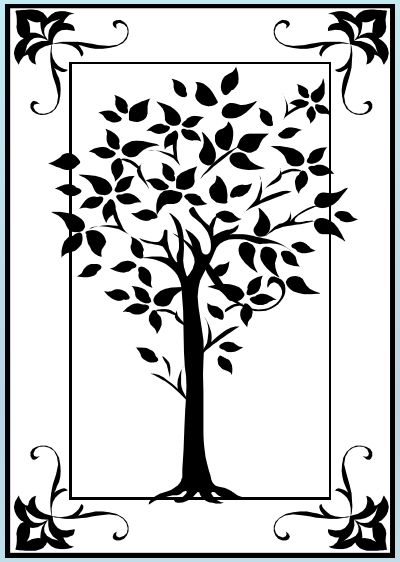
METADATA AND NUMERICAL DATA CAPTURE:
Heat Capacities C_p
(2 – Components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components**
Heat Capacities C_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:

Excess Molar Volume, Viscosity and Heat capacities for the Mixtures of Ethylene Glycol-Water from273.15 K to 353.15 K

Changsheng Yang, Peisheng Ma *, Fengming Jing and Duoqiang Tang

P. O. Box6888 State Key of C_1 Chemistry and Technology

School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China

Heat Capacities C_p for the binary system
Ethylene glycol + water
at p = 101.3 kPa and various temperatures

Table 5. The heat capacities for the ethylene glycol (1) + water (2)

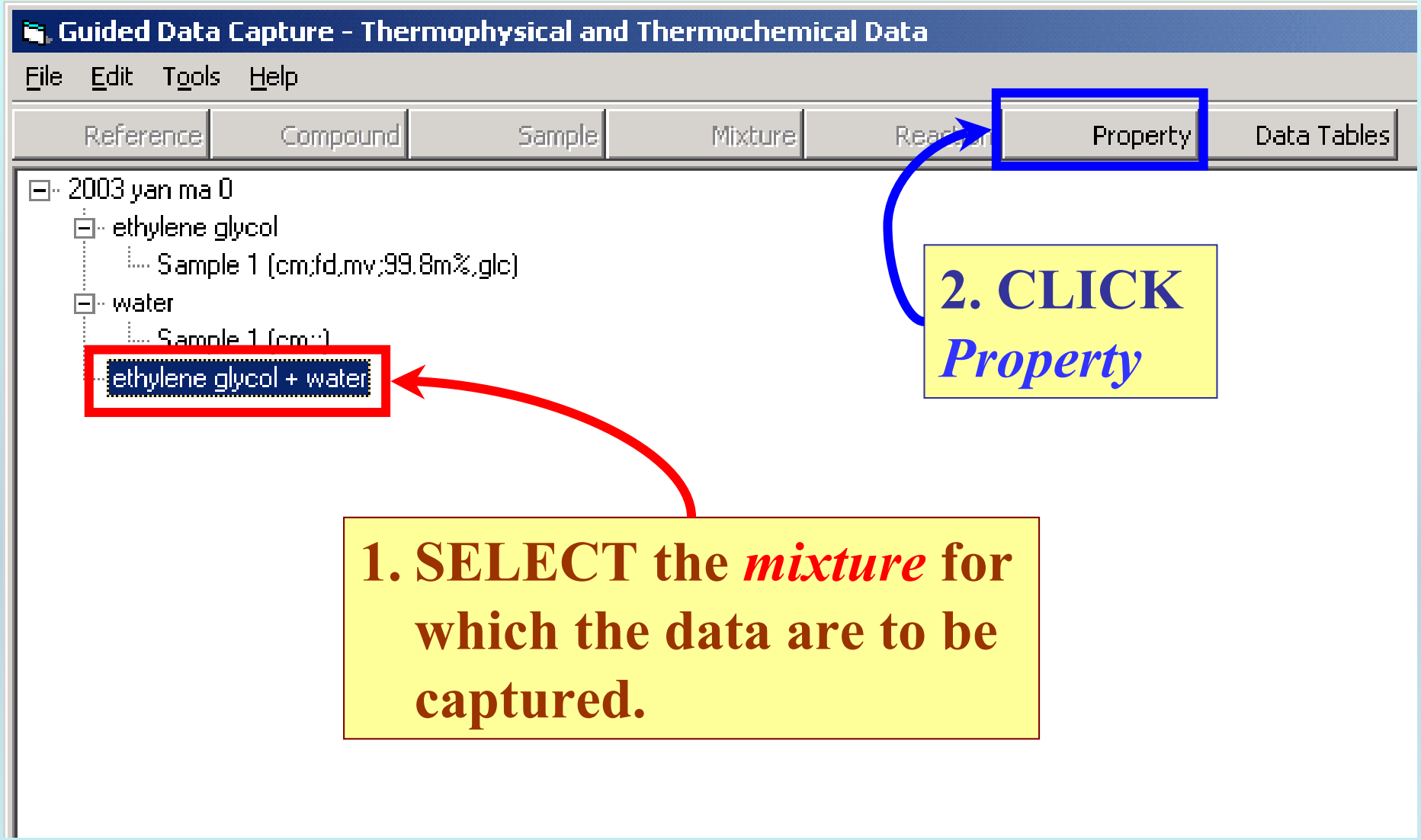
T/K	x_1										
	0.0000	0.0312	0.0676	0.1105	0.1620	0.2248	0.3031	0.4036	0.5370	0.7230	1.0000
293.15	4.179	4.540	4.173	3.789	3.554	3.353	3.136	2.924	2.743	2.565	2.376
303.15	4.184	4.533	4.183	3.804	3.565	3.382	3.161	2.961	2.777	2.596	2.412
313.15	4.175	4.557	4.201	3.823	3.597	3.399	3.198	3.019	2.824	2.631	2.449
323.15	4.176	4.571	4.220	3.825	3.618	3.436	3.248	3.060	2.874	2.675	2.478
333.15	4.175	4.580	4.239	3.835	3.638	3.460	3.264	3.101	2.908	2.715	2.517
343.15	4.181	4.584	4.244	3.859	3.680	3.491	3.304	3.127	2.948	2.769	2.573
353.15	4.190	4.598	4.262	3.888	3.670	3.532	3.347	3.180	2.999	2.819	2.594
363.15	--	4.603	4.268	3.901	3.718	3.568	3.396	3.214	3.043	2.851	2.658
373.15	--	--	--	3.912	3.733	3.590	3.426	3.241	3.077	2.895	2.714

This data set is considered here.

