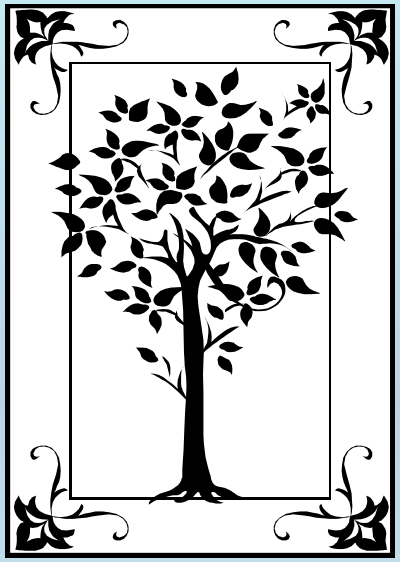
METADATA AND NUMERICAL DATA CAPTURE:
Liquid-Liquid Equilibrium
TEMPERATURES (2-components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
LLE TEMPERATURES
for 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 is from:

892 *J. Chem. Eng. Data* 1999, *44*, 892−895

Thermodynamic Properties of *N*-Alkoxyethanols + Organic Solvent Mixtures. X. Liquid−Liquid Equilibria of Systems Containing 2-Methoxyethanol, 2-(2-Methoxyethoxy)ethanol or 2-(2-Ethoxyethoxy)ethanol, and Selected Alkanes

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Liquid−liquid equilibria (LLE) data are reported for 2-methoxyethanol + heptane, + methylcyclohexane, or + 2,2,4-trimethylpentane and for 2-(2-methoxyethoxy)ethanol + 2,2,4-trimethylpentane and 2-(2-ethoxyethoxy)ethanol + methylcyclohexane mixtures between 281.8 K and the upper critical solution temperatures (UCSTs). The coexistence curves were determined visually. They have a rather horizontal top and are skewed to the region of higher mole fractions of the alkoxyethanol, x_1, for systems with 2-methoxyethanol, and to the region of lower x_1 values for the mixtures including the other two hydroxyethers. The (x_1, T) data were fitted to the equation $T = T_c + k|y - y_c|^m$, where $y = \alpha x_1/\{1 + x_1(\alpha - 1)\}$ and $y_c = \alpha x_{1c}/\{1 + x_{1c}(\alpha - 1)\}$. T_c and x_{1c} are the coordinates of the critical points fitted together with k, m, and α. Results are briefly discussed on the basis of the existence of inter- and intramolecular H-bonds as well as of dipole interactions, which occur in solutions containing hydroxyethers.

Experimental method information:

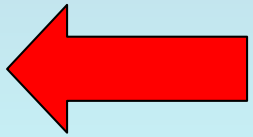
The coexistence curves of the binary mixtures were determined visually (Loven and Rice, 1963; Young, 1969; Snyder and Eckert, 1973). The samples in the sealed Pyrex tubes were placed in a thermostat bath a few hundreths of a degree above the expected temperature, and the appearance of a second phase upon slow cooling (4 K h^{-1}) was noted. The separation temperatures were reproducible to ±0.02 K for temperatures near the upper critical solution temperature. The precision of the equilibrum composition is expected to be better than 0.0005 mole fraction.

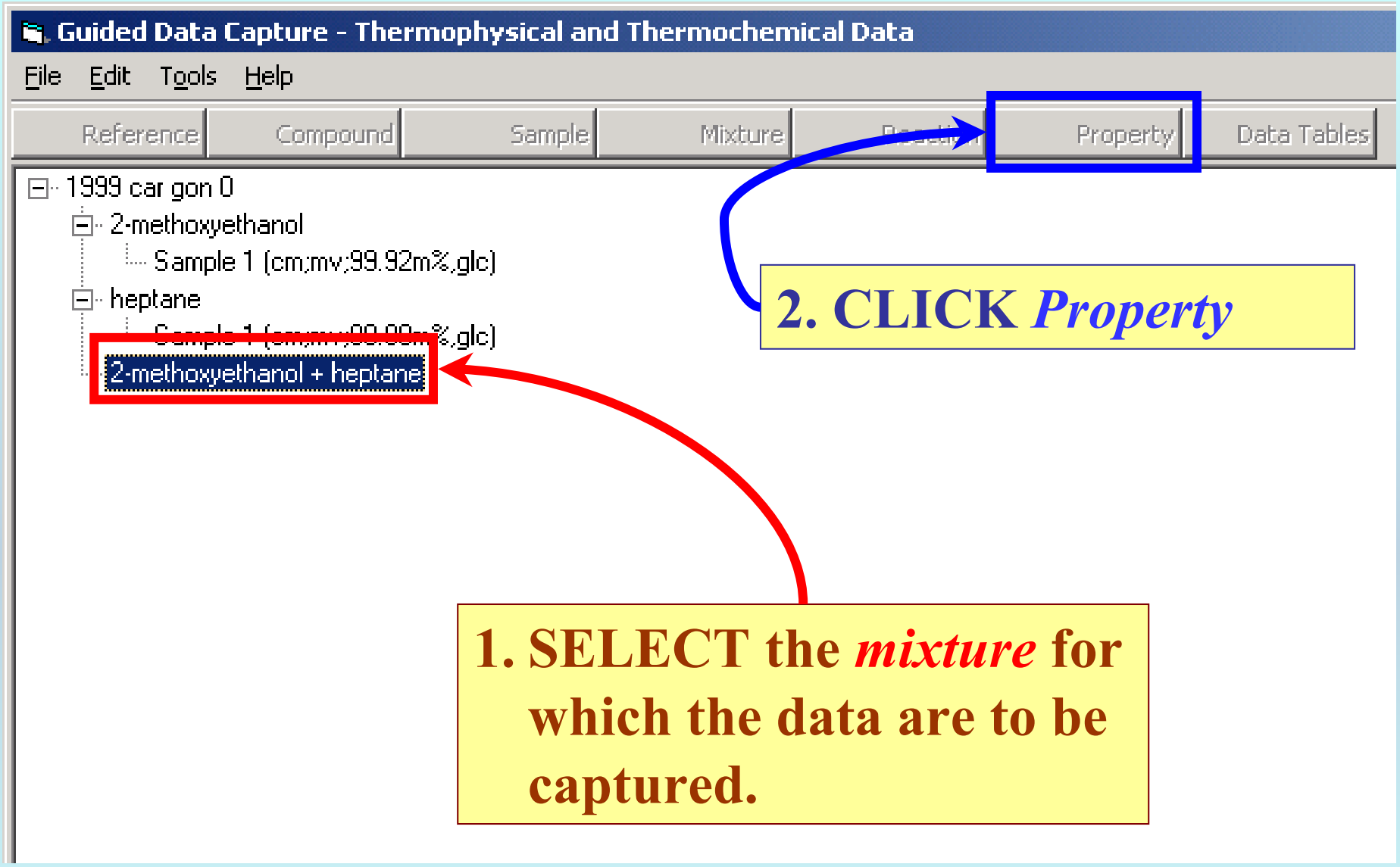
Liquid-Liquid Equilibrium temperatures (2 components) for **2-methoxyethanol (1) + heptane (2)**

