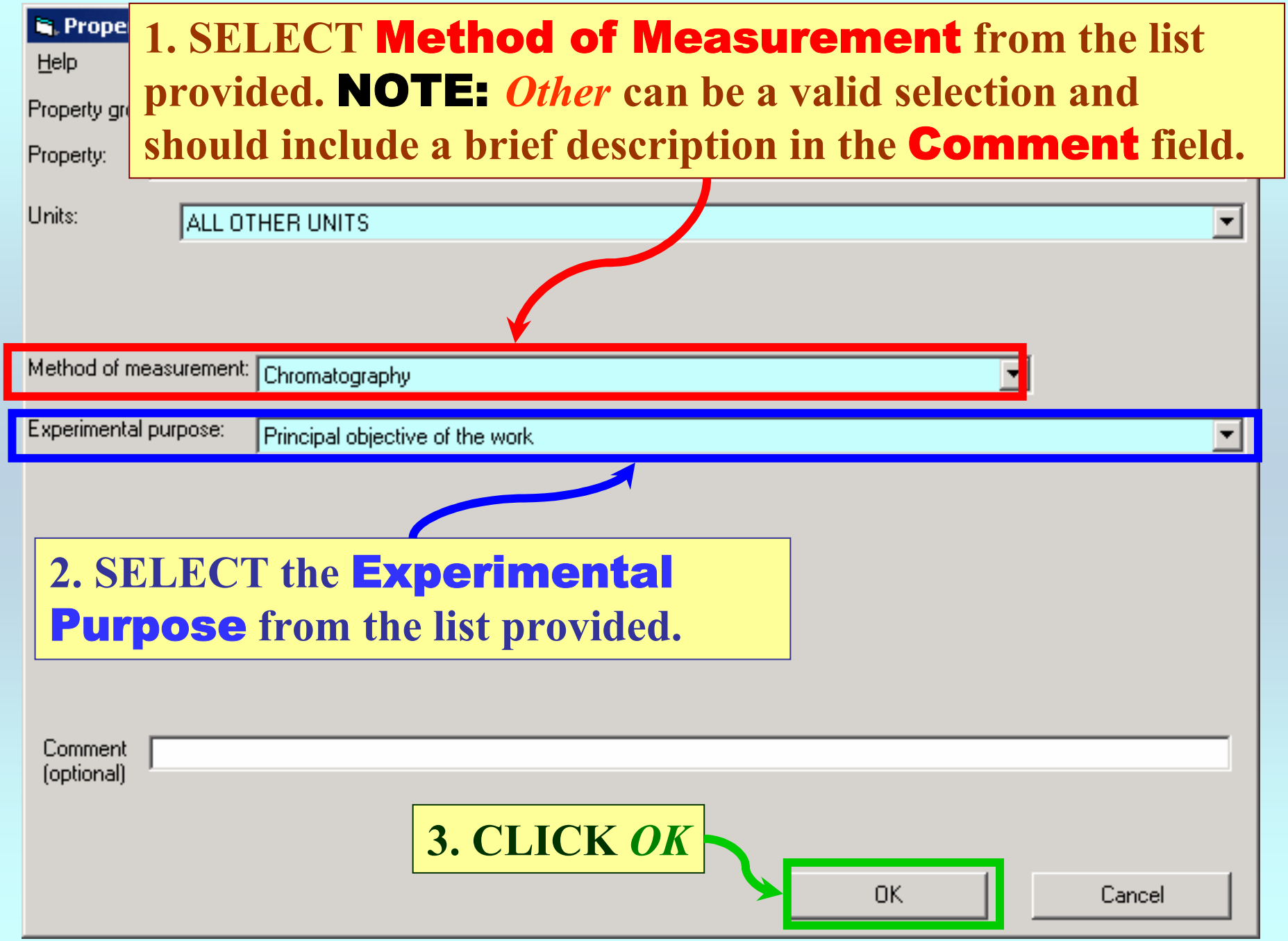
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for benzene + water
Help
Property group:
Composition at phase equilibrium
Property:
Mole fraction of benzene
Units:
Dimensionless
ALL OTHER UNITS
Method of measurement:
Experimental purpose:
OK
Cancel
1. SELECT the Property Group: Composition at phase equilibrium from the menu.
2. SELECT the Property: Mole fraction of benzene, for the example.
3. The Units: Dimensionless are selected automatically in this case based on the property.
SELECT ALL OTHER UNITS to add a multiplier (i.e., x 10-4) as in the present example.