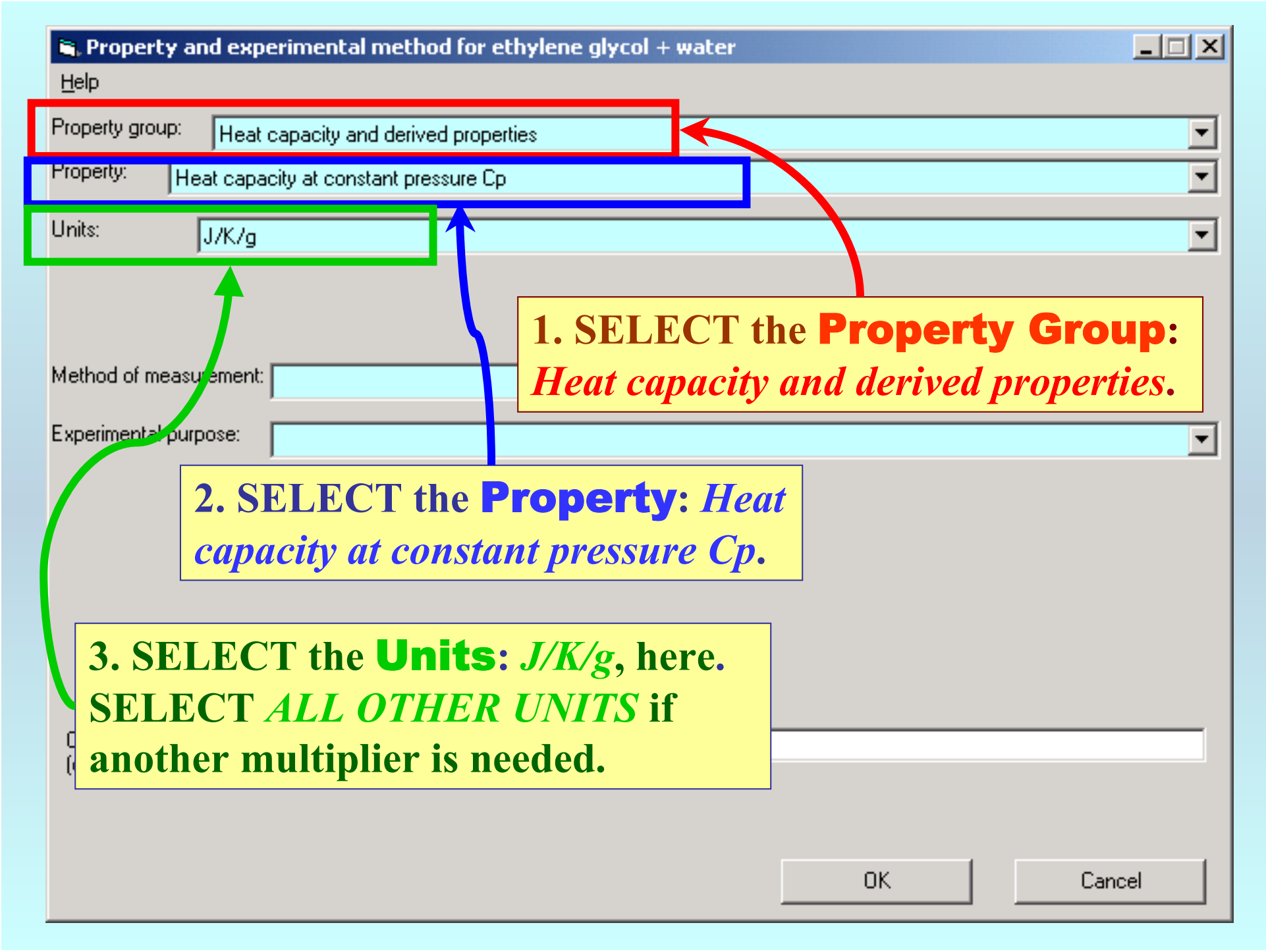
Experimental Method & Uncertainties Info:

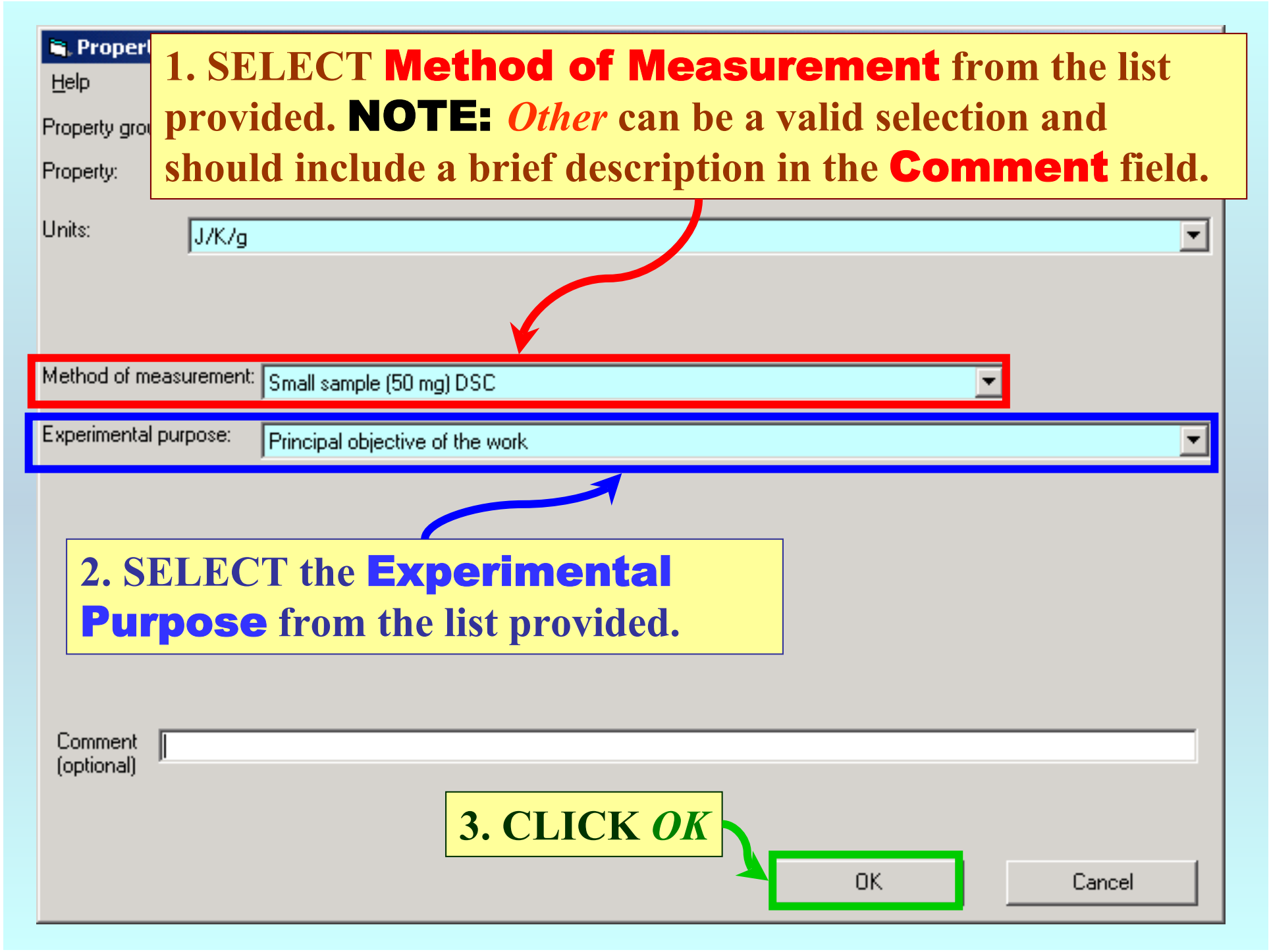
Method: DSC

Uncertainty: 1%

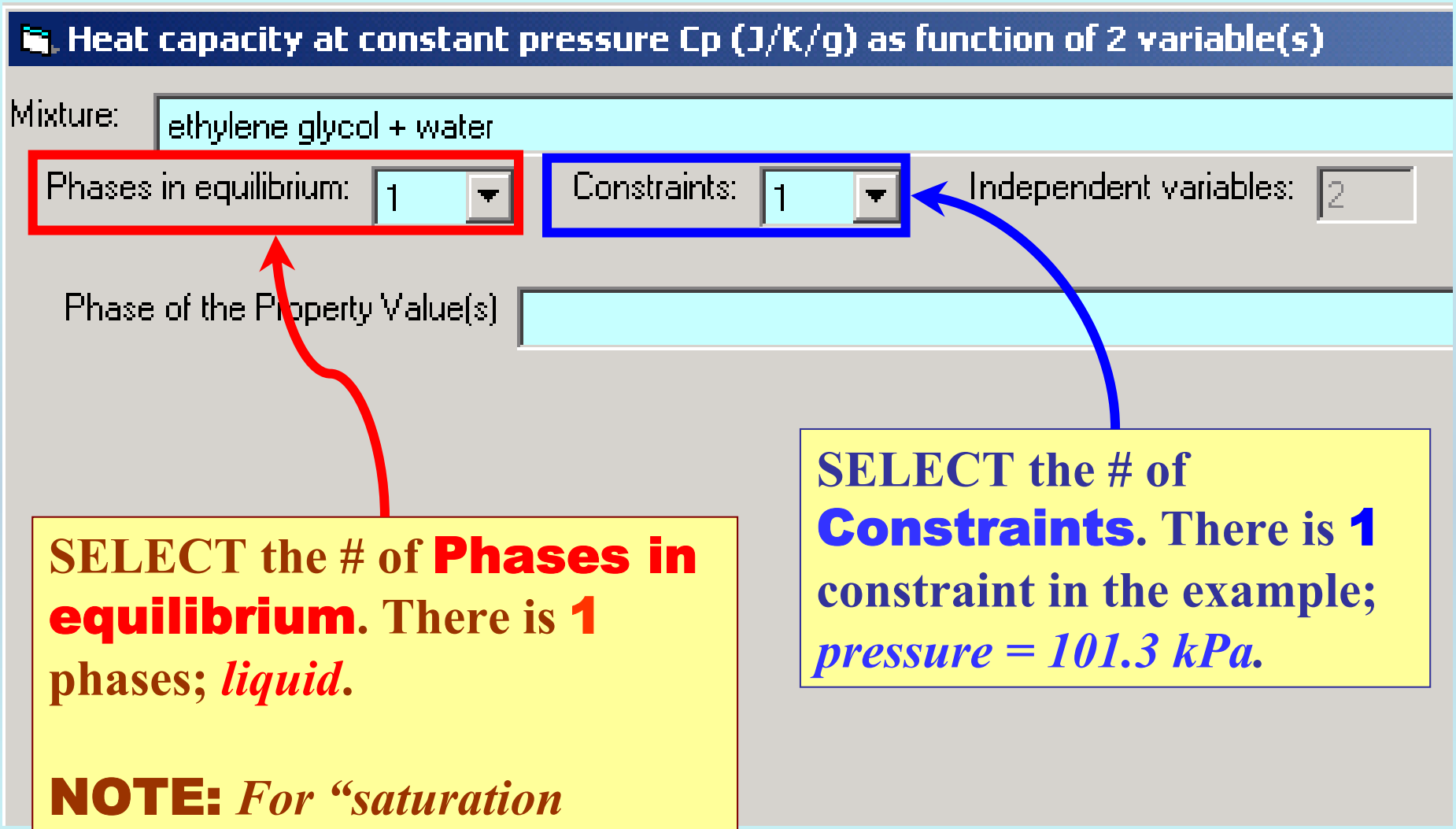


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for ethylene glycol + water
Help
Property group:
Heat capacity and derived properties
Property:
Heat capacity at constant pressure Cp
Units:
J/K/g
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Heat capacity and derived properties.
2. SELECT the Property: Heat capacity at constant pressure Cp.
3. SELECT the Units: J/K/g, here. SELECT ALL OTHER UNITS if another multiplier is needed.
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.
Help
Property:
Units:
J/K/g
Method of measurement:
Small sample (50 mg) DSC
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK OK
OK
Cancel

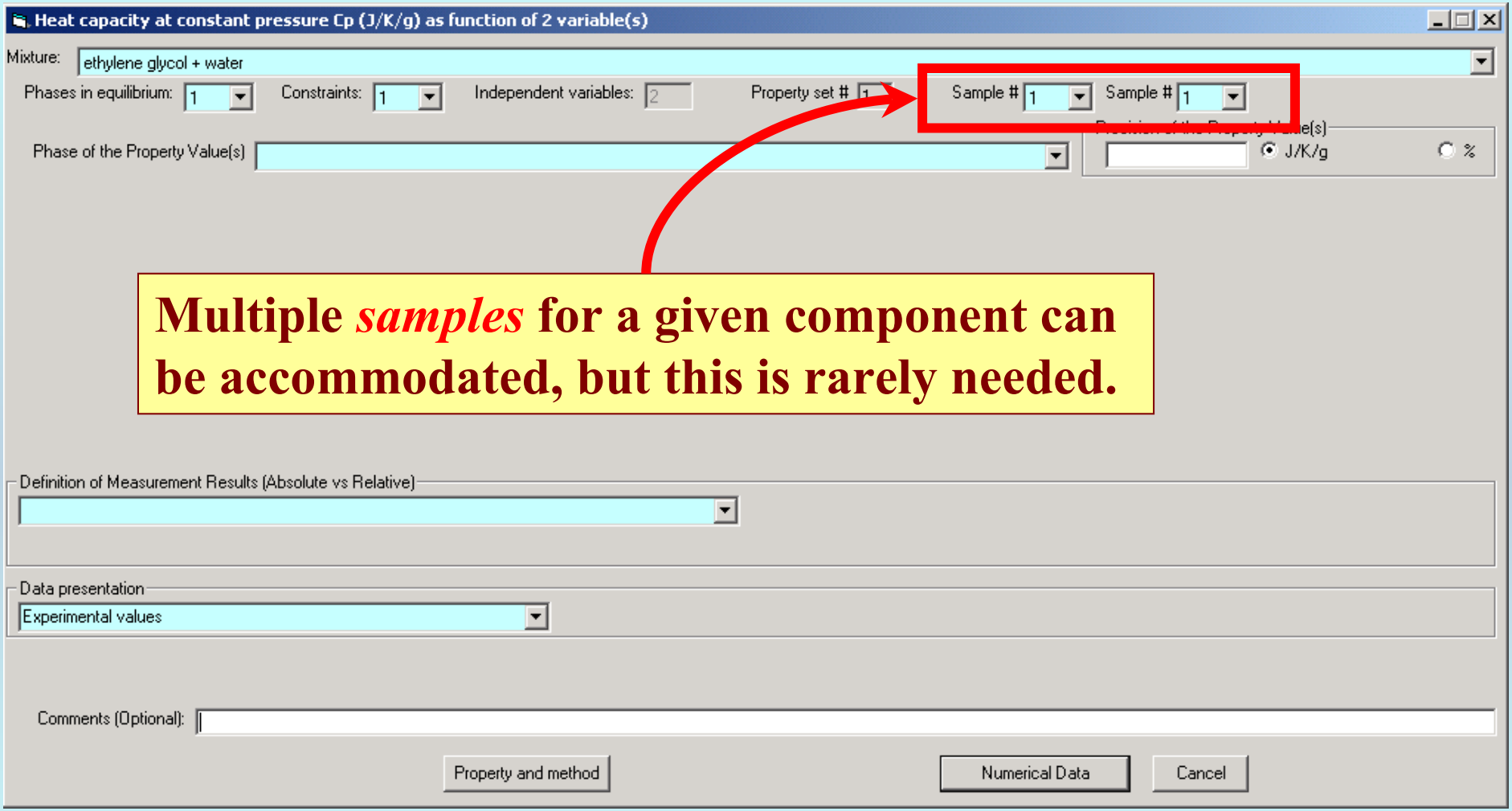
SELECTION of # of Phases in Equilibrium and # of Constraints