Table 2. Experimental Liquid−Liquid Equilibrium Temperatures for the 2-Methoxyethanol (1) + Heptane (2) Mixture

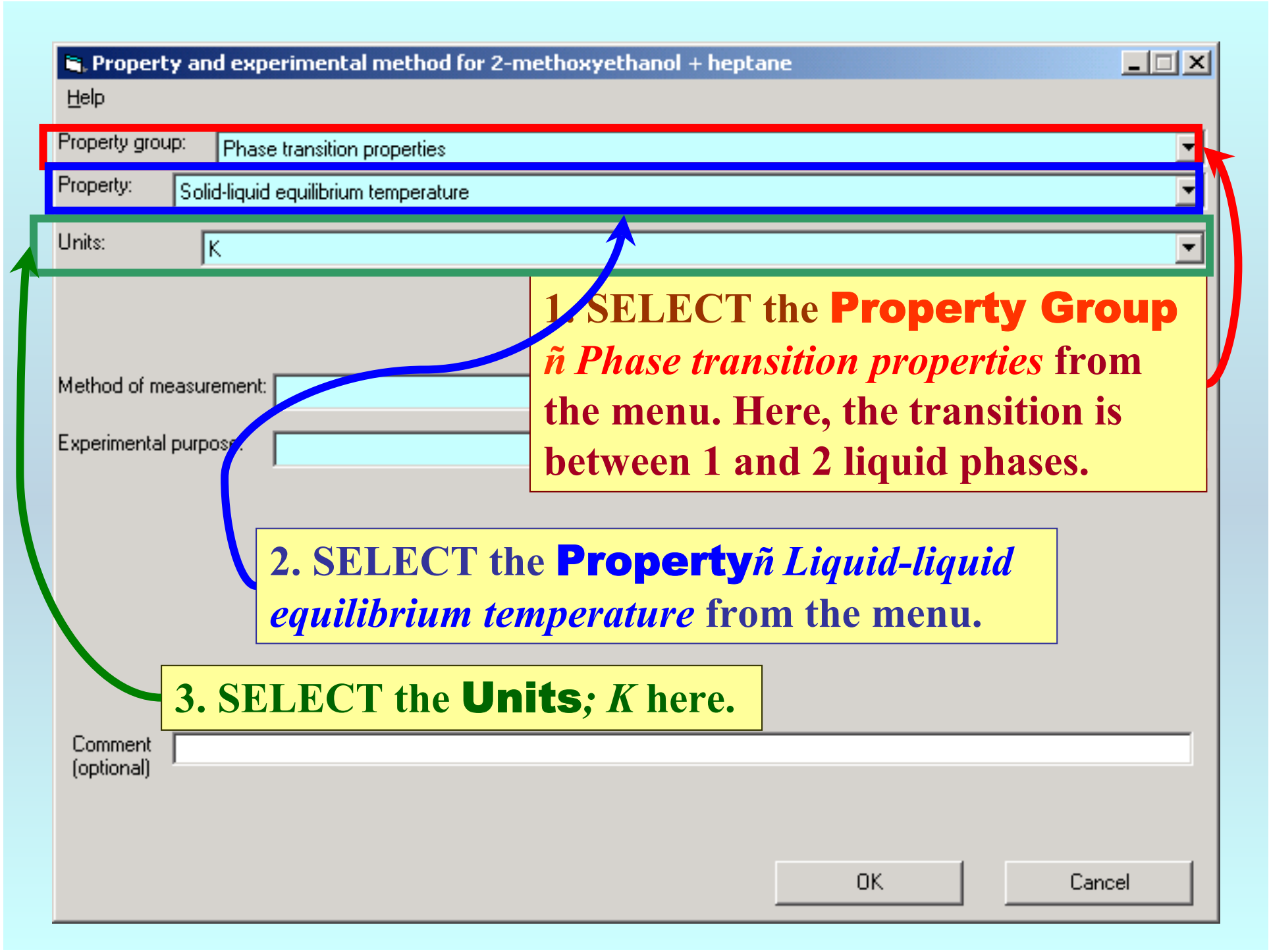
x_1	T/K	x_1	T/K
0.1933	308.57	0.5327	319.72
0.2133	310.29	0.5513	319.74
0.2207	311.26	0.5747	319.80
0.2411	312.25	0.6012	319.73
0.2602	313.55	0.6022	319.80
0.2875	315.31	0.6232	319.67
0.3058	315.99	0.6447	319.55
0.3113	316.41	0.6668	319.23
0.3327	317.02	0.6875	319.04
0.3506	317.67	0.6896	318.90
0.3773	318.53	0.7092	318.37
0.4129	319.07	0.7332	317.47
0.4140	319.08	0.7540	316.45
0.4323	319.33	0.7764	314.86
0.4686	319.59	0.7864	314.03
0.4955	319.69	0.8074	311.71
0.5058	319.82	0.8400	306.71
0.5077	319.74		

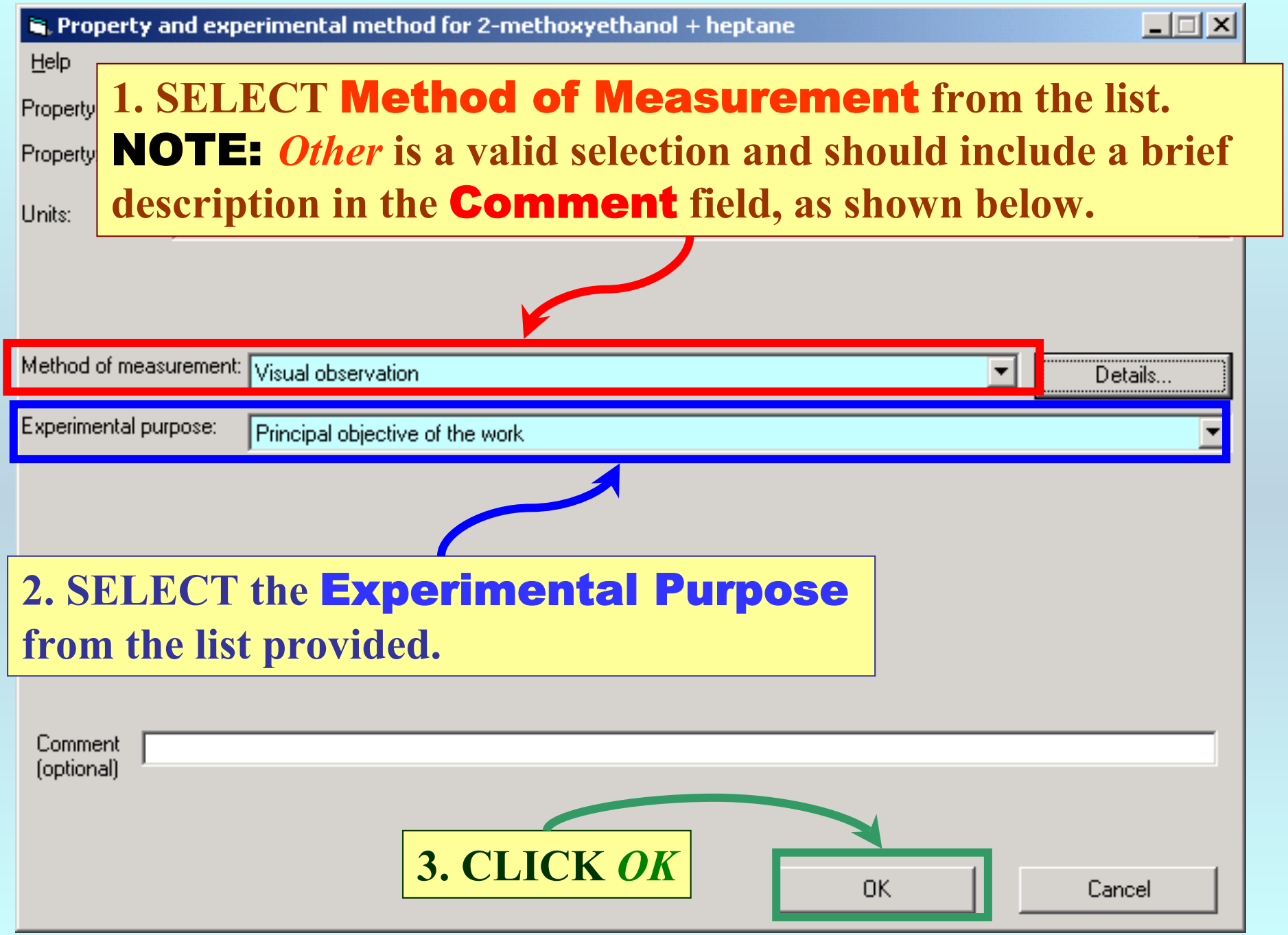
This data set is considered here.