1. TYPE the conversion factor to convert the values in the manuscript table to ì mole fraction of benzene.î



2. CLICK *OK*

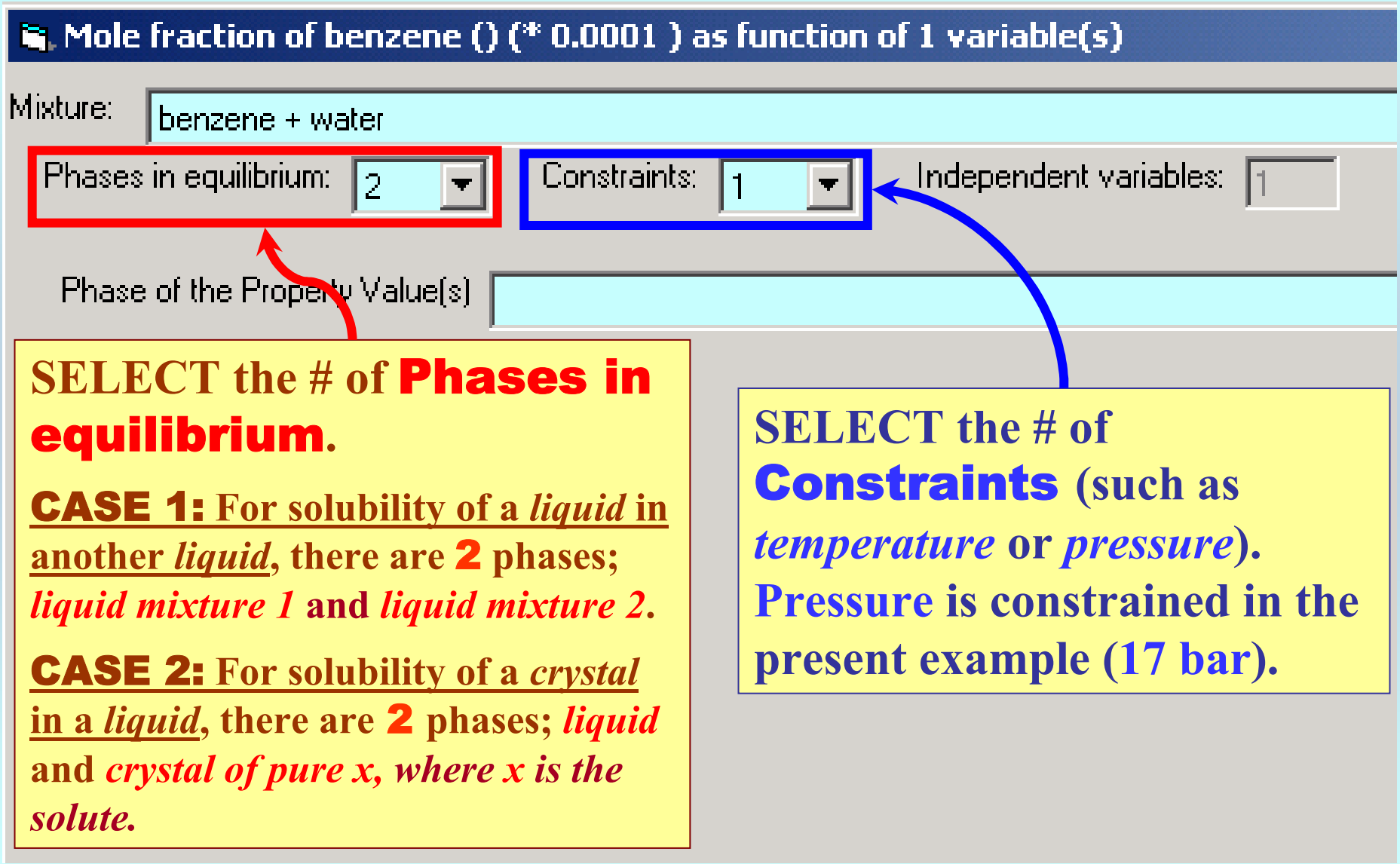


1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

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

3. CLICK *OK*

SELECTION of # of Phases in Equilibrium and # of Constraints

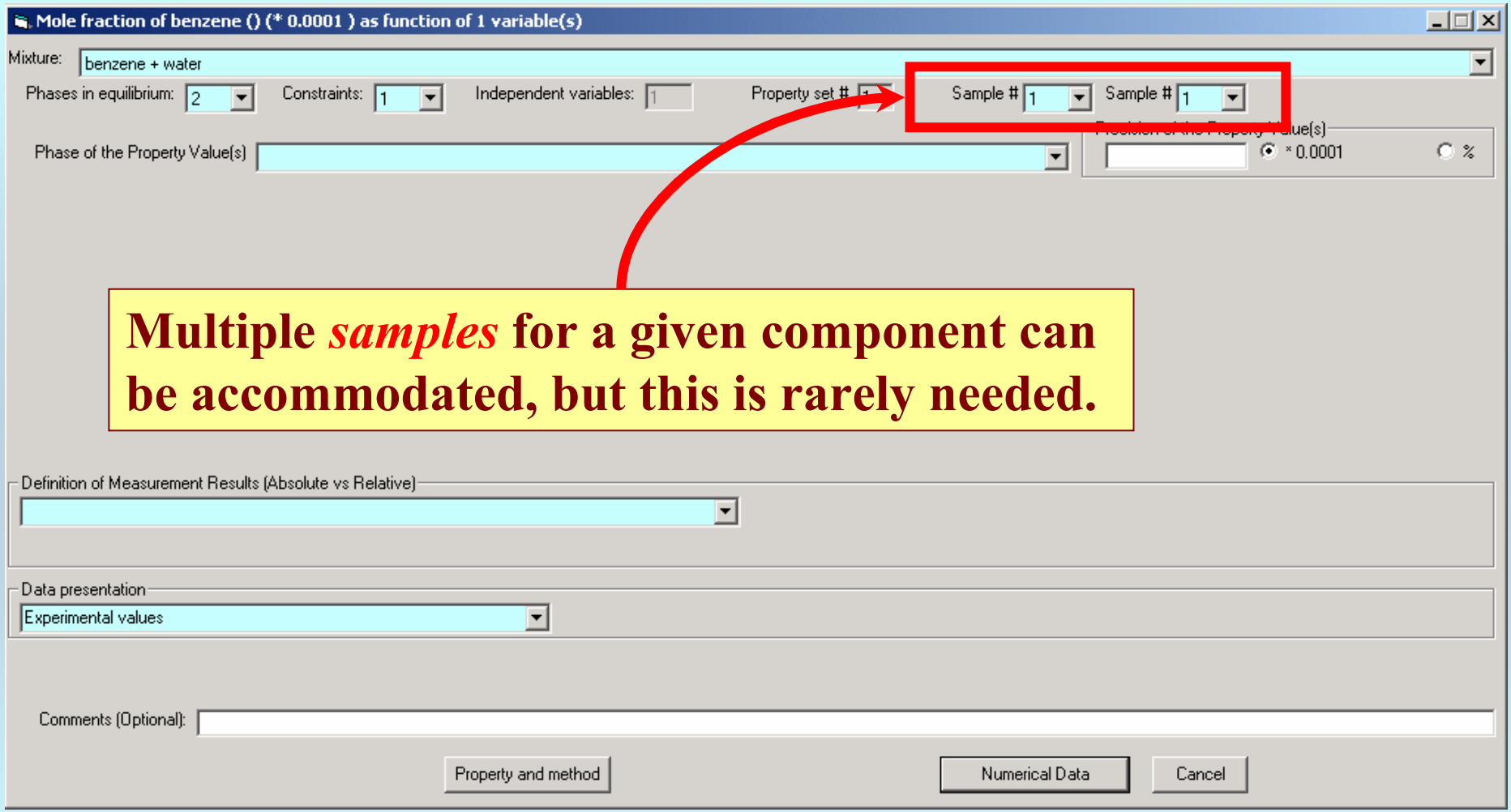


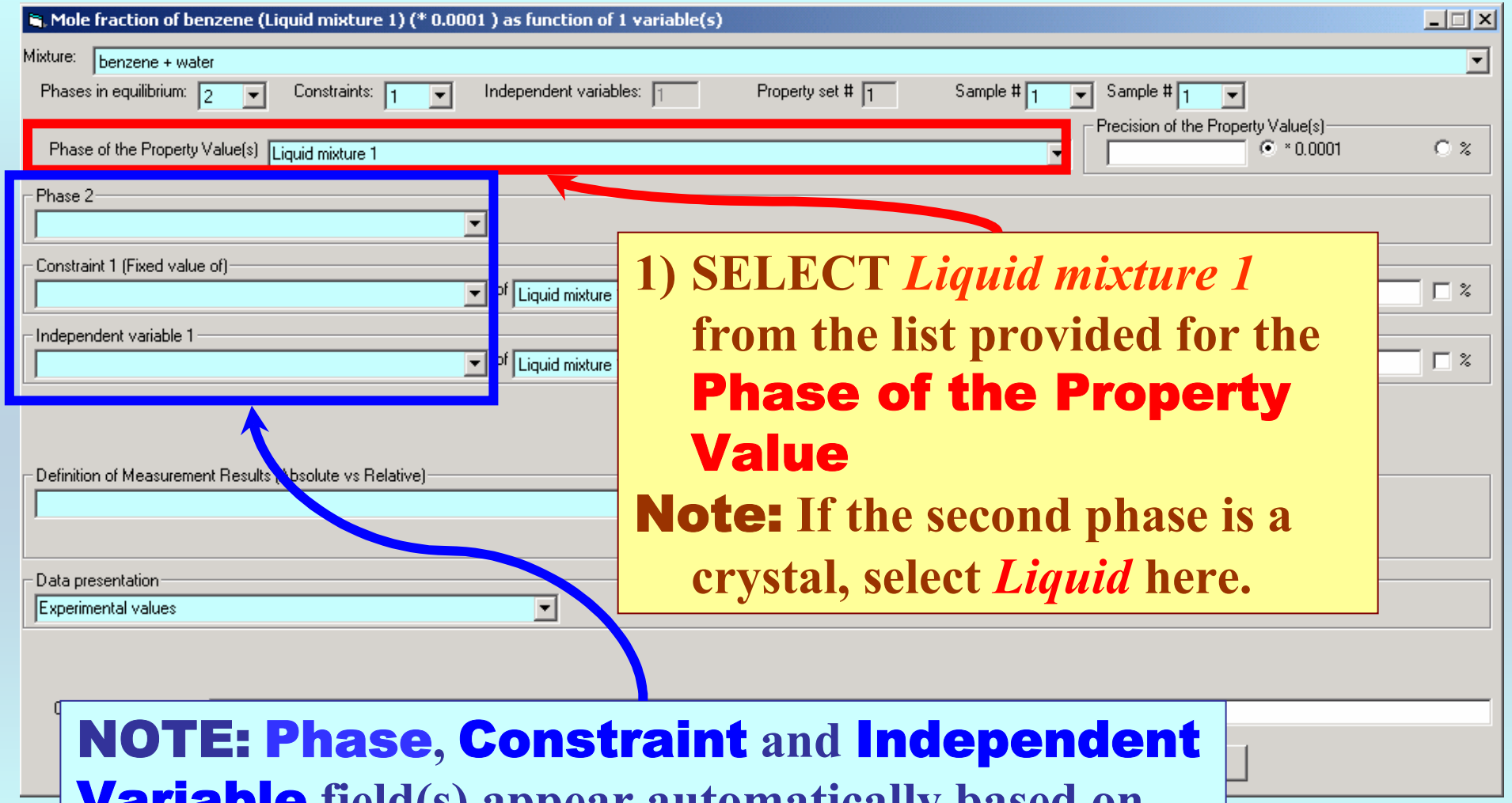
SELECT the # of Phases in equilibrium.

CASE 1: For solubility of a *liquid* in another *liquid*, there are **2** phases; *liquid mixture 1* and *liquid mixture 2*.

CASE 2: For solubility of a *crystal* in a *liquid*, there are **2** phases; *liquid* and *crystal of pure x, where x is the solute.*

SELECT the # of Constraints (such as *temperature* or *pressure*). Pressure is constrained in the present example (17 bar).


