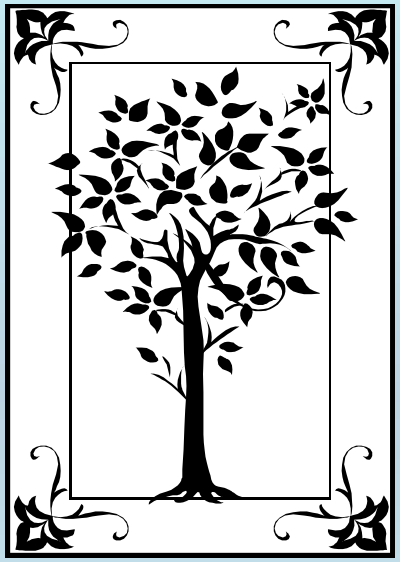
METADATA AND NUMERICAL DATA CAPTURE:
Temperature and Pressure of Liquid-Liquid-Vapor Equilibrium

Guided Data Capture (GDC)



This tutorial describes

METADATA AND NUMERICAL DATA CAPTURE

Temperature and Pressure of Liquid-Liquid-Vapor (L_1L_2V) Equilibrium

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:

Fluid Phase Equilibria of Binary n-Alkane + Squalane Systems

Diana E. Nanu[1], Wim Poot[1], Dan Geanã[2], Theodoor W. de Loos[1*]

[1]Delft University of Technology, Department of Chemical Technology, Laboratory of Applied Thermodynamics and Phase Equilibria, Julianalaan 136, 2628 BL Delft, The Netherlands

[2]University "Politehnica" Bucharest, Department of Applied Physical Chemistry and Electrochemistry, Spl. Independentei 313, 78126 Bucharest, Romania

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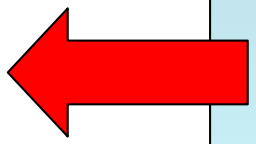
Temperature and Pressure of Liquid-Liquid-Vapor (L_1L_2V) Equilibrium for (ethane + squalane)

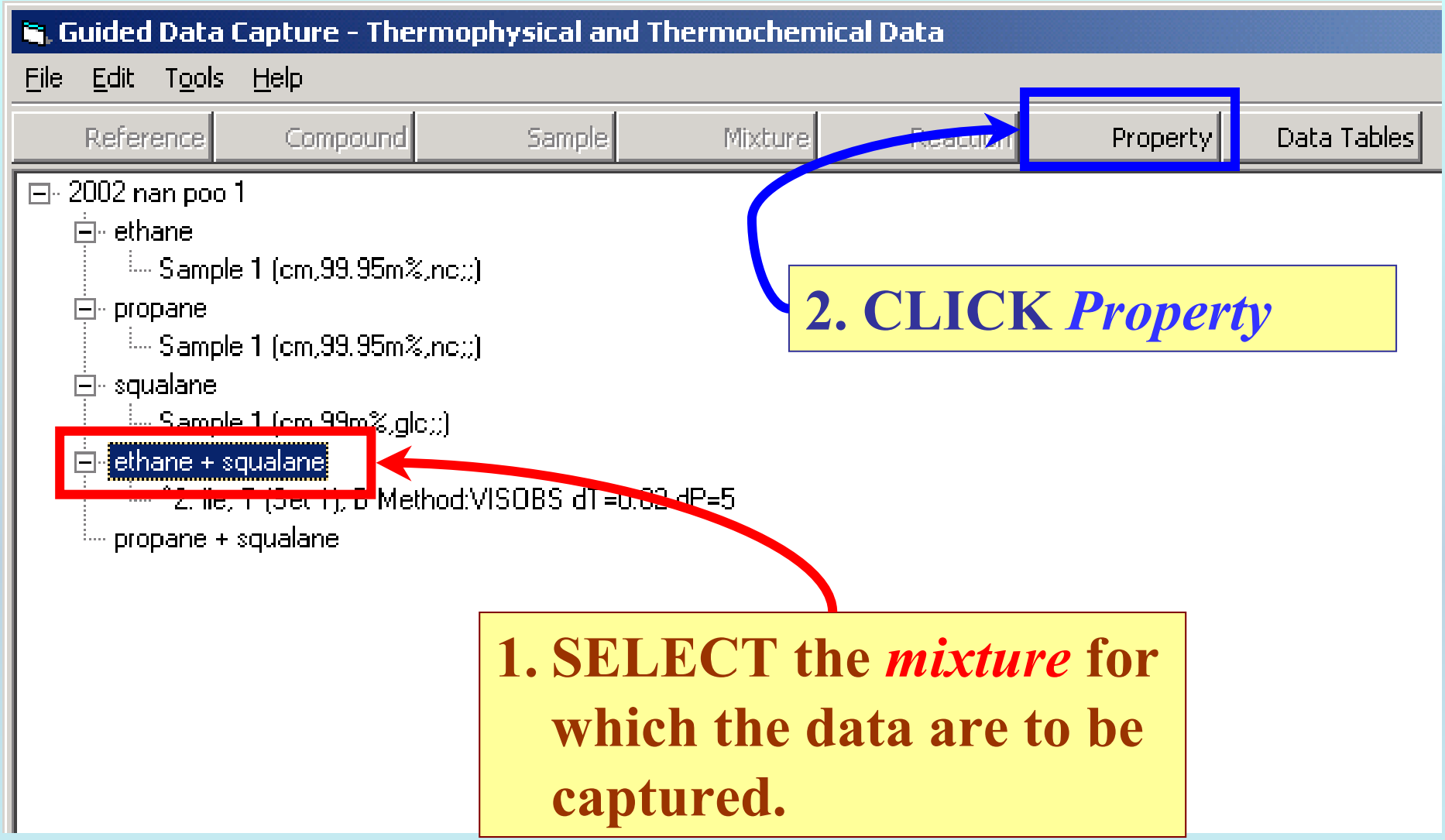
Table 2. Experimental Data of the Three-Phase Equilibrium L_1L_2V in the Ethane-Squalane System

T/K	p/MPa
295.57	3.930[a]
295.71	3.961
296.00	3.979
296.53	4.028
297.38	4.105
297.89	4.166
298.30	4.196
298.79	4.231
299.33	4.287
300.34	4.374
300.94	4.436
301.35	4.474
302.37	4.570
302.53	4.581
303.43	4.685
304.42	4.775
305.32	4.865
306.51	4.996
306.69	5.013[b]