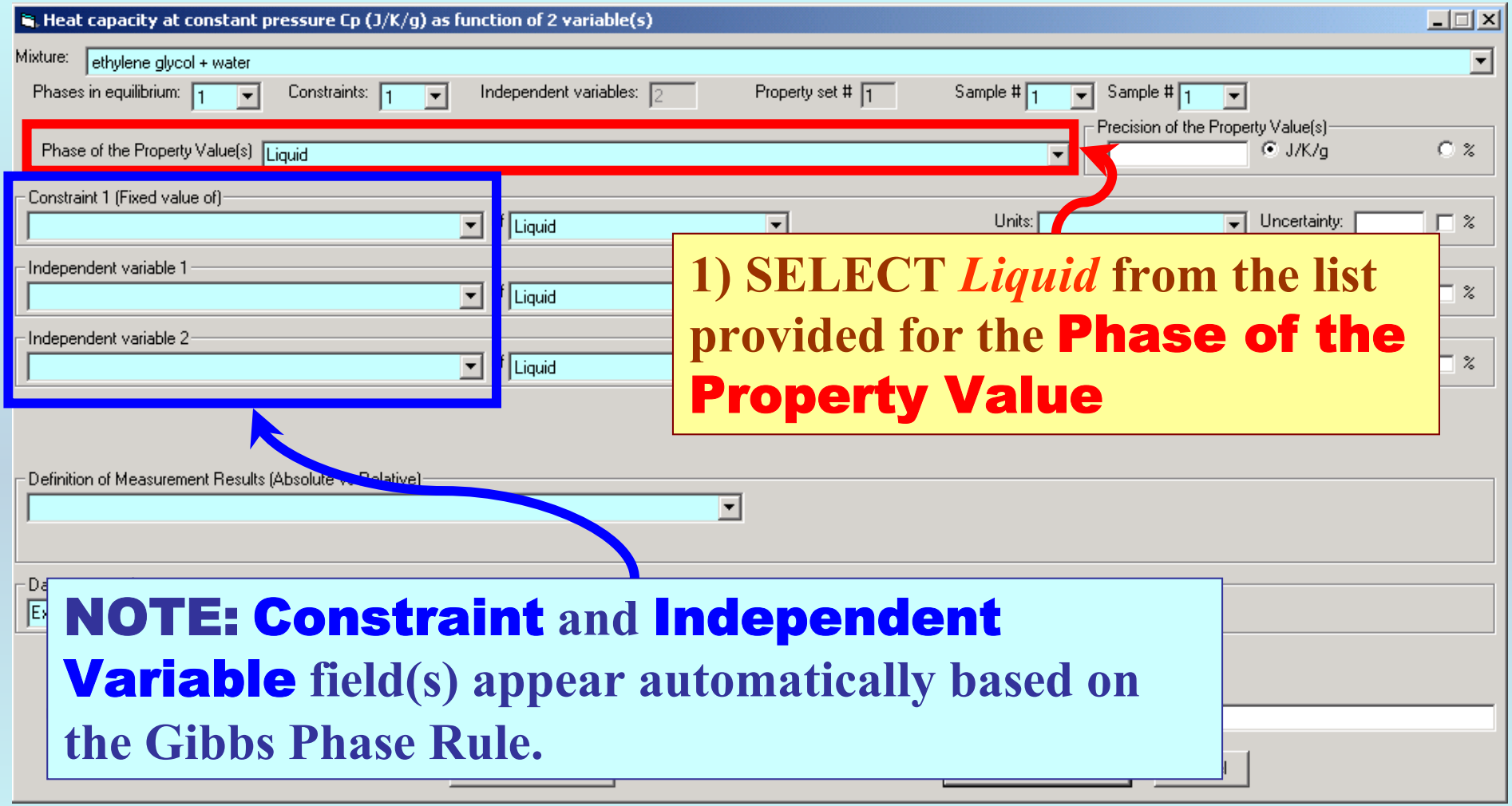


SELECT the # of **Phases in equilibrium**. There is **1** phases; *liquid*.