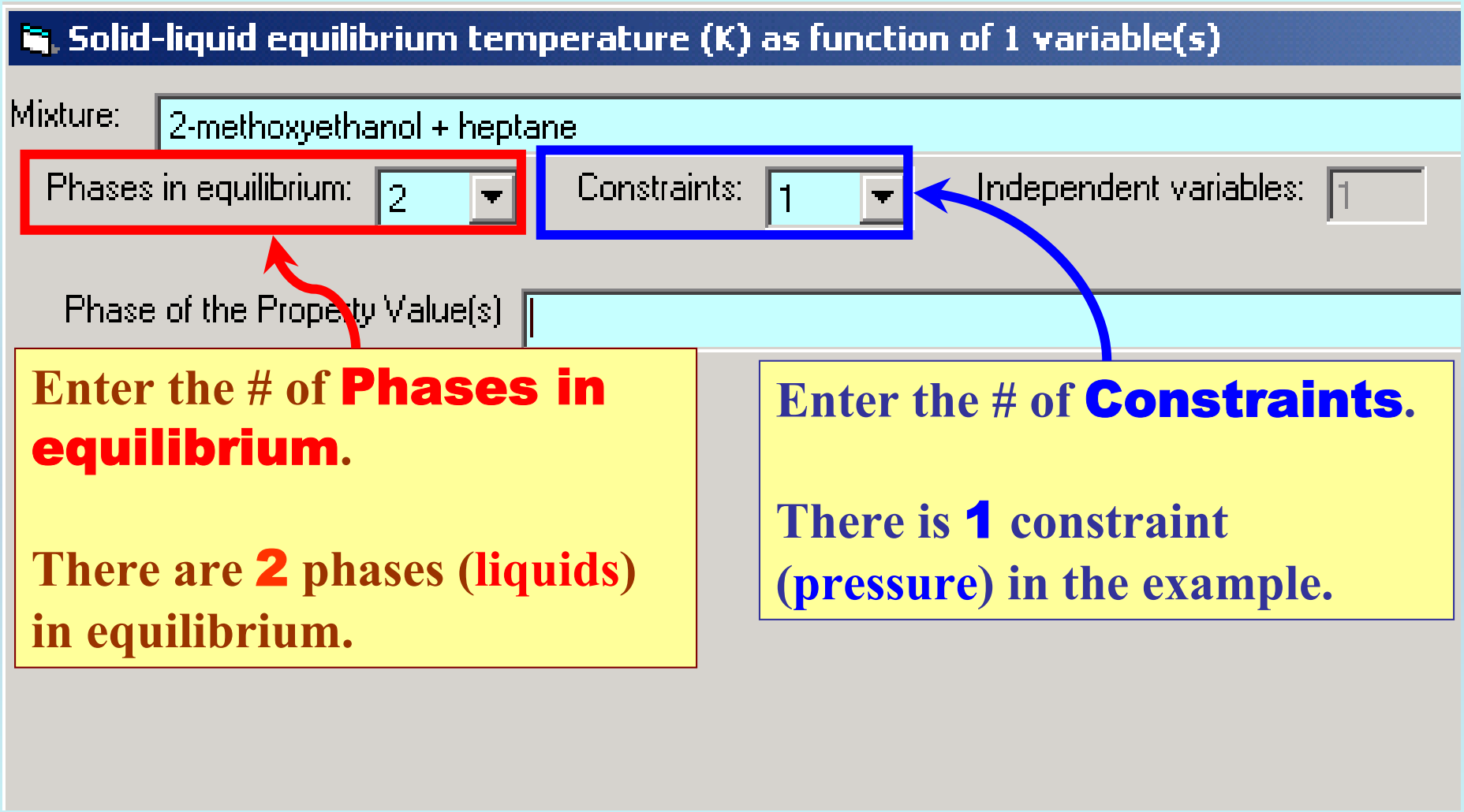


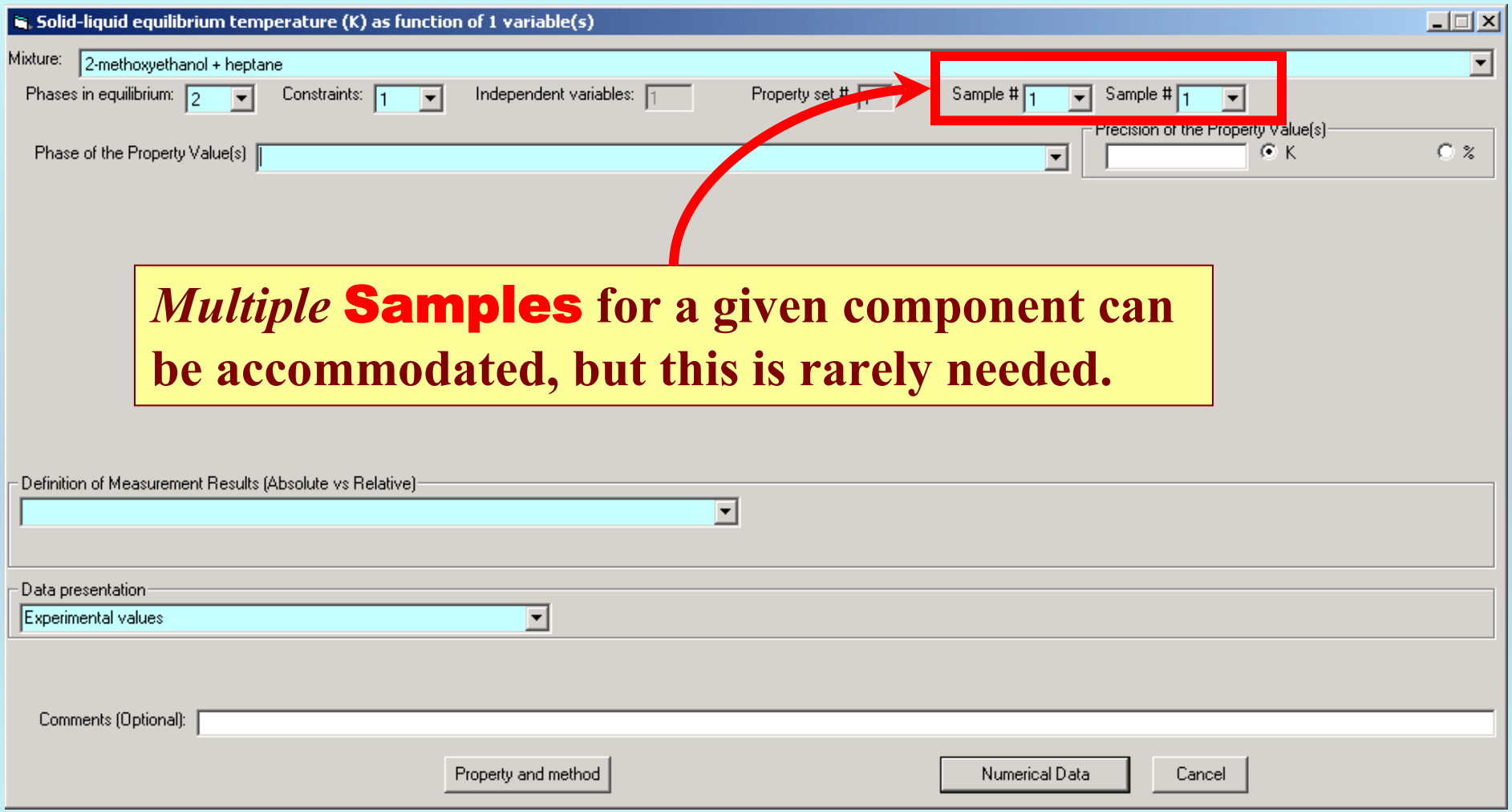
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

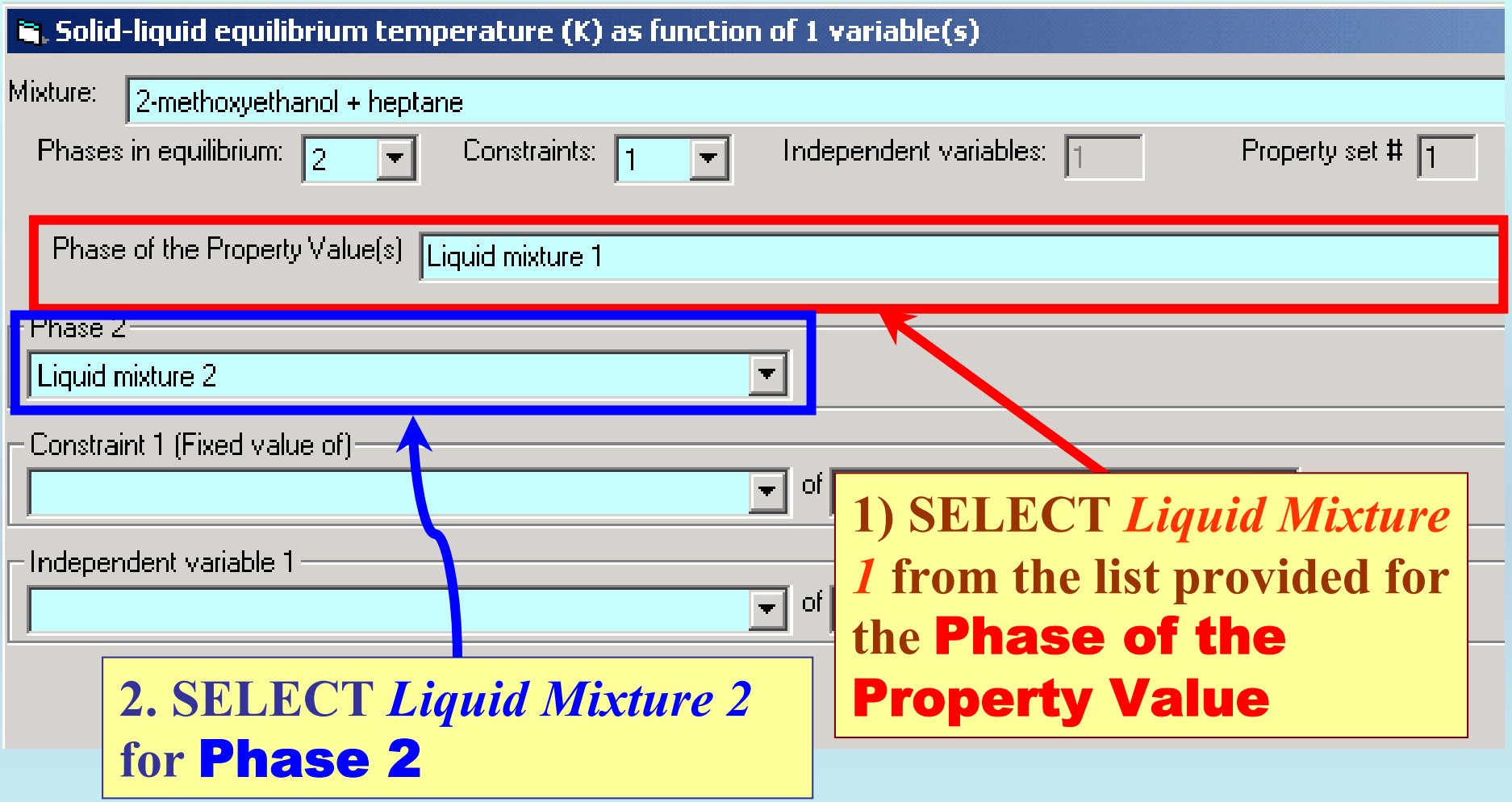

Property and experimental method for 2-methoxyethanol + heptane
Help
Property group:
Phase transition properties
Property:
Solid-liquid equilibrium temperature
Units:
K
Method of measurement:
Experimental purpose:
1. SELECT the Property Group ñ Phase transition properties from the menu. Here, the transition is between 1 and 2 liquid phases.
2. SELECT the Property ñ Liquid-liquid equilibrium temperature from the menu.
3. SELECT the Units; K here.
Comment (optional)
OK
Cancel


Property and experimental method for 2-methoxyethanol + heptane
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, as shown below.
Method of measurement:
Visual observation
Details...
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK OK
OK
Cancel