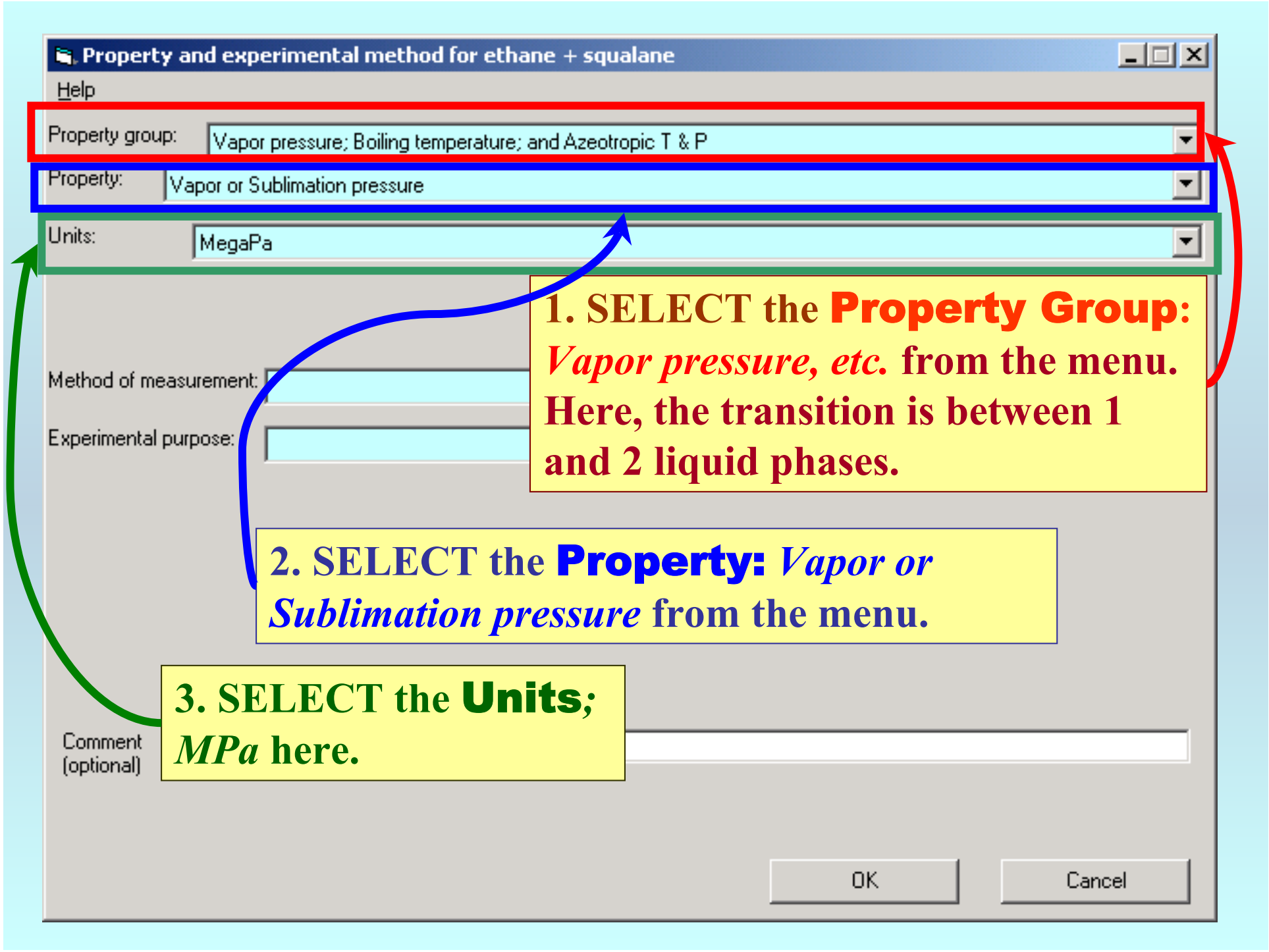
[a] LCEP ($L_2 = L_1 + V$). [b] UCEP ($L_2 + L_1 = V$).

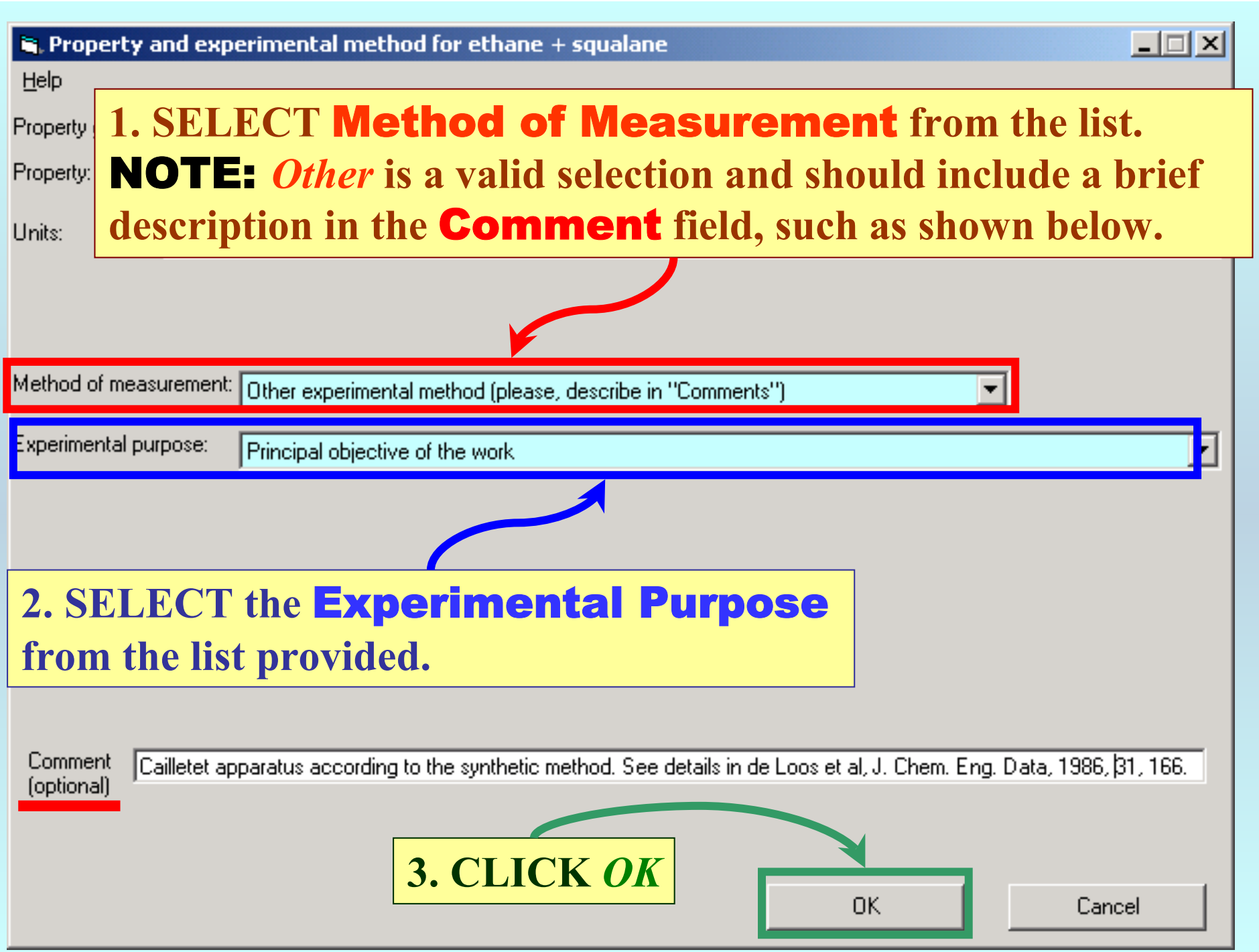
This data set is considered here.