NOTE: *For "saturation conditions, this value would be 2; liquid & gas)*

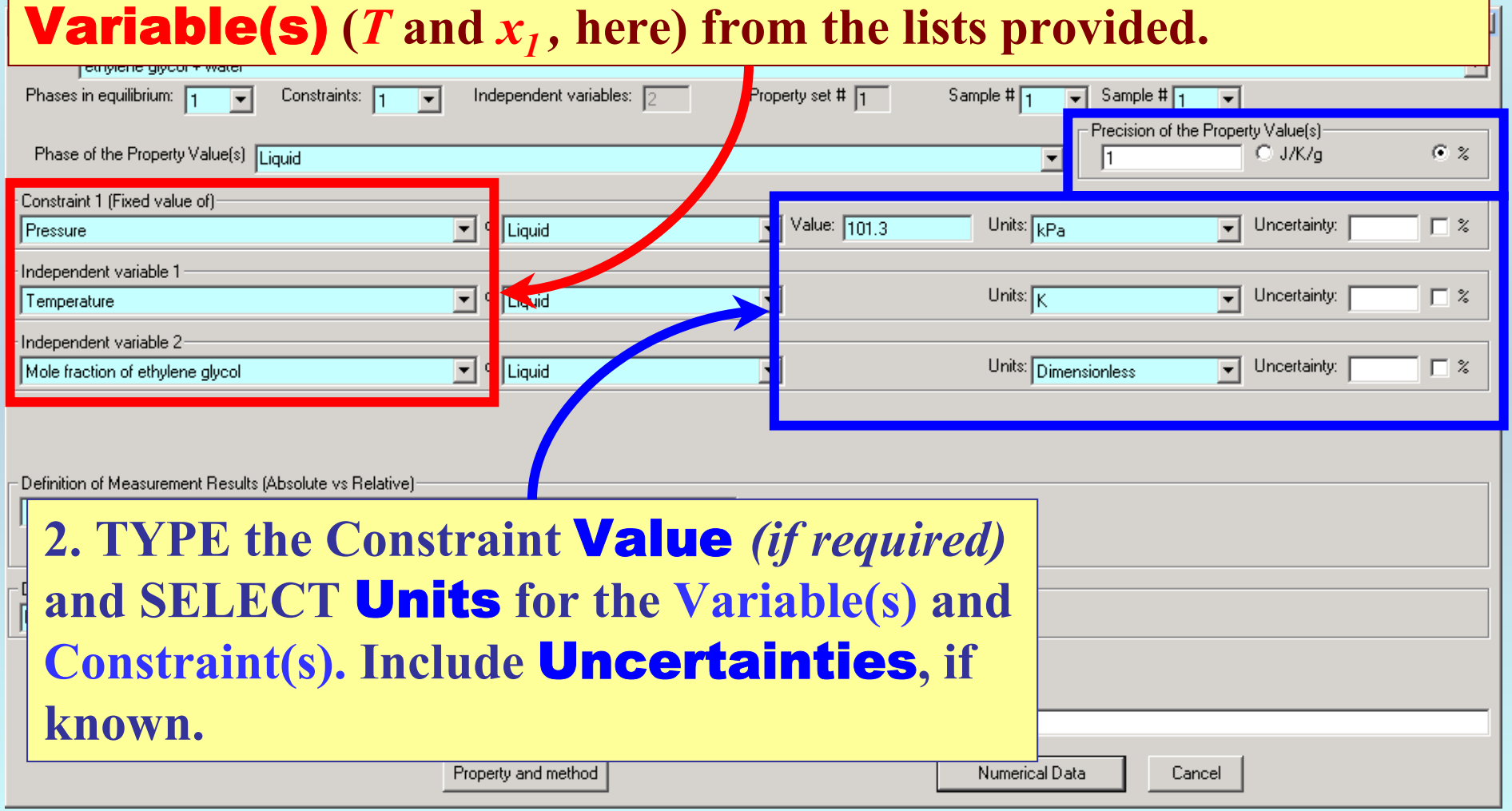
SELECT the # of **Constraints**. There is **1** constraint in the example; *pressure = 101.3 kPa*.


Heat capacity at constant pressure Cp (J/K/g) as function of 2 variable(s)
Mixture:
ethylene glycol + water
Phases in equilibrium:
1
Constraints:
1
Independent variables:
2
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
J/K/g
%
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


Heat capacity at constant pressure Cp (J/K/g) as function of 2 variable(s)
Mixture:
ethylene glycol + water
Phases in equilibrium:
Constraints:
Independent variables:
Property set #
Sample #
Sample #
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
J/K/g
%
Constraint 1 (Fixed value of)
Liquid
Units:
Uncertainty:
Independent variable 1
Liquid
Independent variable 2
Liquid
Definition of Measurement Results (Absolute vs. Relative)
1) SELECT Liquid from the list provided for the Phase of the Property Value
NOTE: Constraint and Independent Variable field(s) appear automatically based on the Gibbs Phase Rule.

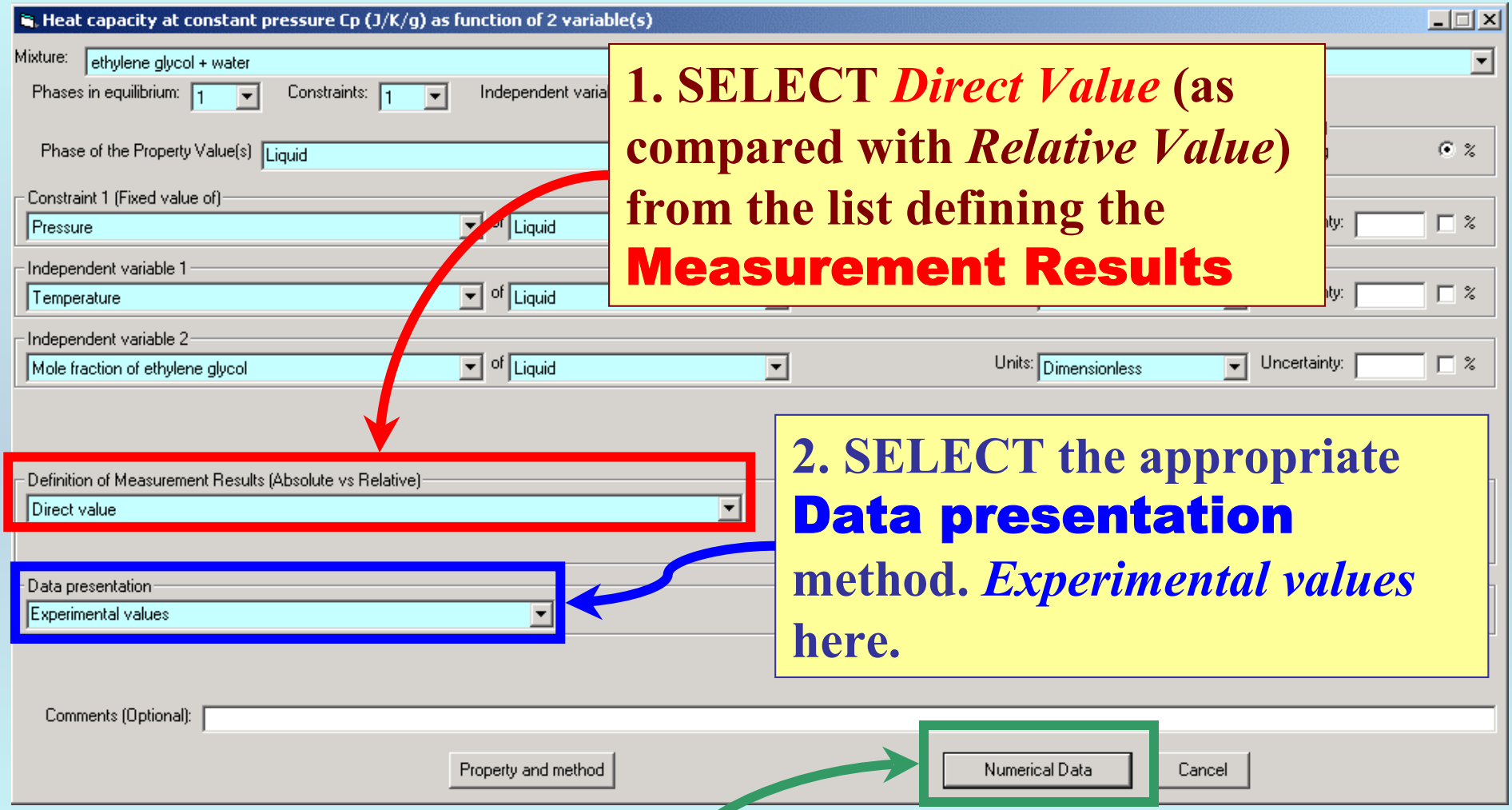
Specification of constraints, constraint values, and constraint units