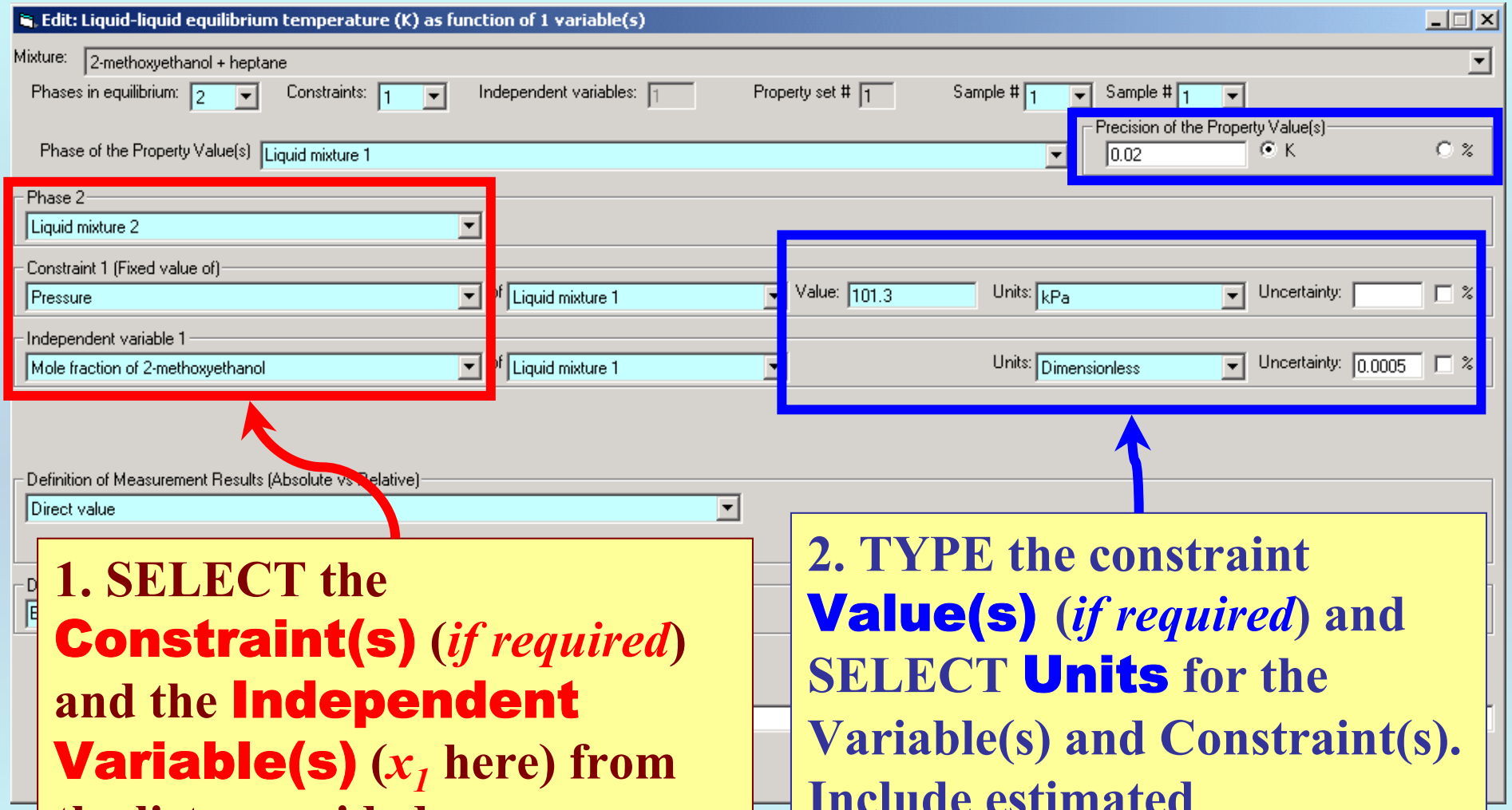
SELECTION of # of Phases in Equilibrium and # of Constraints




Solid-liquid equilibrium temperature (K) as function of 1 variable(s)
Mixture:
2-methoxyethanol + heptane
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
Precision 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


Solid-liquid equilibrium temperature (K) as function of 1 variable(s)
Mixture:
2-methoxyethanol + heptane
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
1
Phase of the Property Value(s)
Liquid mixture 1
Phase 2
Liquid mixture 2
Constraint 1 (Fixed value of)
of
Independent variable 1
of
1) SELECT Liquid Mixture 1 from the list provided for the Phase of the Property Value
2. SELECT Liquid Mixture 2 for Phase 2

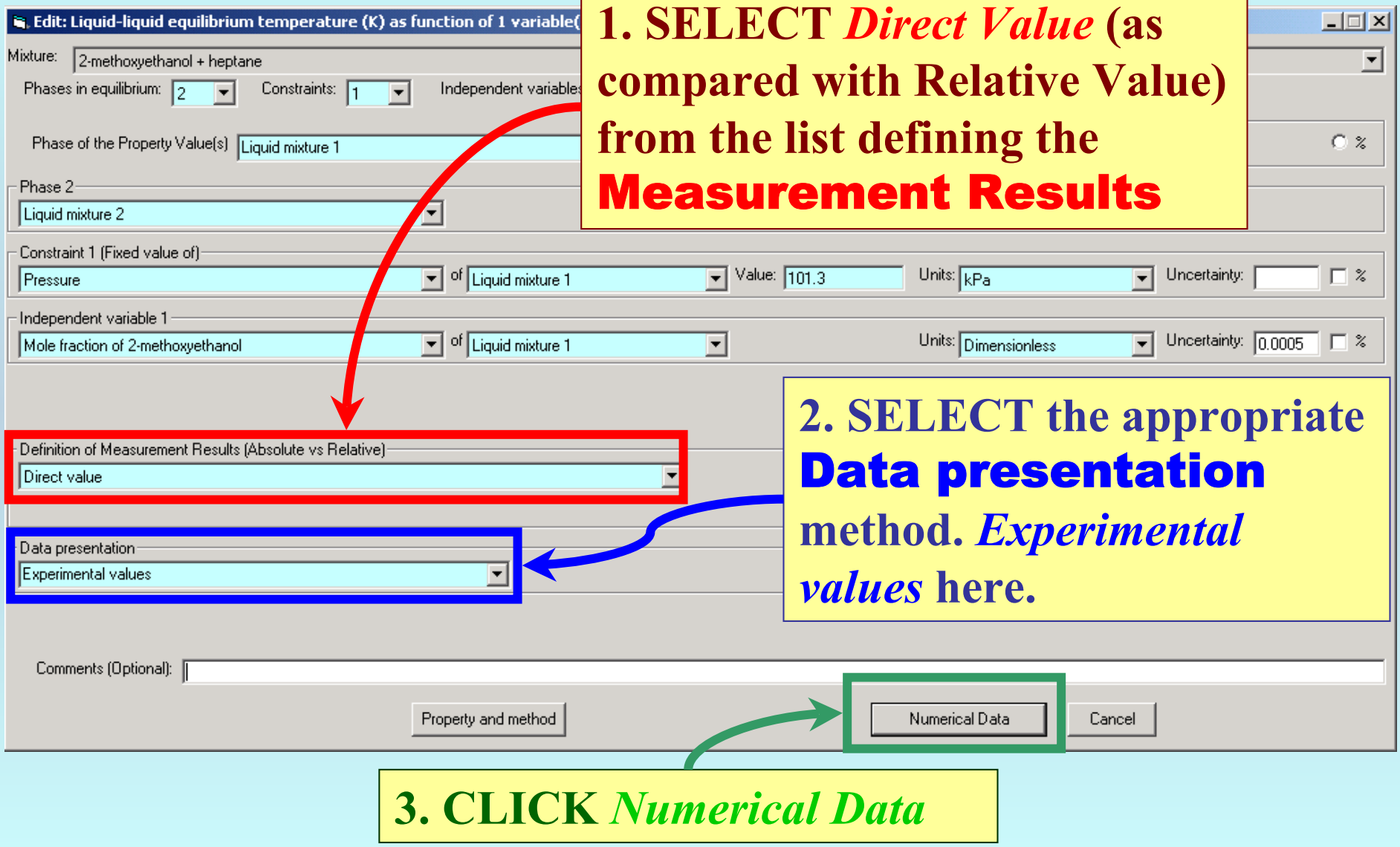
Specification of constraints, constraint values, and constraint units