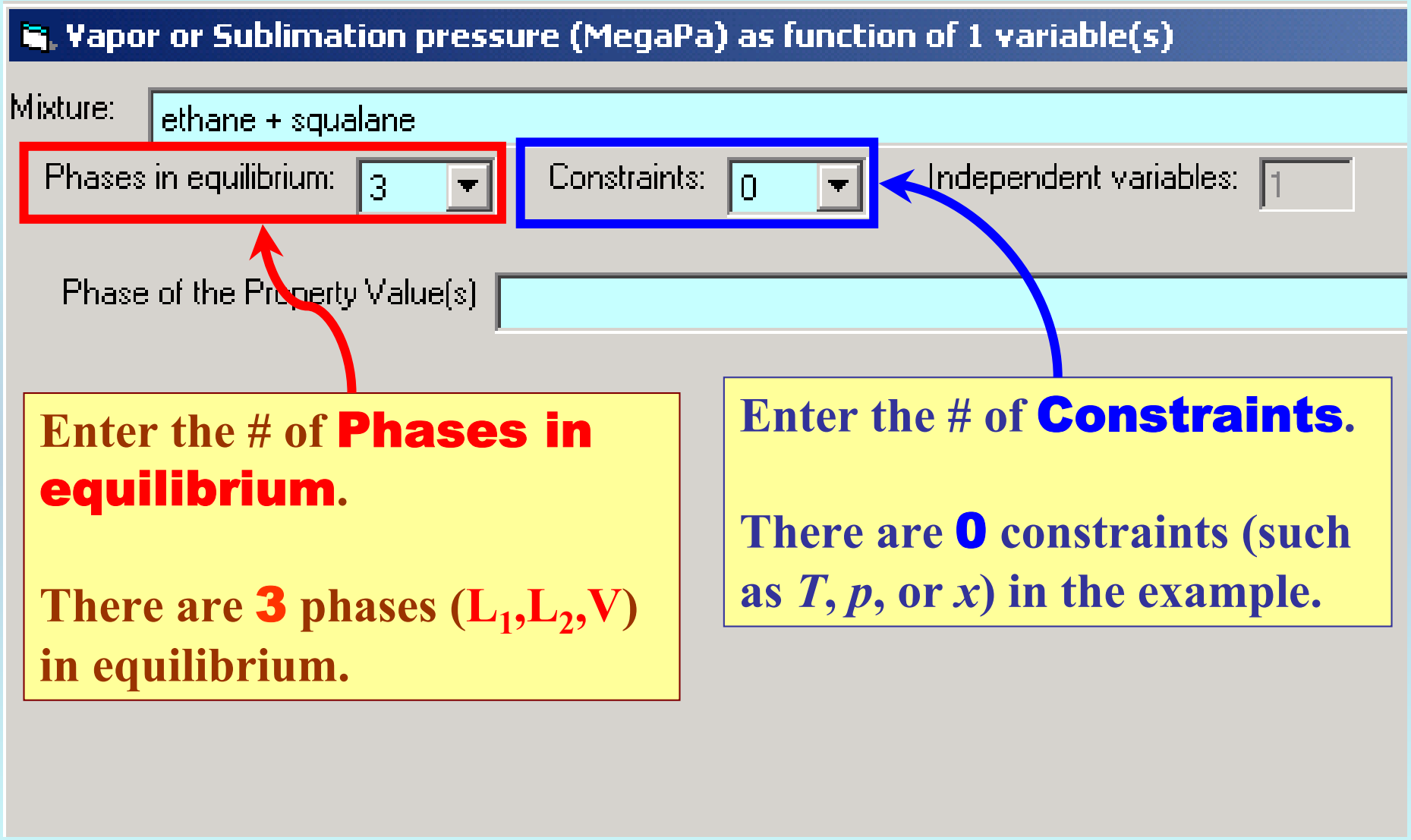


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for ethane + squalane
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Vapor or Sublimation pressure
Units:
MegaPa
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Vapor pressure, etc. from the menu. Here, the transition is between 1 and 2 liquid phases.
2. SELECT the Property: Vapor or Sublimation pressure from the menu.
3. SELECT the Units; MPa here.
Comment (optional)
OK
Cancel


Property and experimental method for ethane + squalane
Help
Property
Property:
Units:
1. SELECT Method of Measurement from the list.
NOTE: Other is a valid selection and should include a brief description in the Comment field, such as shown below.
Method of measurement:
Other experimental method (please, describe in "Comments")
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
Cailletet apparatus according to the synthetic method. See details in de Loos et al, J. Chem. Eng. Data, 1986, 31, 166.
3. CLICK OK
OK
Cancel