Mole fraction of benzene () (* 0.0001) as function of 1 variable(s)
Mixture:
benzene + water
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
* 0.0001
%
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



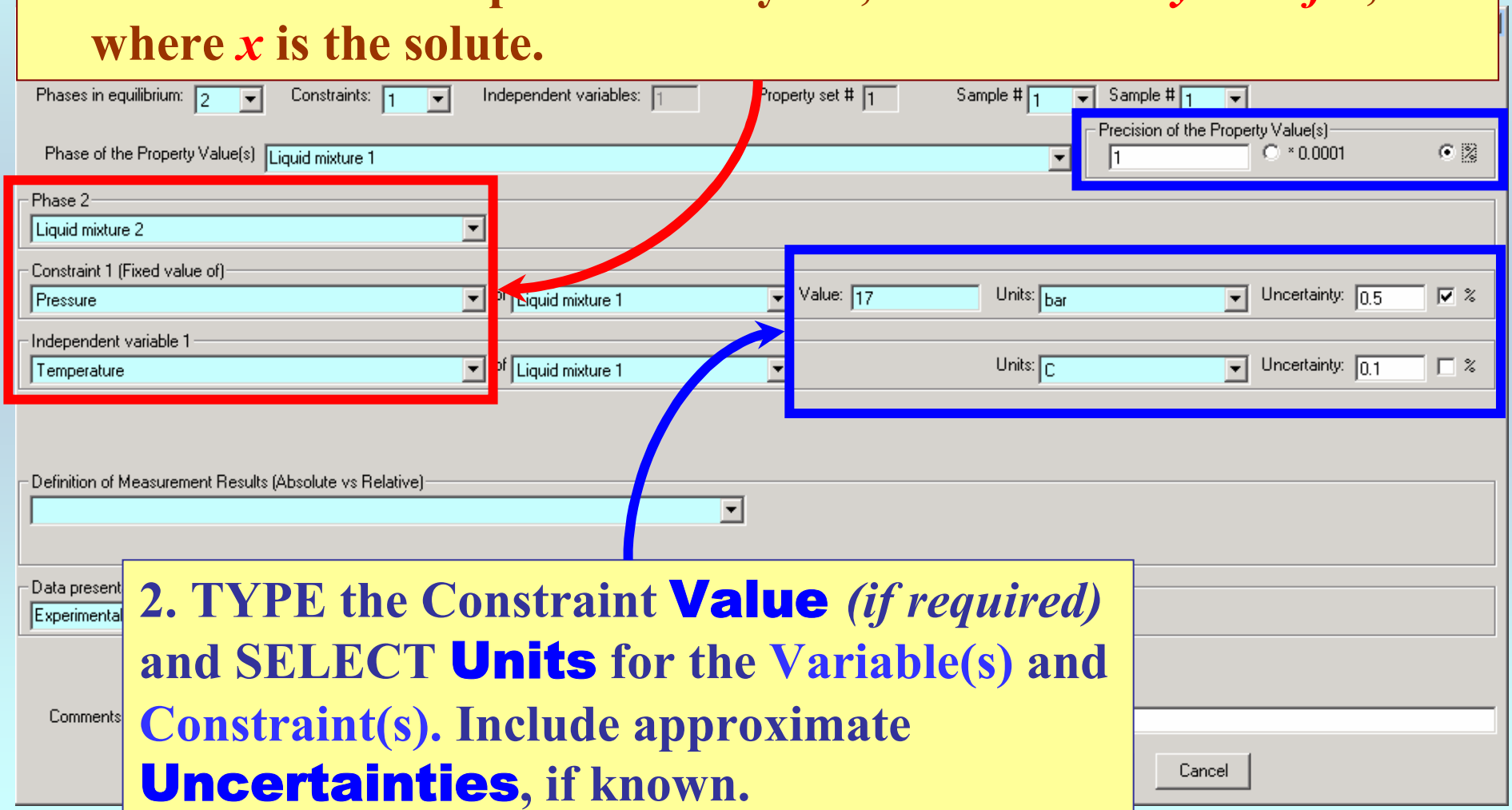
1) SELECT *Liquid mixture 1* from the list provided for the **Phase of the Property Value**

Note: If the second phase is a crystal, select *Liquid* here.

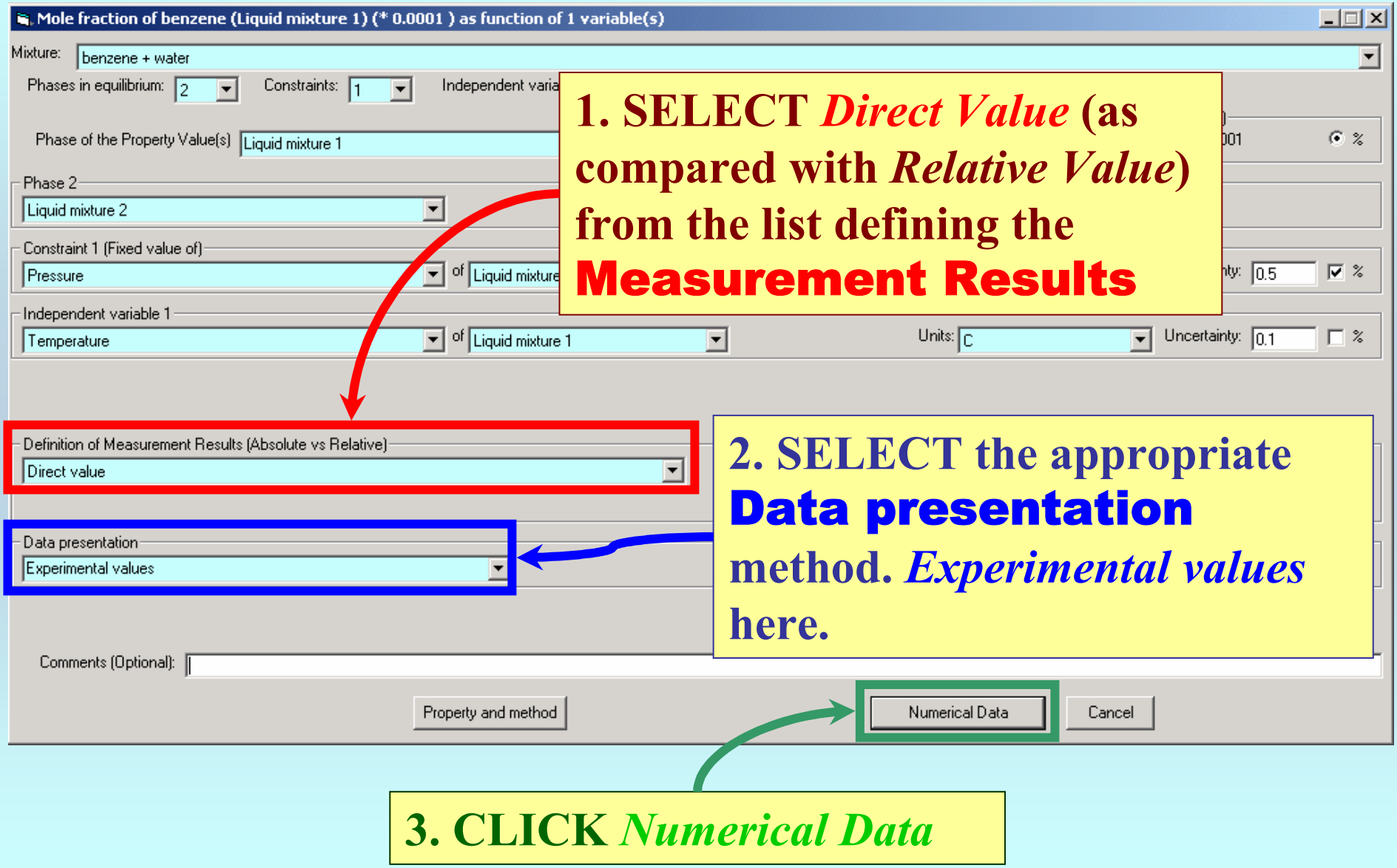
NOTE: Phase, Constraint and **Independent Variable** field(s) appear automatically based on the entered information and the *Gibbs Phase Rule*.