1. SELECT the Constraint(s) (*if required*) and the Independent Variable(s) (x_1 here) from the lists provided.

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

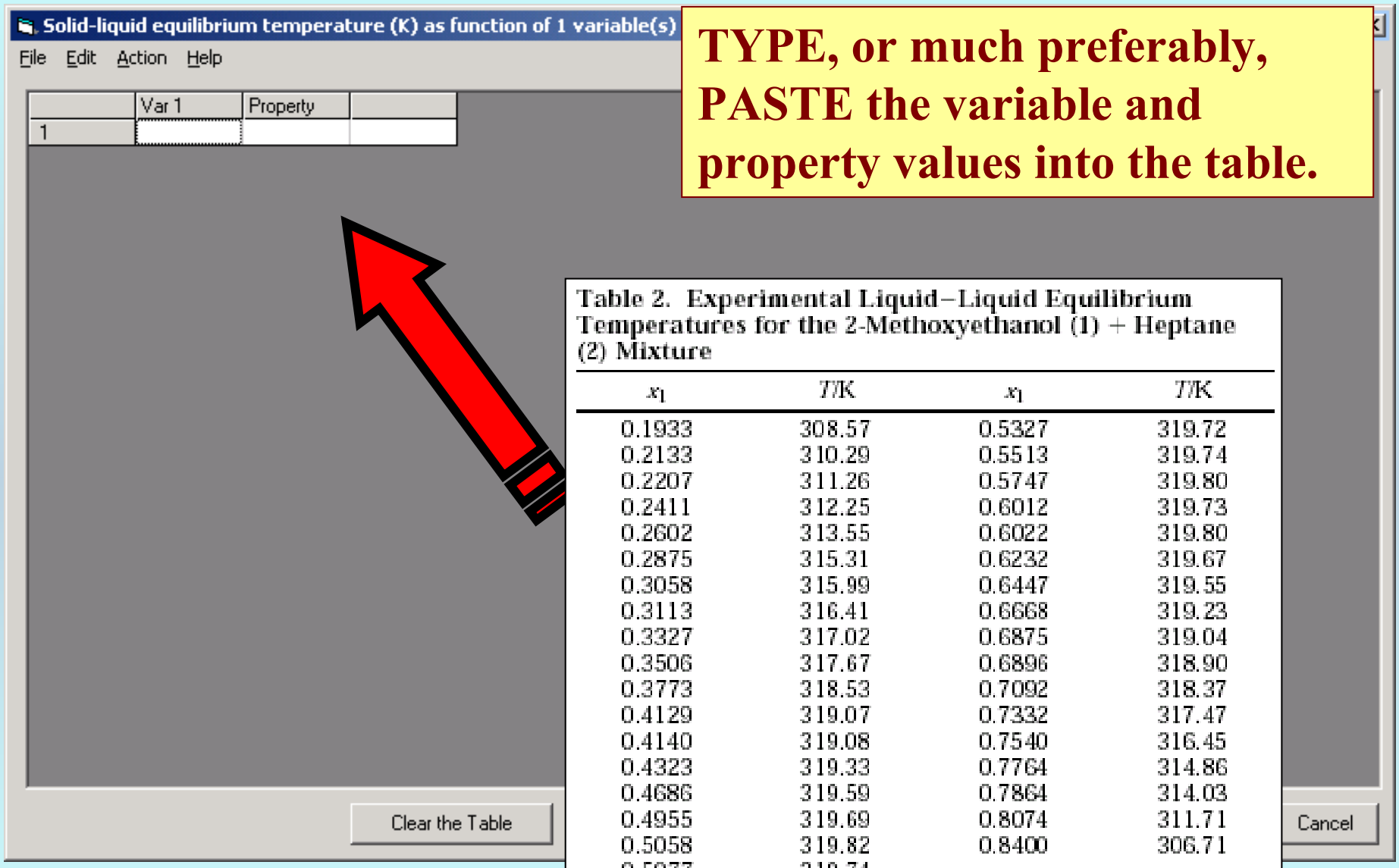
Measurement definition and Data presentation



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*



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

Table 2. Experimental Liquid−Liquid Equilibrium Temperatures for the 2-Methoxyethanol (1) + Heptane (2) Mixture

x_1	T/K	x_1	T/K
0.1933	308.57	0.5327	319.72
0.2133	310.29	0.5513	319.74
0.2207	311.26	0.5747	319.80
0.2411	312.25	0.6012	319.73
0.2602	313.55	0.6022	319.80
0.2875	315.31	0.6232	319.67
0.3058	315.99	0.6447	319.55
0.3113	316.41	0.6668	319.23
0.3327	317.02	0.6875	319.04
0.3506	317.67	0.6896	318.90
0.3773	318.53	0.7092	318.37
0.4129	319.07	0.7332	317.47
0.4140	319.08	0.7540	316.45
0.4323	319.33	0.7764	314.86
0.4686	319.59	0.7864	314.03
0.4955	319.69	0.8074	311.71
0.5058	319.82	0.8400	306.71
0.5077	319.74		

Solid-liquid equilibrium temperature (K) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	0.1933	308.57
2	0.2133	310.29
3	0.2207	311.26
4	0.2411	312.25
5	0.2602	313.55
6	0.2875	315.31
7	0.3058	315.99
8	0.3113	316.41
9	0.3327	317.02
10	0.3506	317.67
11	0.3773	318.53
12	0.4129	319.07
13	0.4140	319.08
14	0.4323	319.33
15	0.4686	319.59
16	0.4955	319.69
17	0.5058	319.82
18	0.5077	319.74
19	0.5327	319.72
20	0.5513	319.74
21	0.5747	319.80
22	0.6012	319.73
23	0.6022	319.80
24	0.6232	319.67
25	0.6447	319.55