SELECTION of # of Phases in Equilibrium and # of Constraints

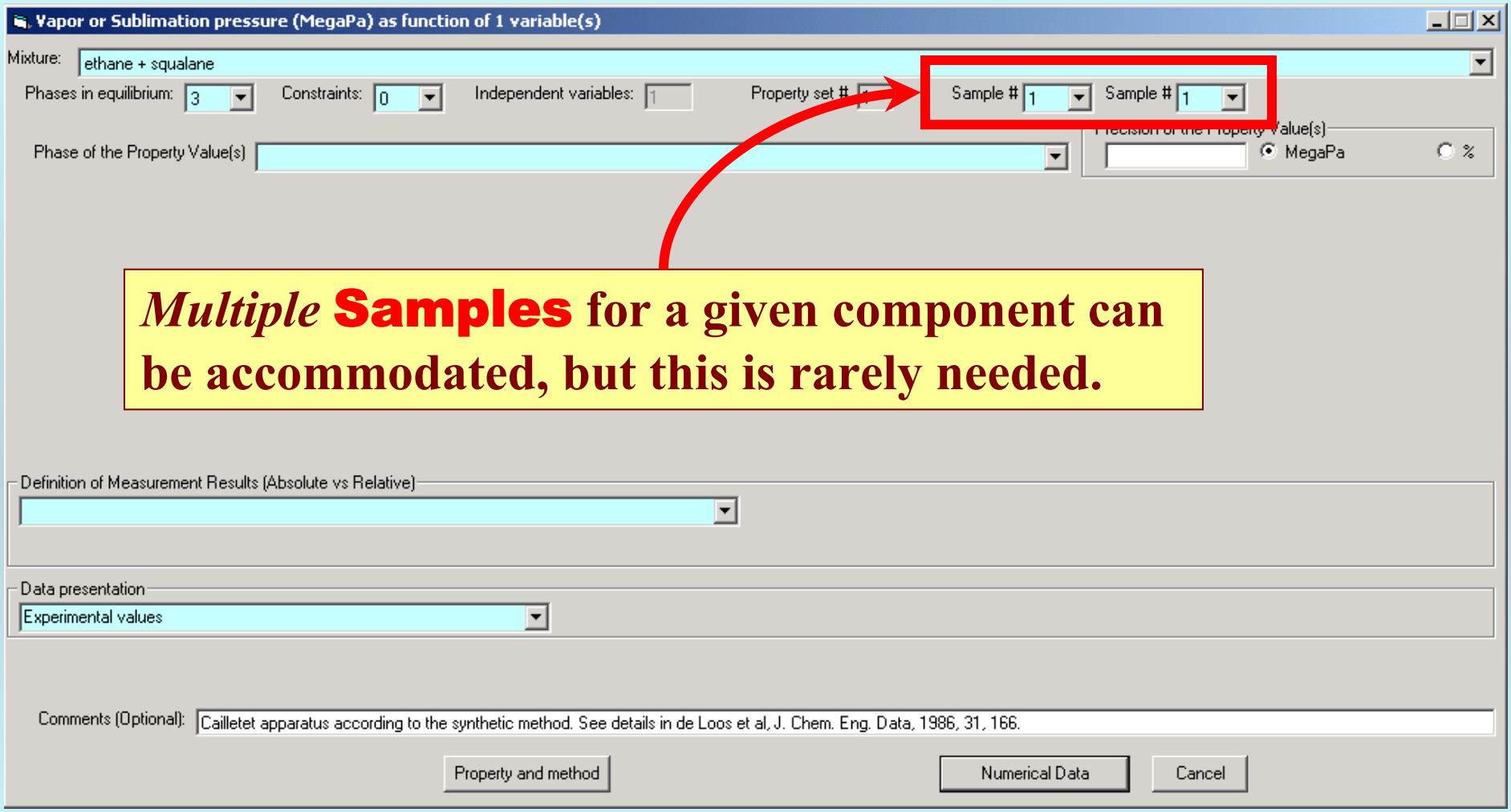


Enter the # of **Phases in equilibrium**.

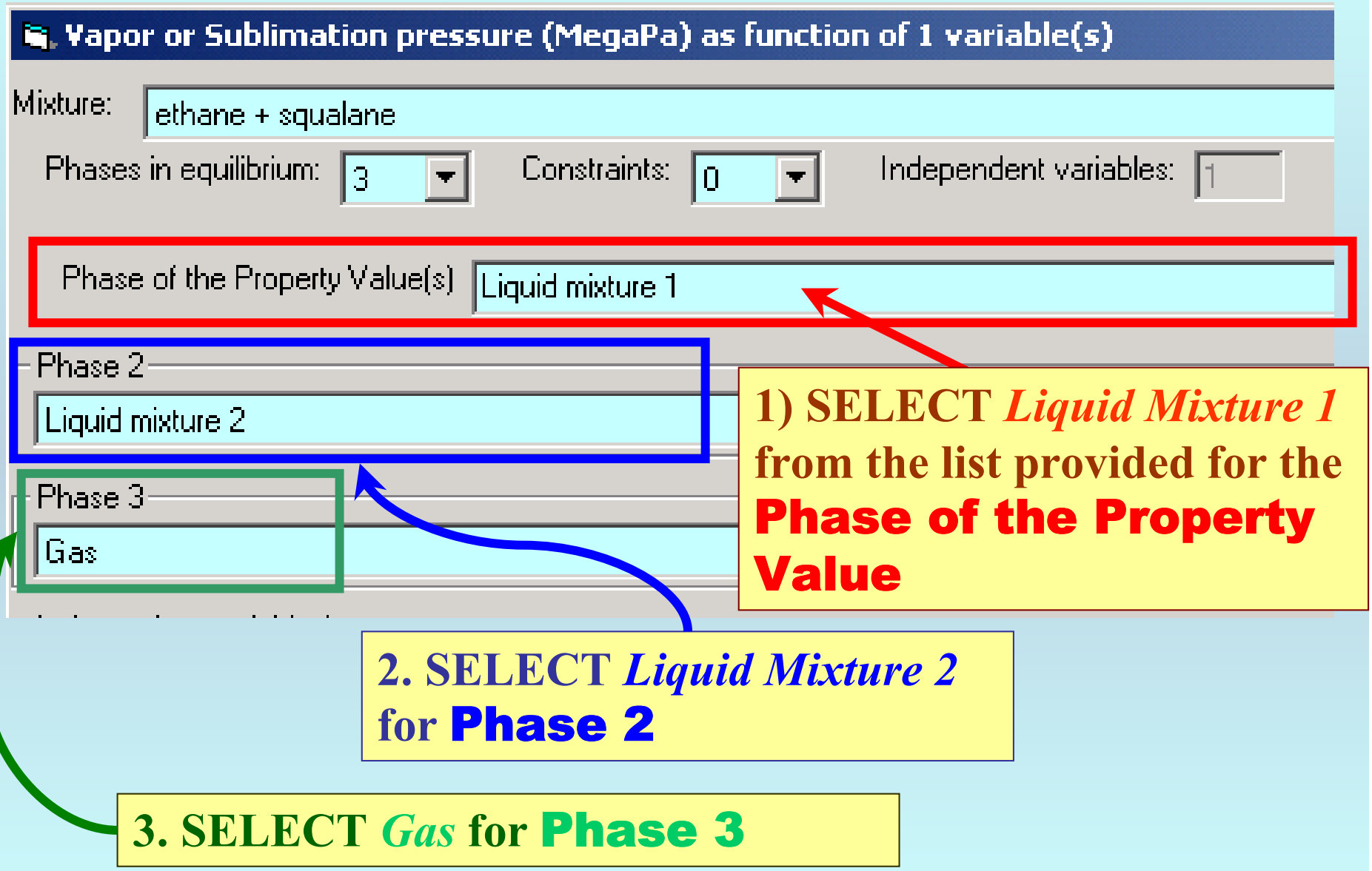
There are **3** phases (L_1,L_2,V) in equilibrium.

Enter the # of **Constraints**.