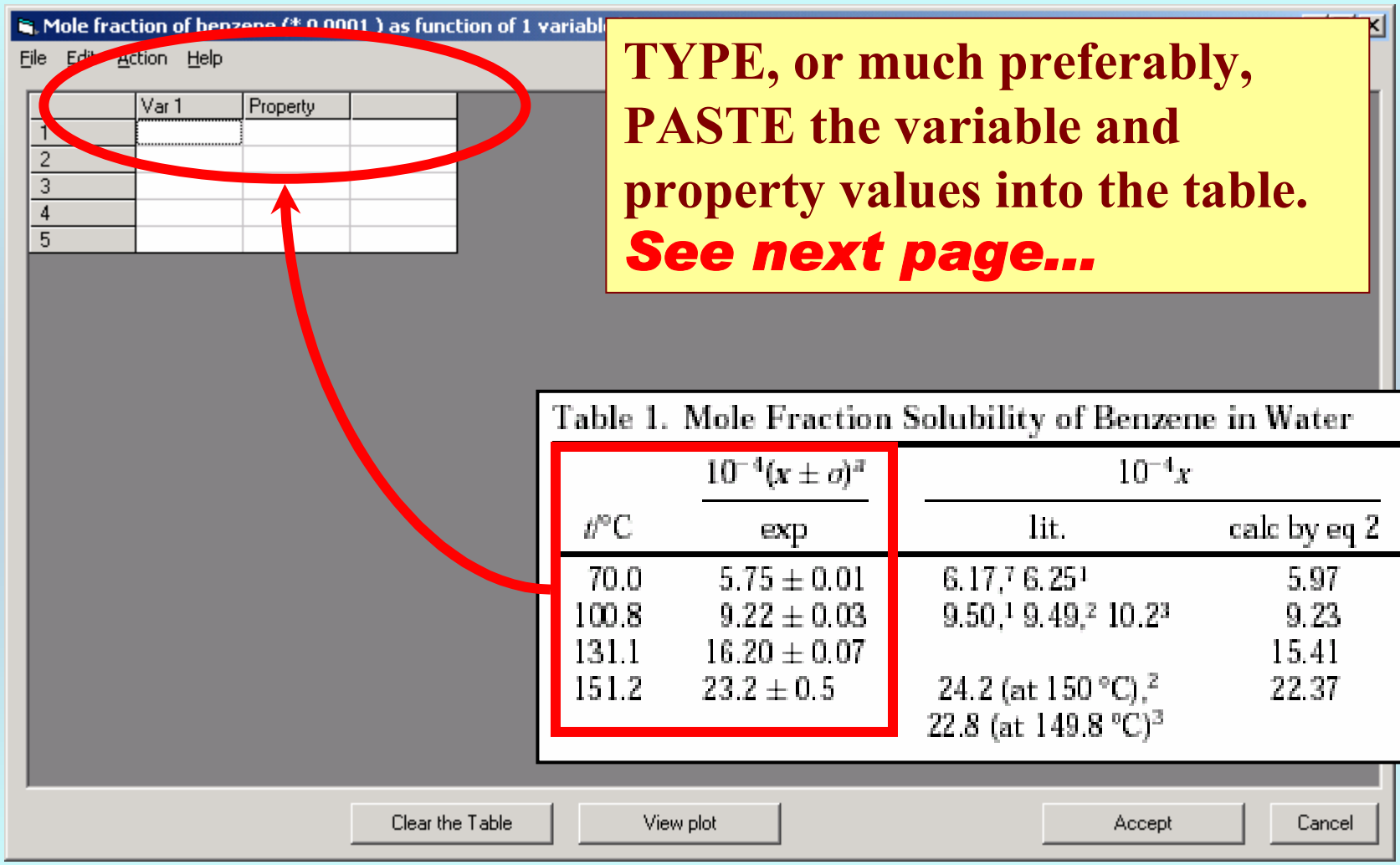
1. SELECT **Phase 2** (*Liquid mixture 2*), **Constraint(s)** (*Pressure*) and the **Independent Variable(s)** (*Temperature*) from the menus.