Clear the Table

Table 2. Experimental Liquid−Liquid Equilibrium Temperatures for the 2-Methoxyethanol (1) + Heptane (2) Mixture

x_1	T/K	x_1	T/K
0.1933	308.57	0.5327	319.72
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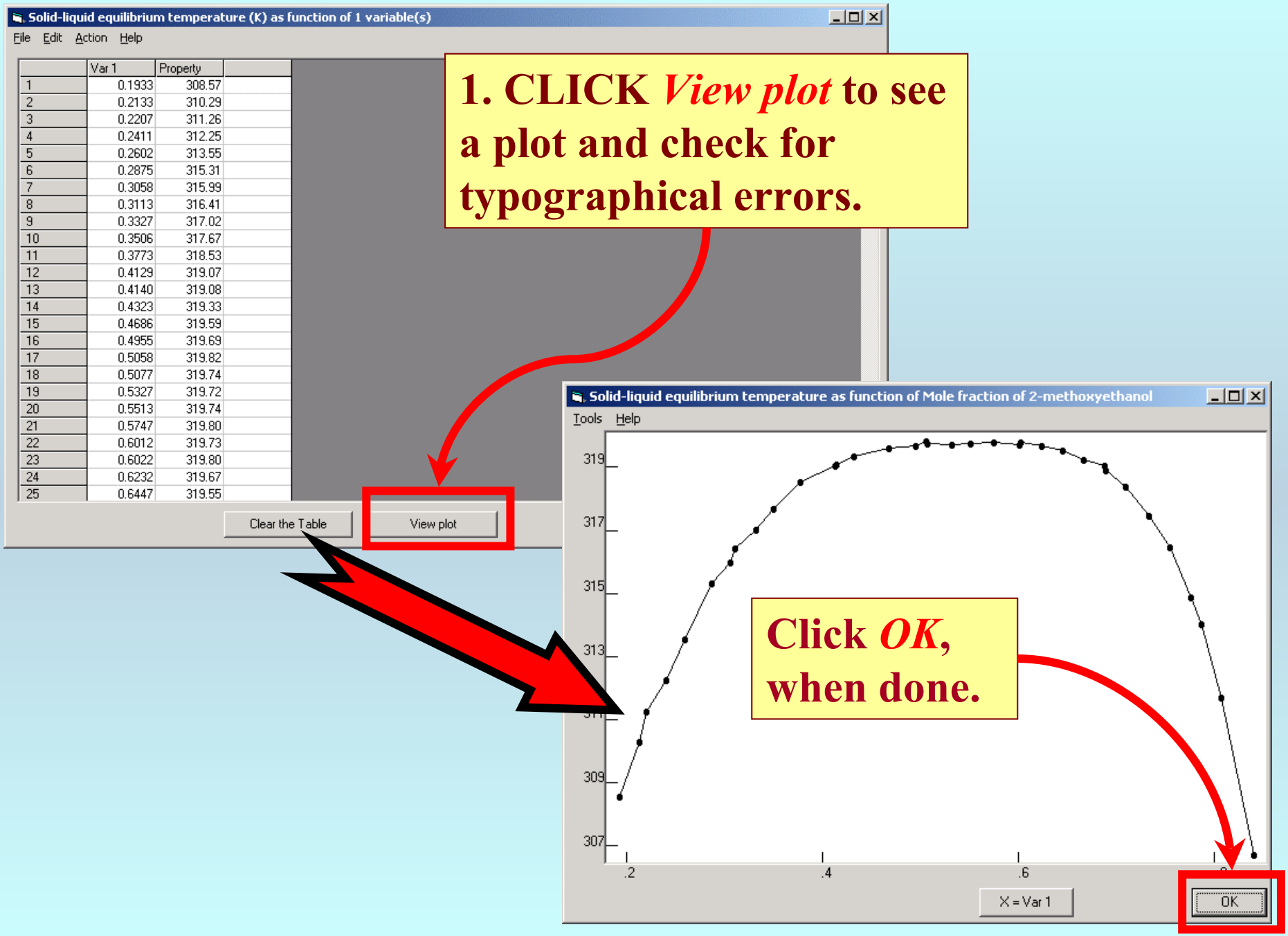
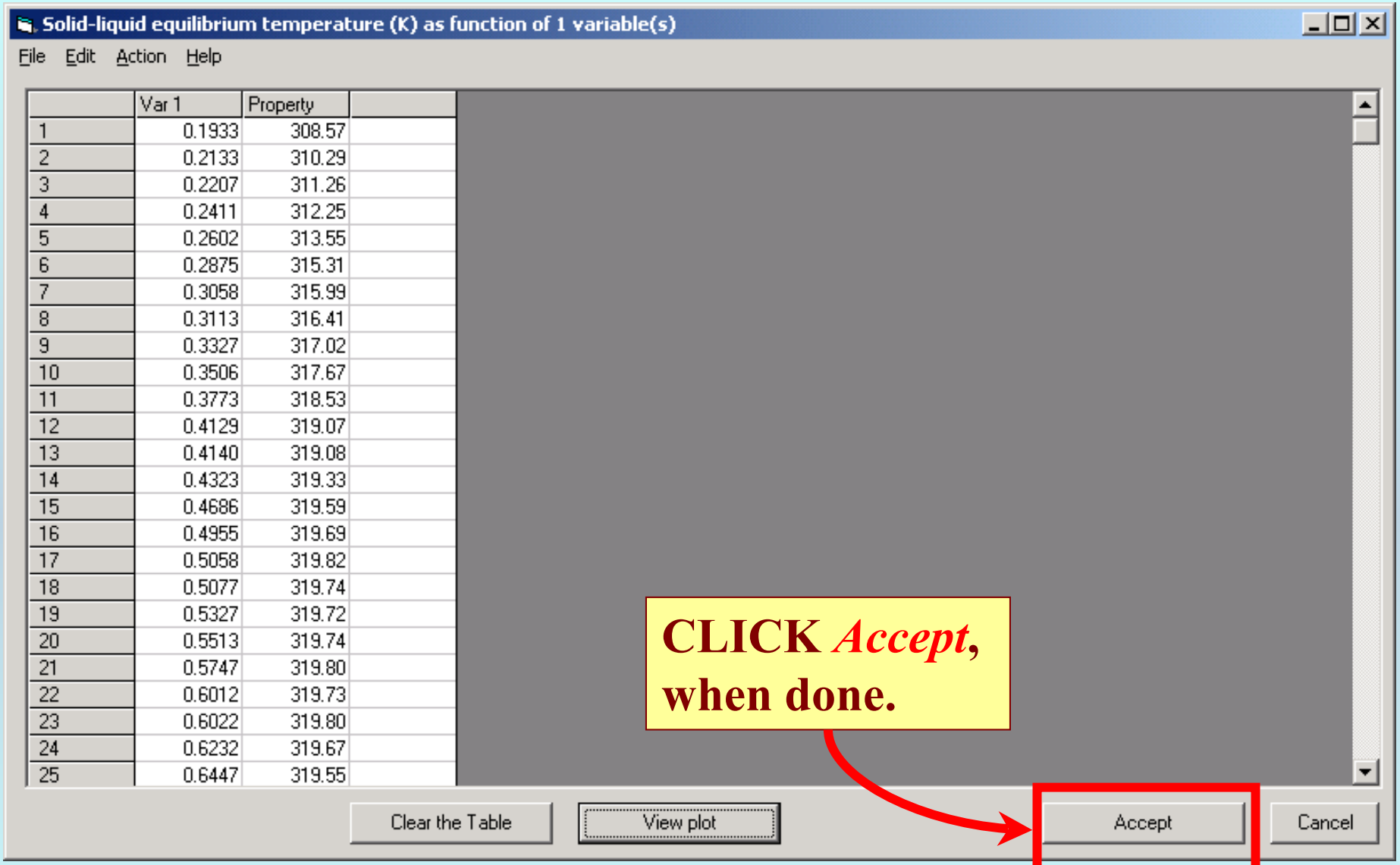
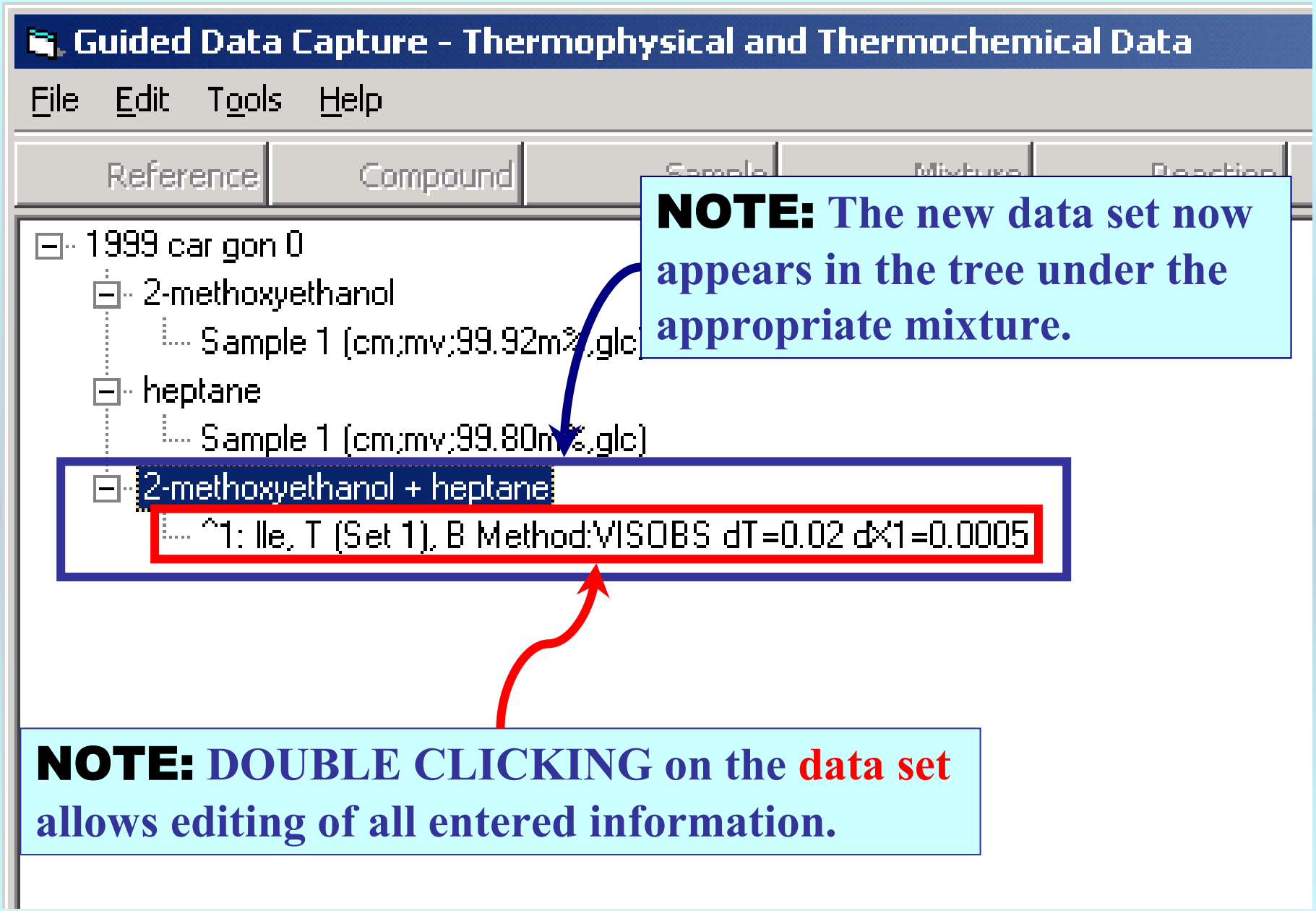
0.2411	312.25	0.6012	319.73
0.2602	313.55	0.6022	319.80
0.2875	315.31	0.6232	319.67
0.3058	315.99	0.6447	319.55
0.3113	316.41	0.6668	319.23
0.3327	317.02	0.6875	319.04
0.3506	317.67	0.6896	318.90
0.3773	318.53	0.7092	318.37
0.4129	319.07	0.7332	317.47
0.4140	319.08	0.7540	316.45
0.4323	319.33	0.7764	314.86
0.4686	319.59	0.7864	314.03
0.4955	319.69	0.8074	311.71
0.5058	319.82	0.8400	306.71
0.5077	319.74		