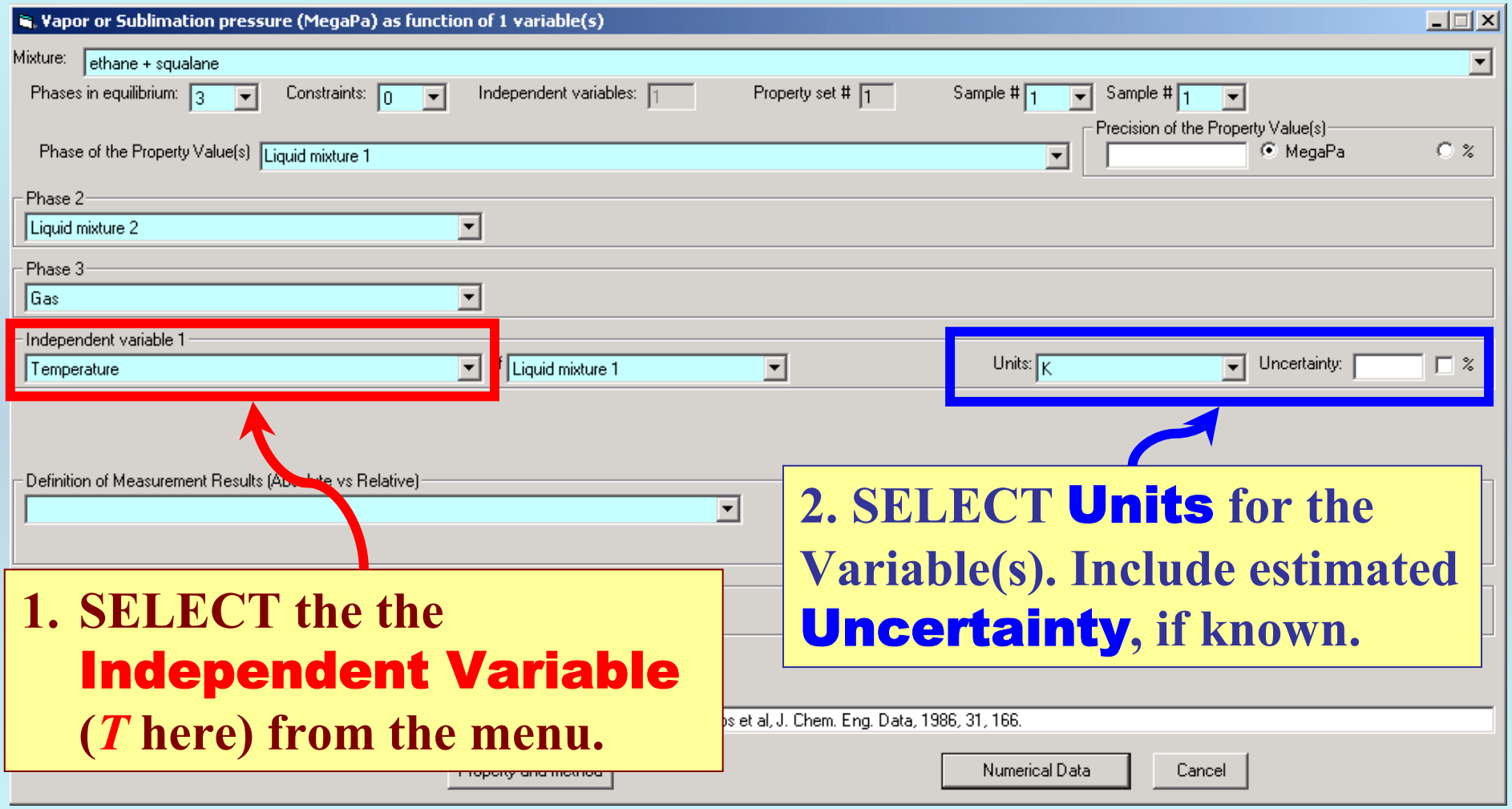
There are **0** constraints (such as *T*, *p*, or *x*) in the example.


Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)
Mixture:
ethane + squalane
Phases in equilibrium:
3
Constraints:
0
Independent variables:
1
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
Precision of the Property Value(s)
MegaPa
%
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):
Cailletet apparatus according to the synthetic method. See details in de Loos et al, J. Chem. Eng. Data, 1986, 31, 166.
Property and method
Numerical Data
Cancel