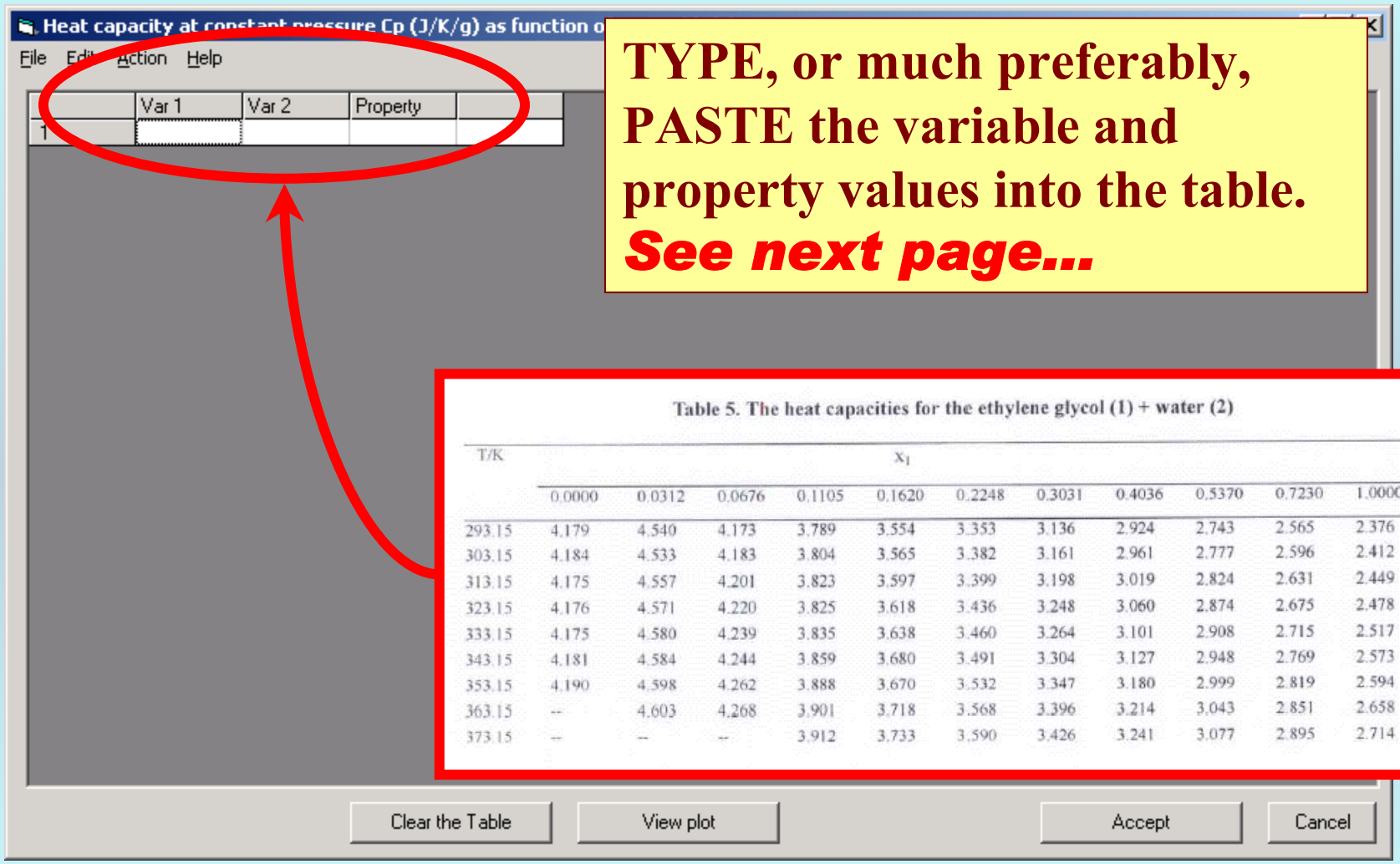
1. SELECT the Constraint(s) (*p* here) and the Independent Variable(s) (*T* and x_1, here) from the lists provided.

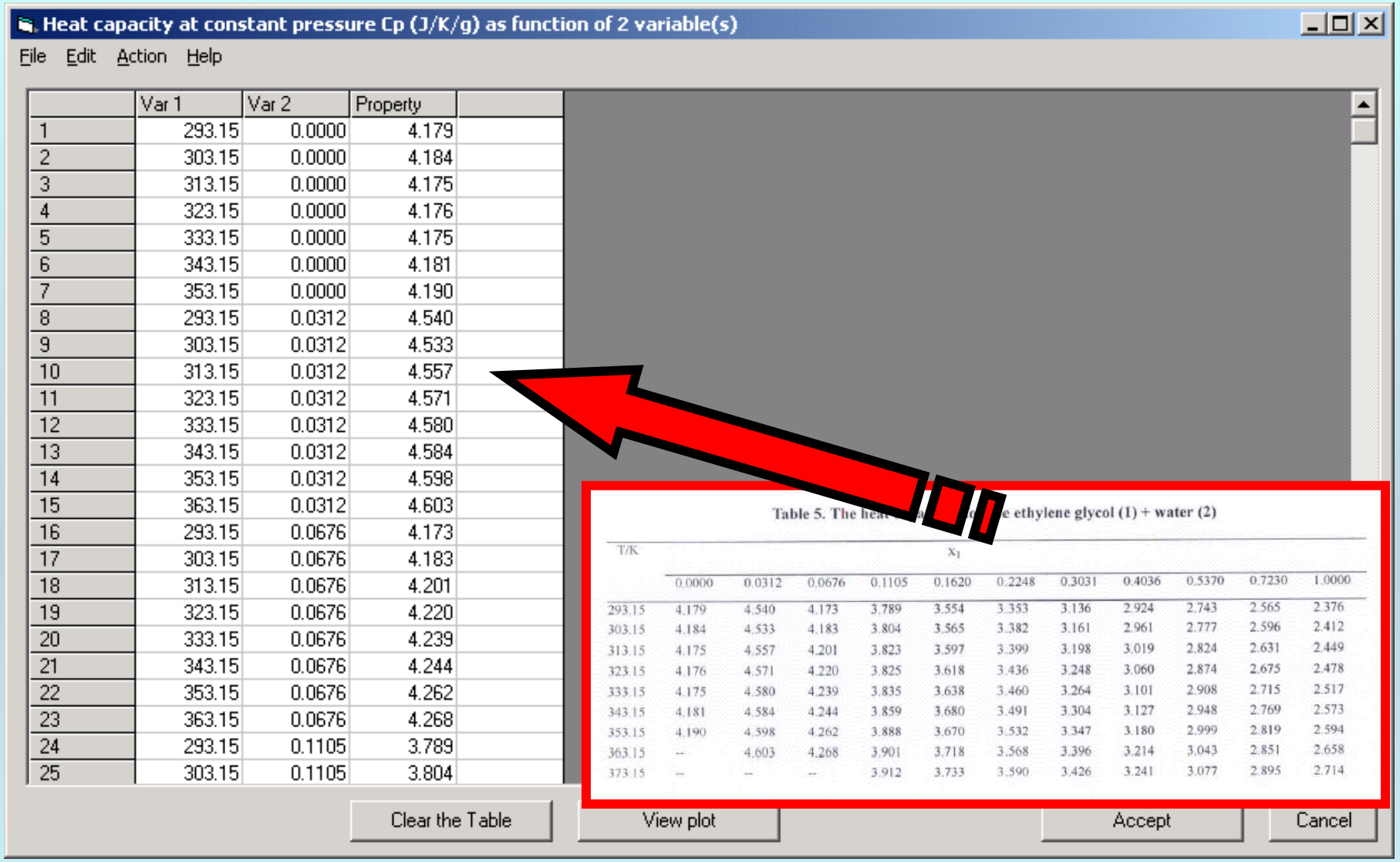


2. TYPE the Constraint Value *(if required)* and SELECT Units for the Variable(s) and Constraint(s). Include Uncertainties, if known.