Note: If the second phase is a crystal, select *Pure crystal of x*, where *x* is the solute.



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


Mole fraction of benzene (Liquid mixture 1) (* 0.0001) as function of 1 variable(s)
Mixture: benzene + water
Phases in equilibrium: 2
Constraints: 1
Phase of the Property Value(s): Liquid mixture 1
Phase 2
Liquid mixture 2
Constraint 1 (Fixed value of)
Pressure
of Liquid mixture
Independent variable 1
Temperature
of Liquid mixture 1
Units: C
Uncertainty: 0.1
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel
1. SELECT Direct Value (as compared with Relative Value) from the list defining the Measurement Results
2. SELECT the appropriate Data presentation method. Experimental values here.
3. CLICK Numerical Data



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131.1	16.20 ± 0.07		15.41
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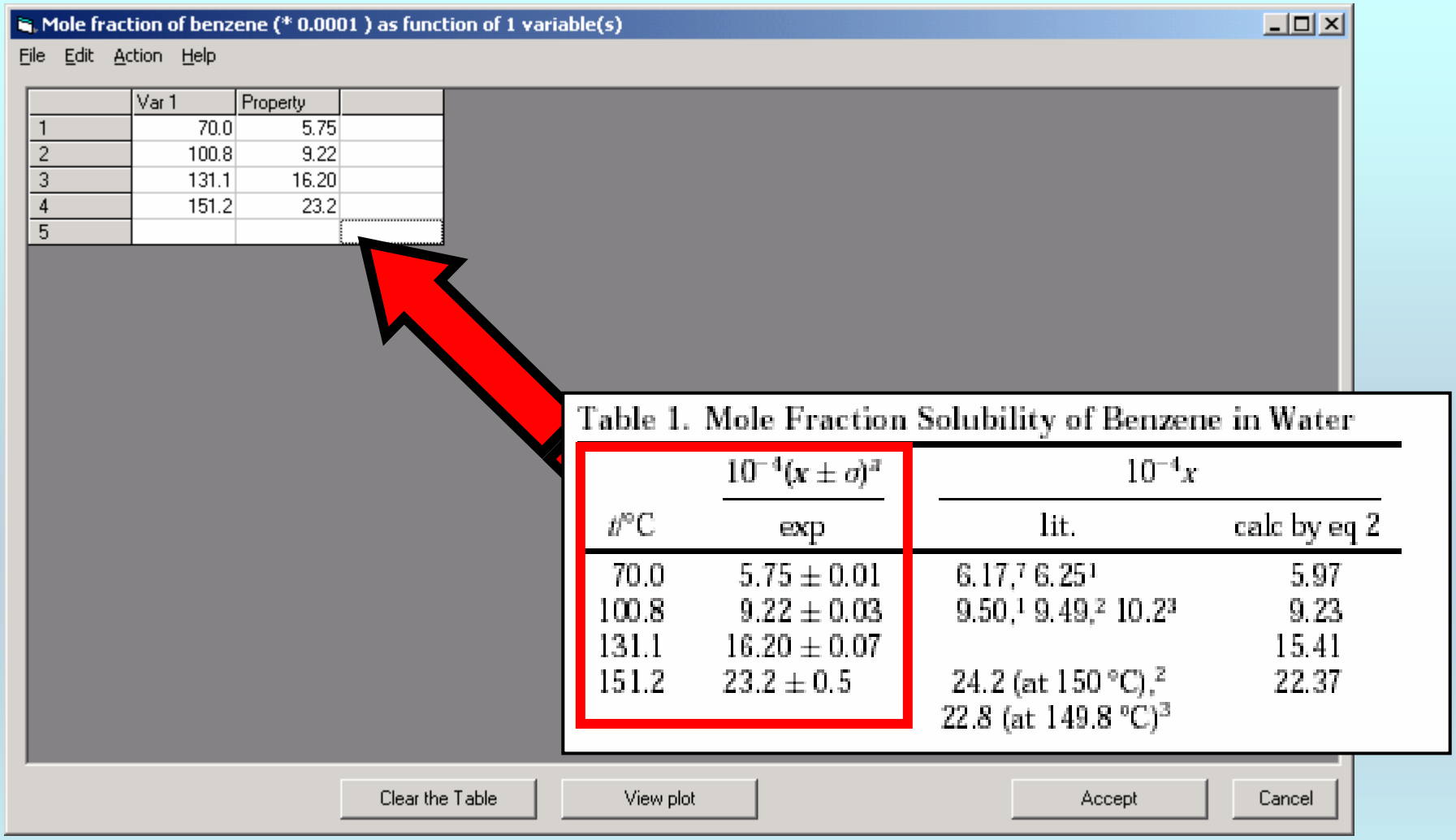
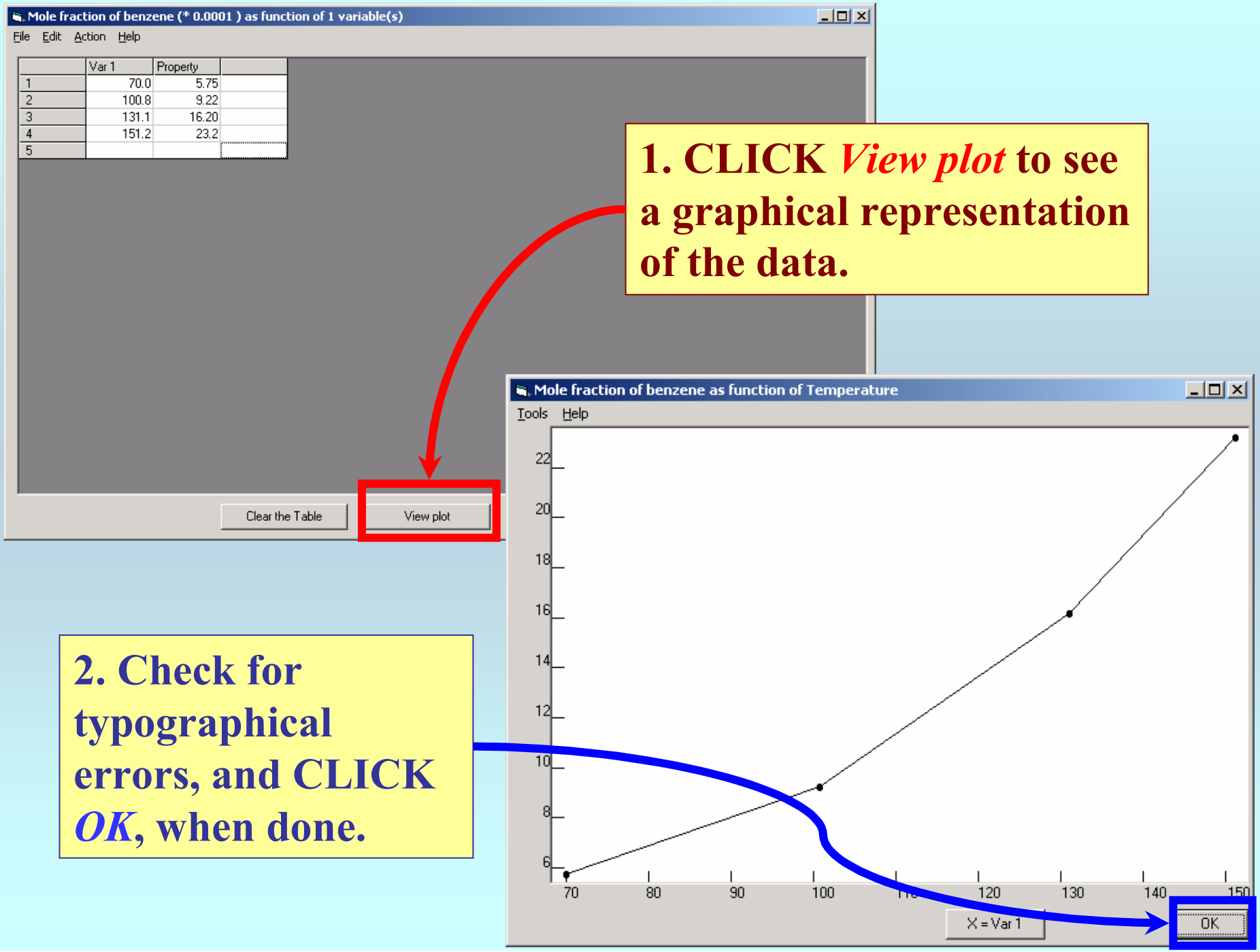
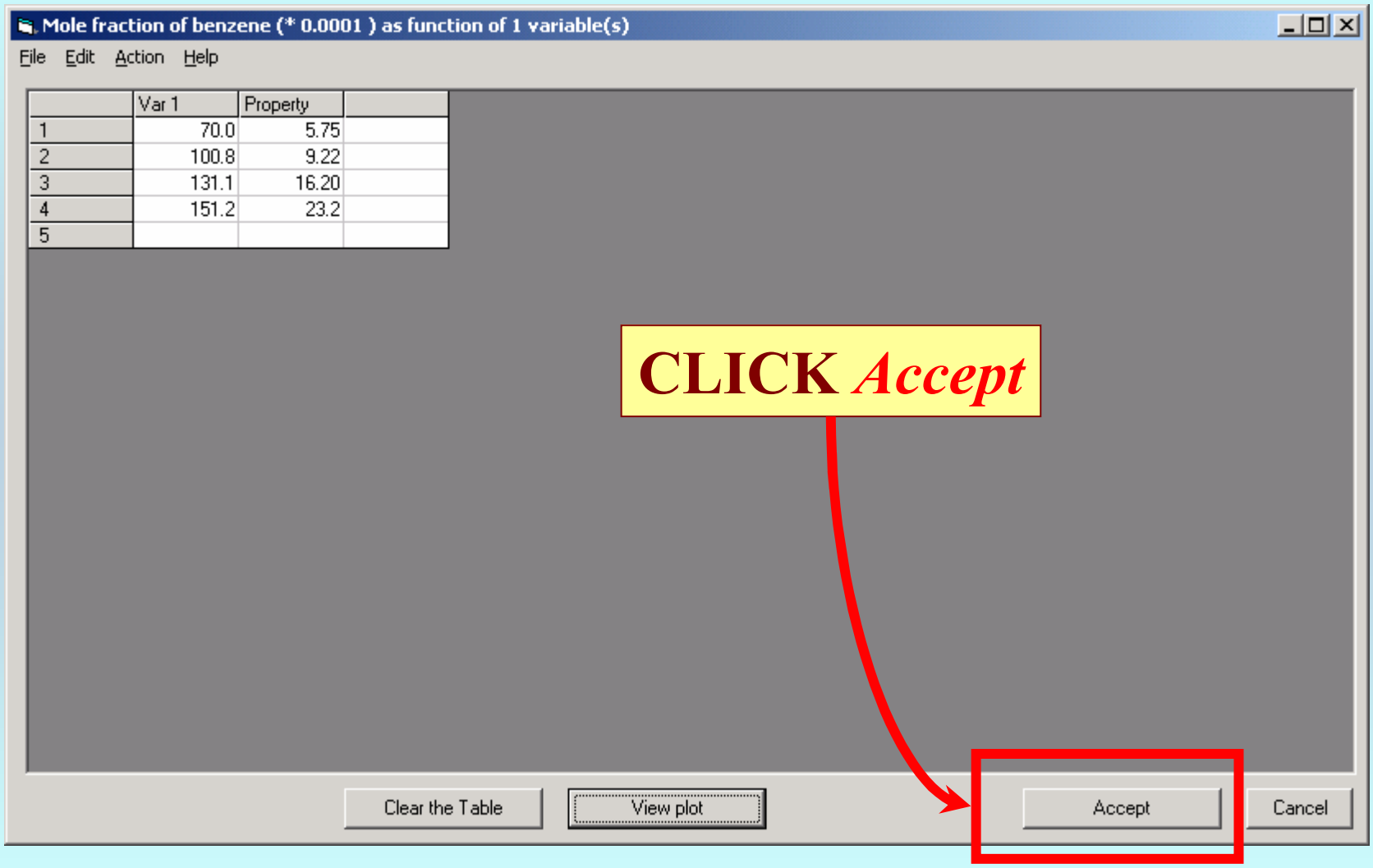
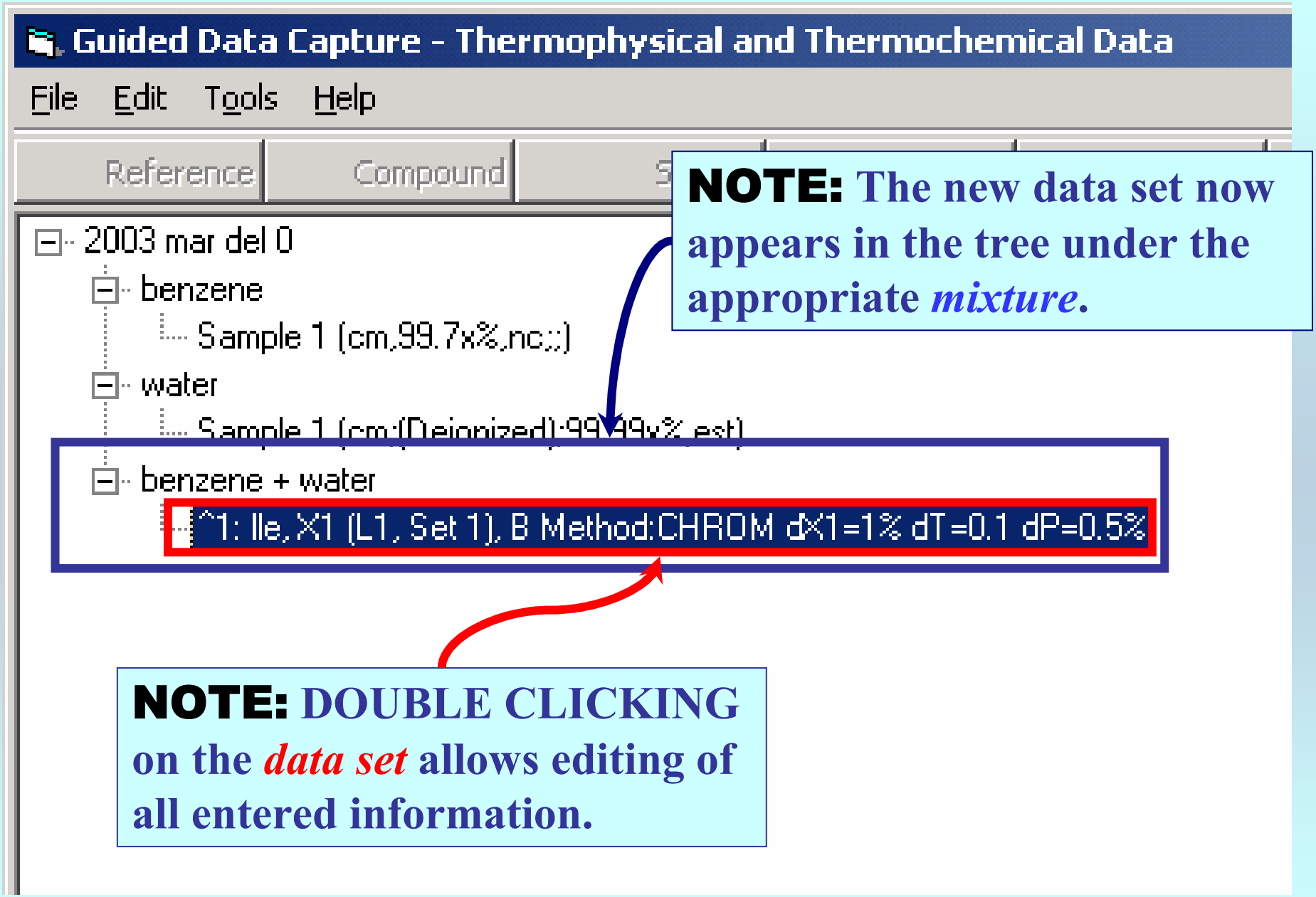


NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)


Mole fraction of benzene (* 0.0001) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 70.0 5.75
2 100.8 9.22
3 131.1 16.20
4 151.2 23.2
5
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
Mole fraction of benzene as function of Temperature
Tools Help
22
20
18
16
14
12
10
8
6
70
80
90
100
120
130
140
150
X = Var 1
OK
2. Check for typographical errors, and CLICK OK, when done.


Mole fraction of benzene (* 0.0001) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 70.0 5.75
2 100.8 9.22
3 131.1 16.20
4 151.2 23.2
5
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
2003 mar del 0
benzene
Sample 1 (cm,99.7x%,nc;;)
water
benzene + water
^1: Ile, X1 (L1, Set 1), B Method:CHROM dX1=1% dT=0.1 dP=0.5%
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.**