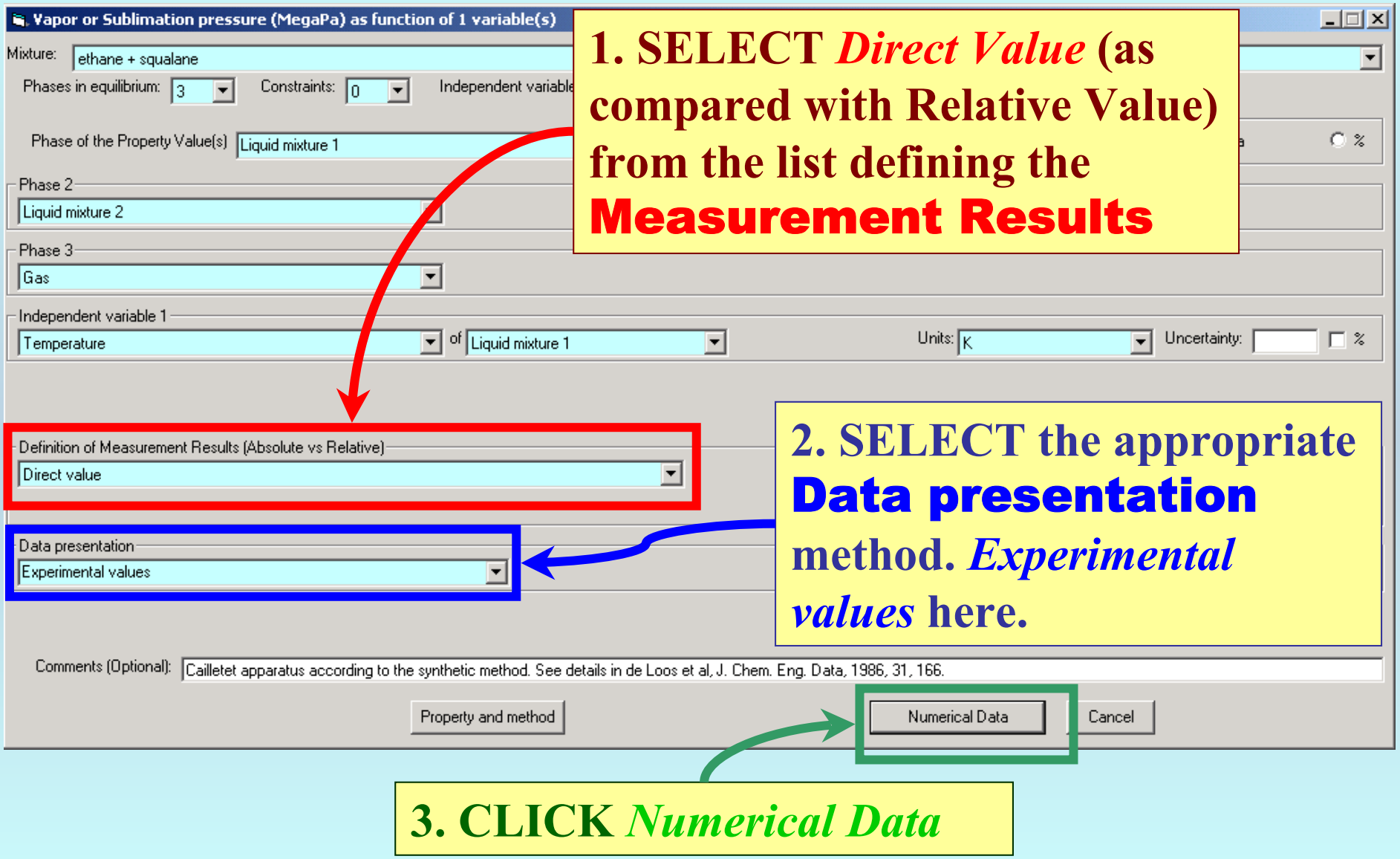
Select phases



Specification of constraints, constraint values, and constraint units



Measurement definition and Data presentation



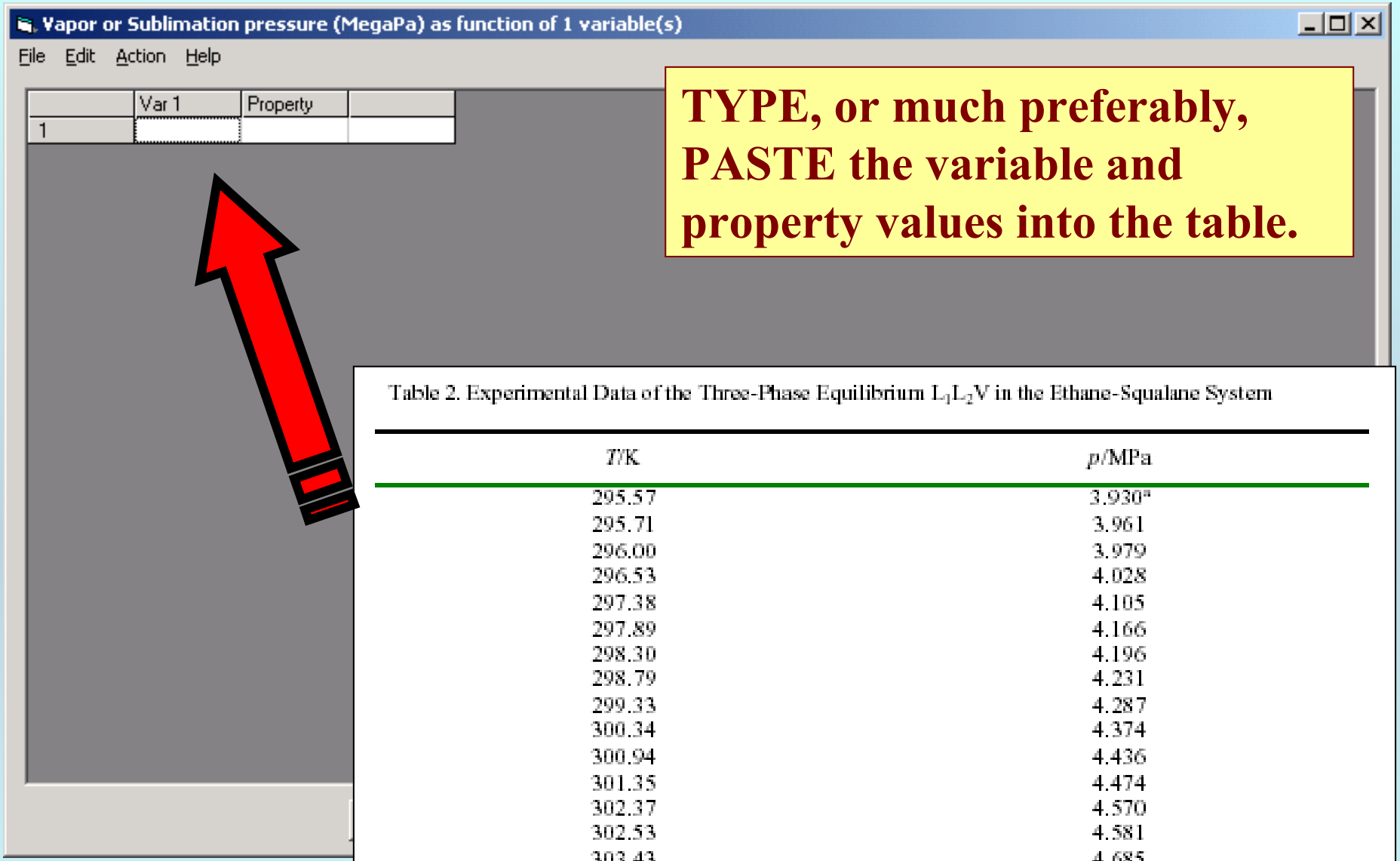


Table 2. Experimental Data of the Three-Phase Equilibrium L_1L_2V in the Ethane-Squalane System

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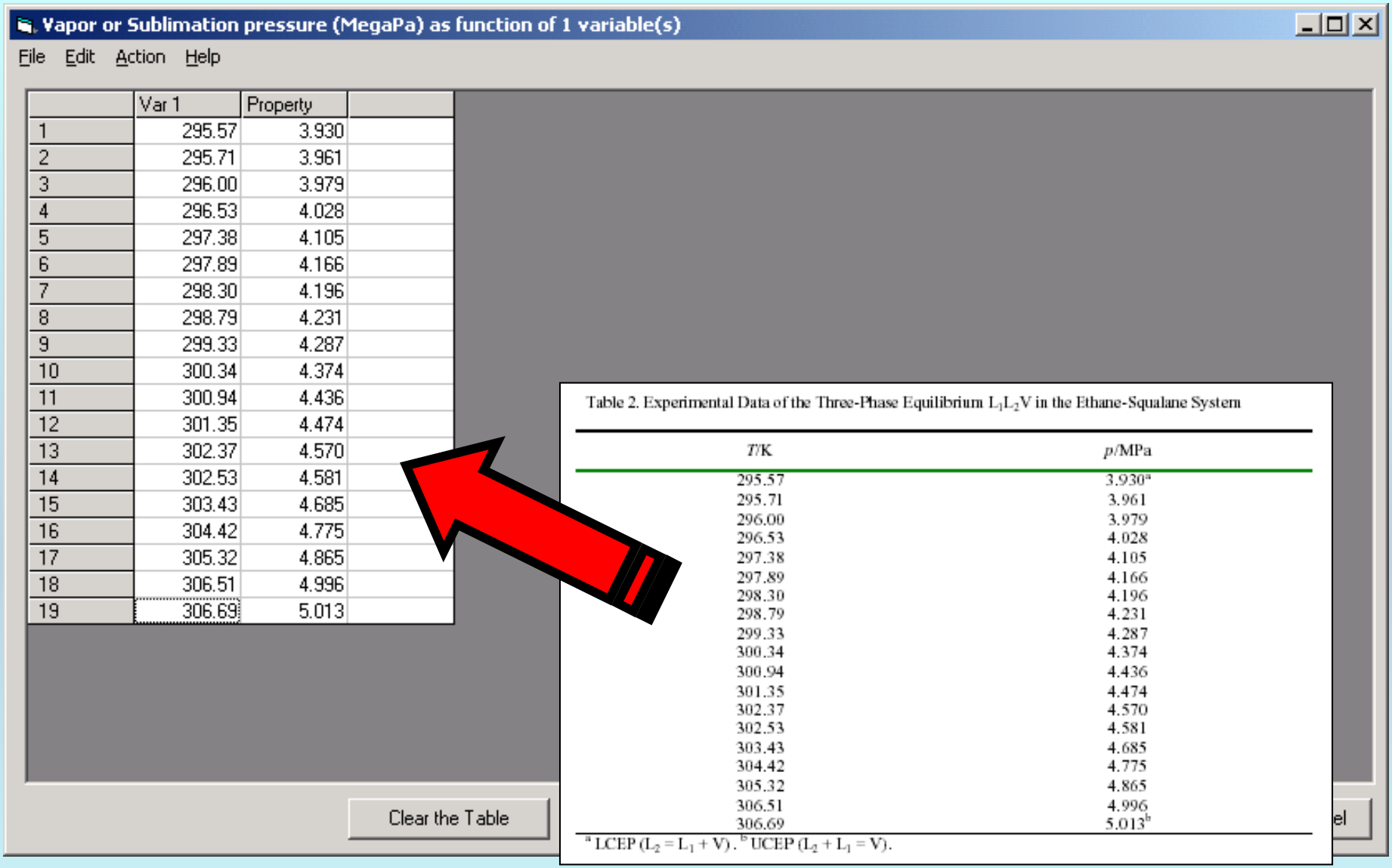
306.51	4.996
306.69	5.013[b]

[a] LCEP ($L_2 = L_1 + V$). [b] UCEP ($L_2 + L_1 = V$).