Measurement definition and Data presentation




Heat capacity at constant pressure Cp (J/K/g) as function o
File Edit Action Help
Var 1
Var 2
Property
1
TYPE, or much preferably, PASTE the variable and property values into the table.
See next page...
Table 5. The heat capacities for the ethylene glycol (1) + water (2)
T/K
x1
0.0000 0.0312 0.0676 0.1105 0.1620 0.2248 0.3031 0.4036 0.5370 0.7230 1.0000
293.15 4.179 4.540 4.173 3.789 3.554 3.353 3.136 2.924 2.743 2.565 2.376
303.15 4.184 4.533 4.183 3.804 3.565 3.382 3.161 2.961 2.777 2.596 2.412
313.15 4.175 4.557 4.201 3.823 3.597 3.399 3.198 3.019 2.824 2.631 2.449
323.15 4.176 4.571 4.220 3.825 3.618 3.436 3.248 3.060 2.874 2.675 2.478
333.15 4.175 4.580 4.239 3.835 3.638 3.460 3.264 3.101 2.908 2.715 2.517
343.15 4.181 4.584 4.244 3.859 3.680 3.491 3.304 3.127 2.948 2.769 2.573
353.15 4.190 4.598 4.262 3.888 3.670 3.532 3.347 3.180 2.999 2.819 2.594
363.15 -- 4.603 4.268 3.901 3.718 3.568 3.396 3.214 3.043 2.851 2.658
373.15 -- -- -- 3.912 3.733 3.590 3.426 3.241 3.077 2.895 2.714
Clear the Table
View plot
Accept
Cancel

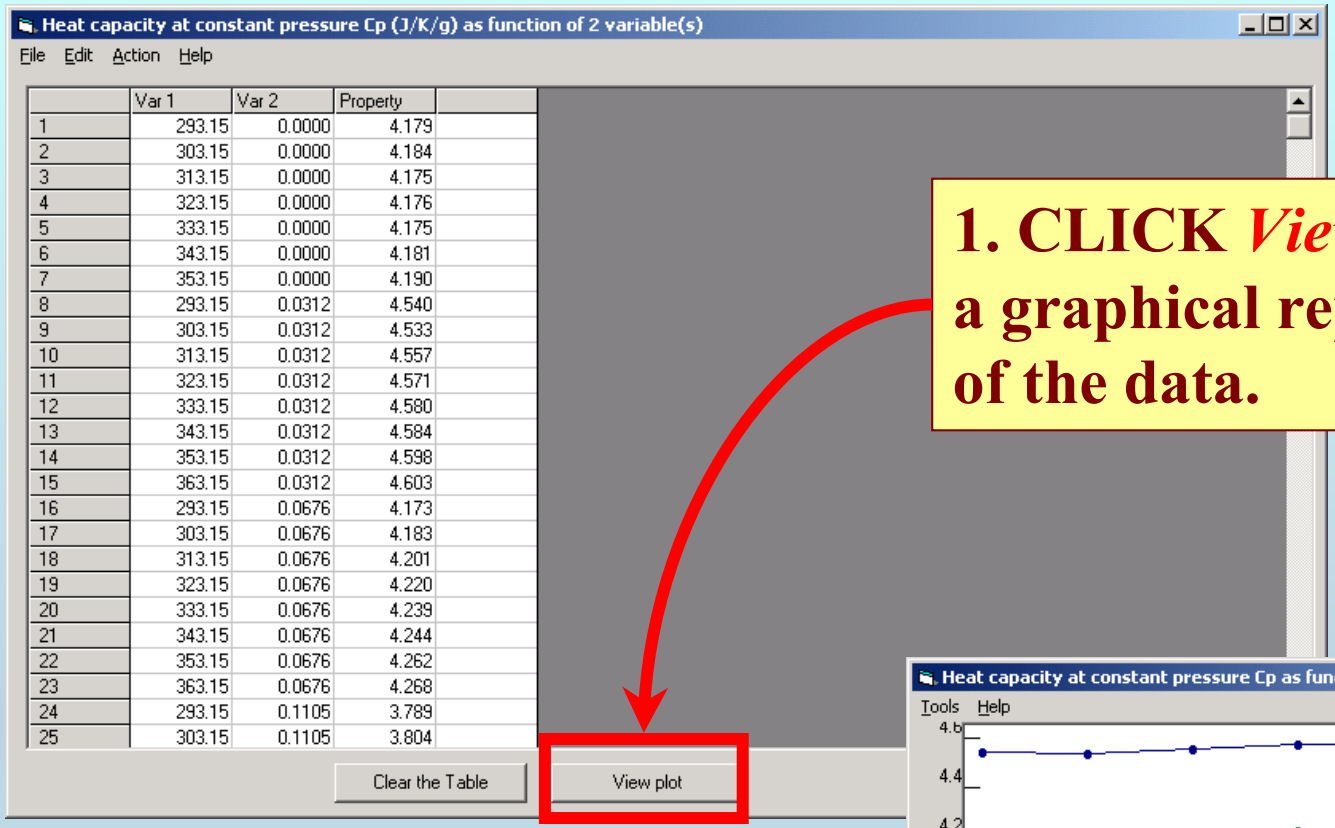


	Var 1	Var 2	Property
1	293.15	0.0000	4.179
2	303.15	0.0000	4.184
3	313.15	0.0000	4.175
4	323.15	0.0000	4.176
5	333.15	0.0000	4.175
6	343.15	0.0000	4.181
7	353.15	0.0000	4.190
8	293.15	0.0312	4.540
9	303.15	0.0312	4.533
10	313.15	0.0312	4.557
11	323.15	0.0312	4.571
12	333.15	0.0312	4.580
13	343.15	0.0312	4.584
14	353.15	0.0312	4.598
15	363.15	0.0312	4.603
16	293.15	0.0676	4.173
17	303.15	0.0676	4.183
18	313.15	0.0676	4.201
19	323.15	0.0676	4.220
20	333.15	0.0676	4.239
21	343.15	0.0676	4.244
22	353.15	0.0676	4.262
23	363.15	0.0676	4.268
24	293.15	0.1105	3.789
25	303.15	0.1105	3.804