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.)


Solid-liquid equilibrium temperature (K) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 0.1933 308.57
2 0.2133 310.29
3 0.2207 311.26
4 0.2411 312.25
5 0.2602 313.55
6 0.2875 315.31
7 0.3058 315.99
8 0.3113 316.41
9 0.3327 317.02
10 0.3506 317.67
11 0.3773 318.53
12 0.4129 319.07
13 0.4140 319.08
14 0.4323 319.33
15 0.4686 319.59
16 0.4955 319.69
17 0.5058 319.82
18 0.5077 319.74
19 0.5327 319.72
20 0.5513 319.74
21 0.5747 319.80
22 0.6012 319.73
23 0.6022 319.80
24 0.6232 319.67
25 0.6447 319.55
Clear the Table
View plot
1. CLICK View plot to see a plot and check for typographical errors.
Solid-liquid equilibrium temperature as function of Mole fraction of 2-methoxyethanol
Tools Help
319
317
315
313
309
307
.2
.4
.6
X = Var 1
OK
Click OK, when done.


Solid-liquid equilibrium temperature (K) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 0.1933 308.57
2 0.2133 310.29
3 0.2207 311.26
4 0.2411 312.25
5 0.2602 313.55
6 0.2875 315.31
7 0.3058 315.99
8 0.3113 316.41
9 0.3327 317.02
10 0.3506 317.67
11 0.3773 318.53
12 0.4129 319.07
13 0.4140 319.08
14 0.4323 319.33
15 0.4686 319.59
16 0.4955 319.69
17 0.5058 319.82
18 0.5077 319.74
19 0.5327 319.72
20 0.5513 319.74
21 0.5747 319.80
22 0.6012 319.73
23 0.6022 319.80
24 0.6232 319.67
25 0.6447 319.55
CLICK Accept, when done.
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
1999 car gon 0
2-methoxyethanol
Sample 1 (cm;mv;99.92m%,glc)
heptane
Sample 1 (cm;mv;99.80m%,glc)
2-methoxyethanol + heptane
^1: Ile, T (Set 1), B Method:VISOBS dT=0.02 dX1=0.0005
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.**