	Var 1	Property
1	295.57	3.930
2	295.71	3.961
3	296.00	3.979
4	296.53	4.028
5	297.38	4.105
6	297.89	4.166
7	298.30	4.196
8	298.79	4.231
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10	300.34	4.374
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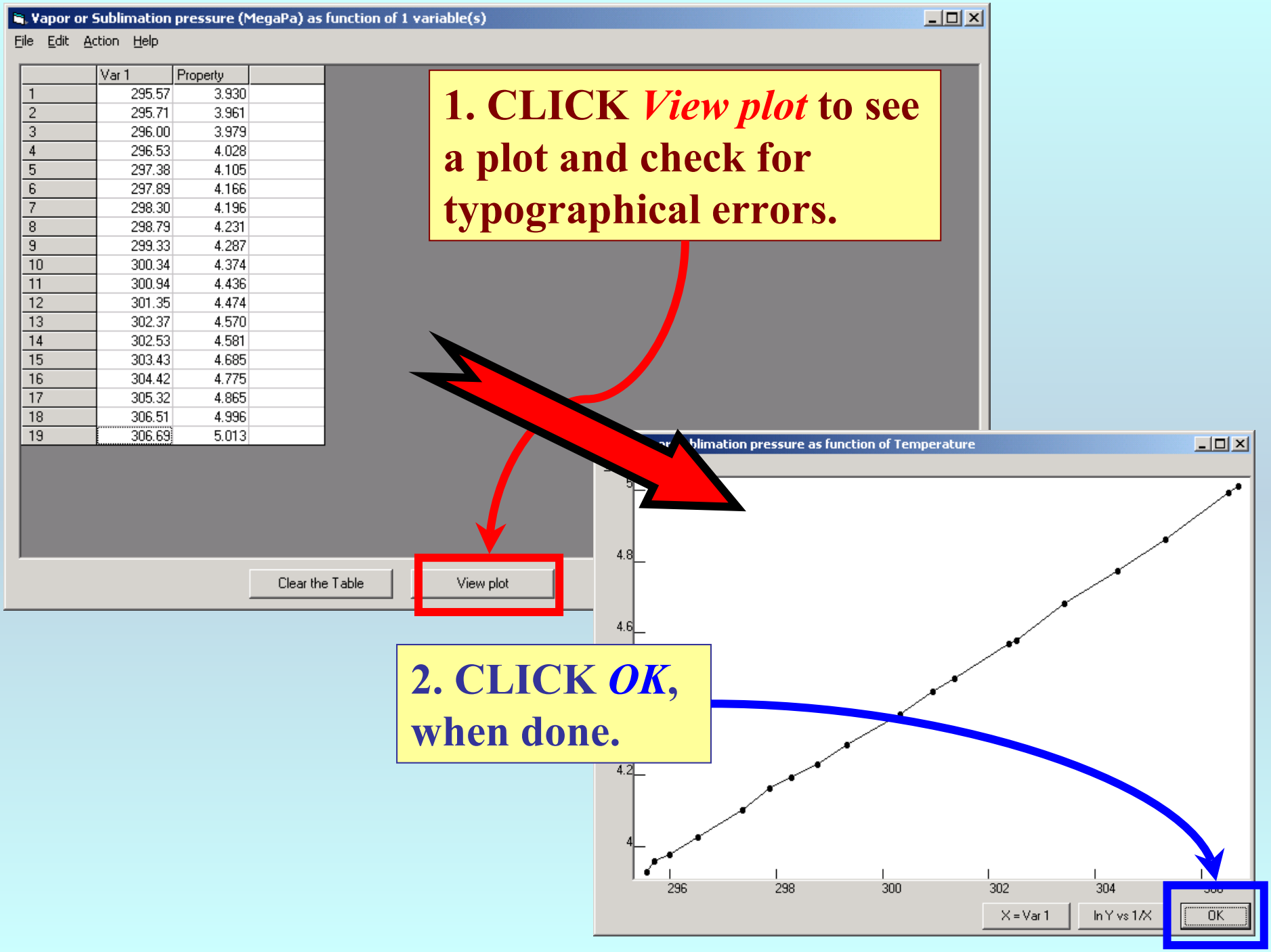
306.69	5.013[b]

[a] LCEP ($L_2 = L_1 + V$). [b] UCEP ($L_2 + L_1 = V$).

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 (MegaPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 295.57 3.930
2 295.71 3.961
3 296.00 3.979
4 296.53 4.028
5 297.38 4.105
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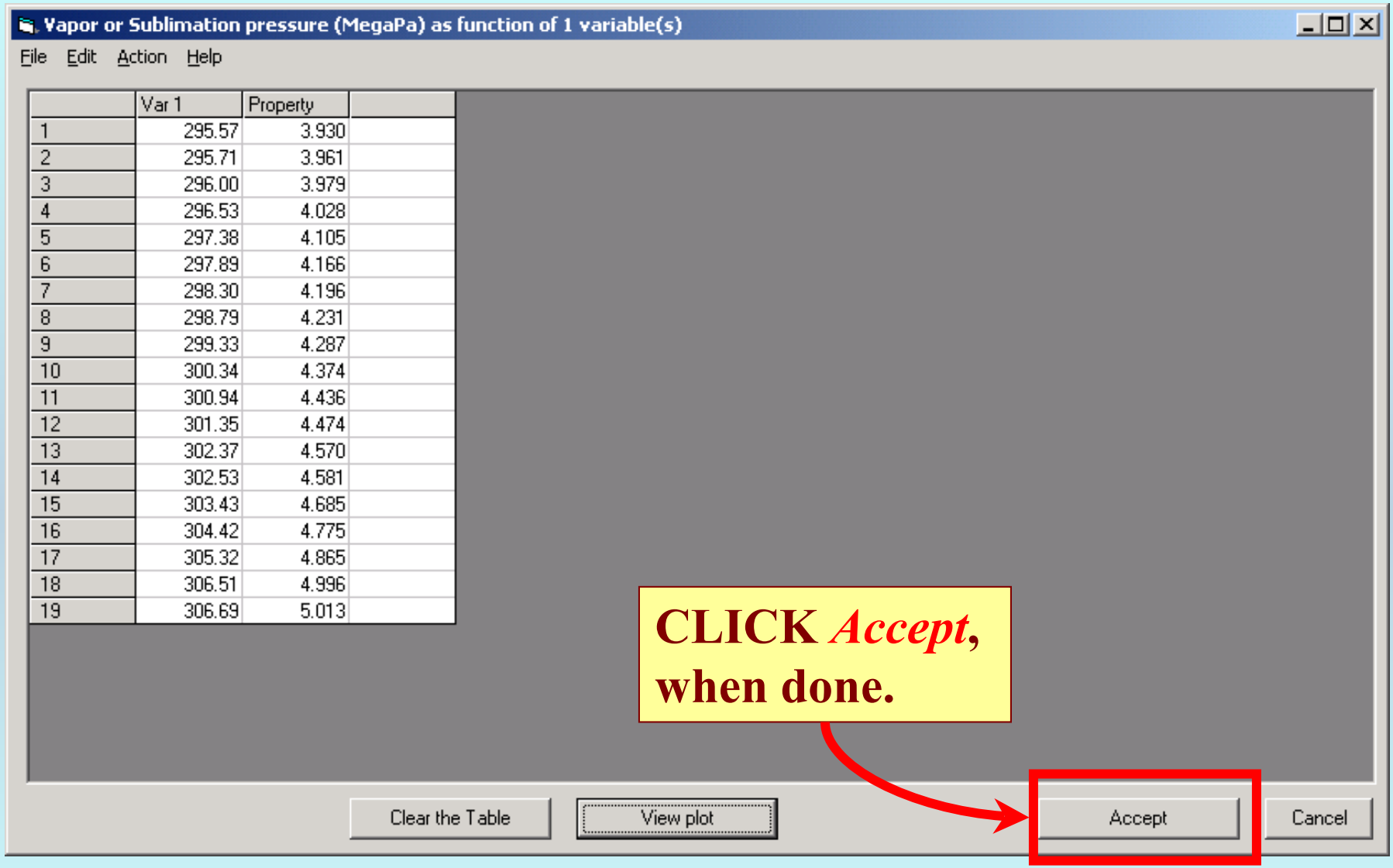
13 302.37 4.570
14 302.53 4.581
15 303.43 4.685
16 304.42 4.775
17 305.32 4.865
18 306.51 4.996
19 306.69 5.013
Clear the Table
View plot
1. CLICK View plot to see a plot and check for typographical errors.
blimation pressure as function of Temperature
4.8
4.6
4.2
4
296
298
300
302
304
X = Var 1
ln Y vs 1/X
OK
2. CLICK OK, when done.


Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 295.57 3.930
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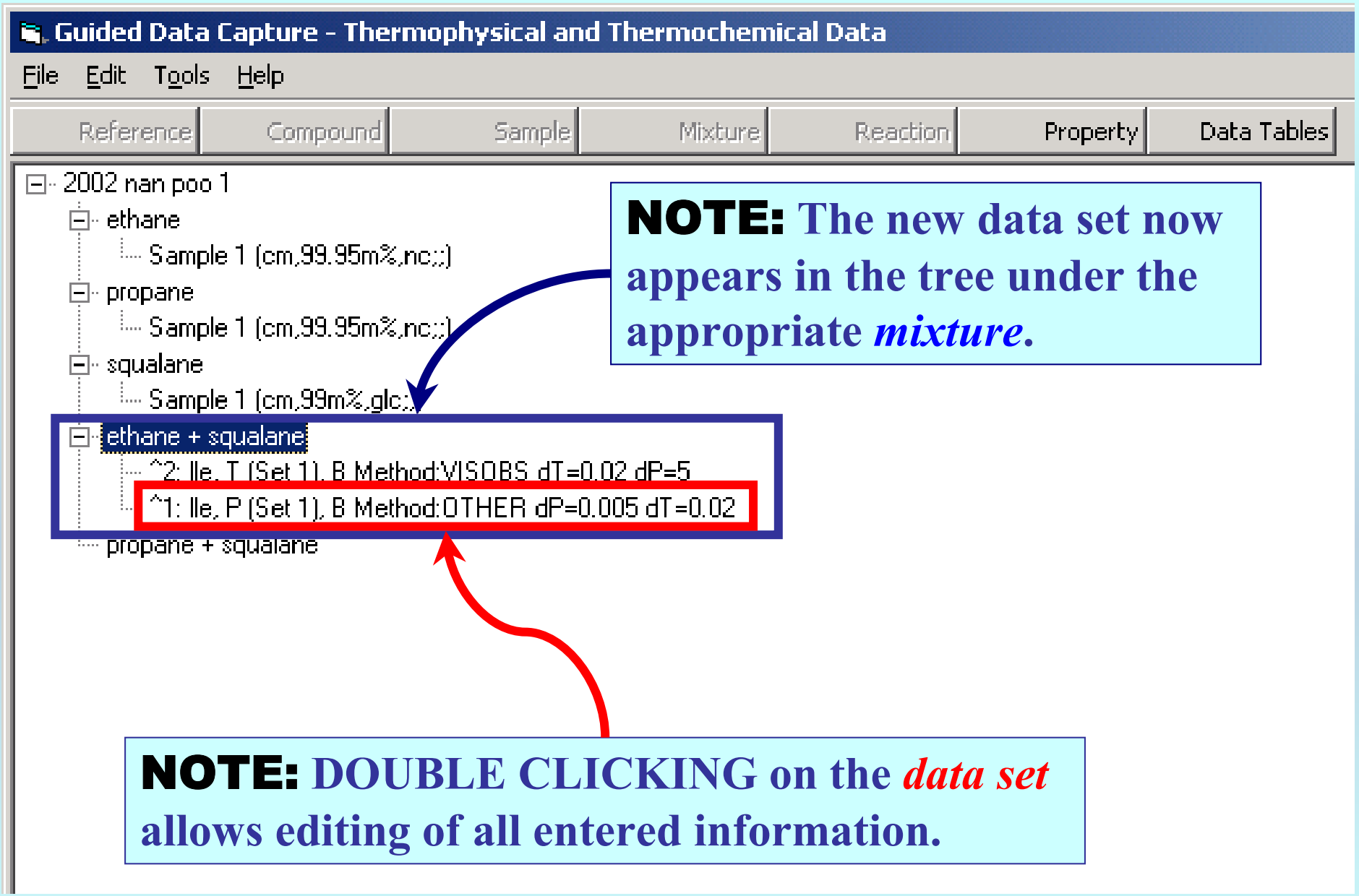
16 304.42 4.775
17 305.32 4.865
18 306.51 4.996
19 306.69 5.013
CLICK Accept, when done.
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property Data Tables
2002 nan poo 1
ethane
Sample 1 (cm,99.95m%,nc;;)
propane
Sample 1 (cm,99.95m%,nc;;)
squalane
Sample 1 (cm,99m%,glc;;)
ethane + squalane
^2: Ile, T (Set 1), B Method:VISOBS dT=0.02 dP=5
^1: Ile, P (Set 1), B Method:OTHER dP=0.005 dT=0.02
propane + squalane
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.**