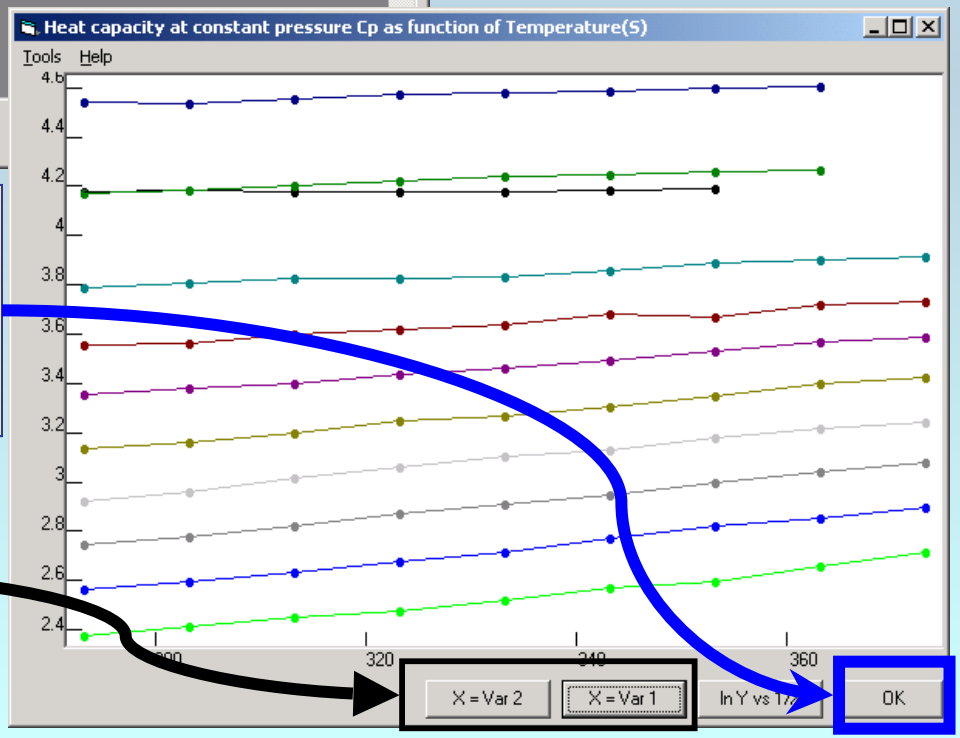
Table 5. The heat [illegible] ethylene glycol (1) + water (2)

T/K	x_1										
	0.0000	0.0312	0.0676	0.1105	0.1620	0.2248	0.3031	0.4036	0.5370	0.7230	1.0000
293.15	4.179	4.540	4.173	3.789	3.554	3.353	3.136	2.924	2.743	2.565	2.376
303.15	4.184	4.533	4.183	3.804	3.565	3.382	3.161	2.961	2.777	2.596	2.412
313.15	4.175	4.557	4.201	3.823	3.597	3.399	3.198	3.019	2.824	2.631	2.449
323.15	4.176	4.571	4.220	3.825	3.618	3.436	3.248	3.060	2.874	2.675	2.478
333.15	4.175	4.580	4.239	3.835	3.638	3.460	3.264	3.101	2.908	2.715	2.517
343.15	4.181	4.584	4.244	3.859	3.680	3.491	3.304	3.127	2.948	2.769	2.573
353.15	4.190	4.598	4.262	3.888	3.670	3.532	3.347	3.180	2.999	2.819	2.594
363.15	--	4.603	4.268	3.901	3.718	3.568	3.396	3.214	3.043	2.851	2.658
373.15	--	--	--	3.912	3.733	3.590	3.426	3.241	3.077	2.895	2.714

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.)

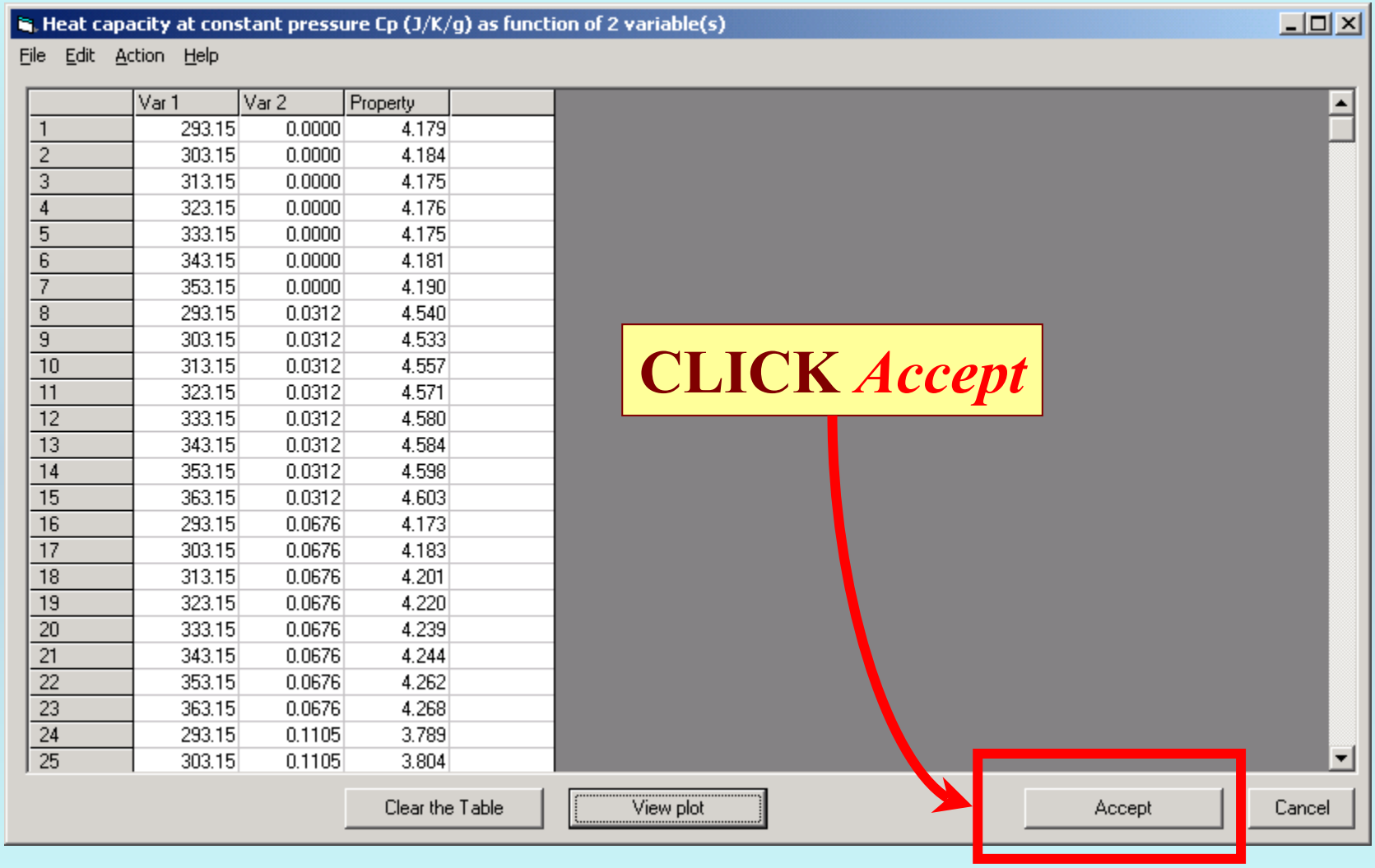


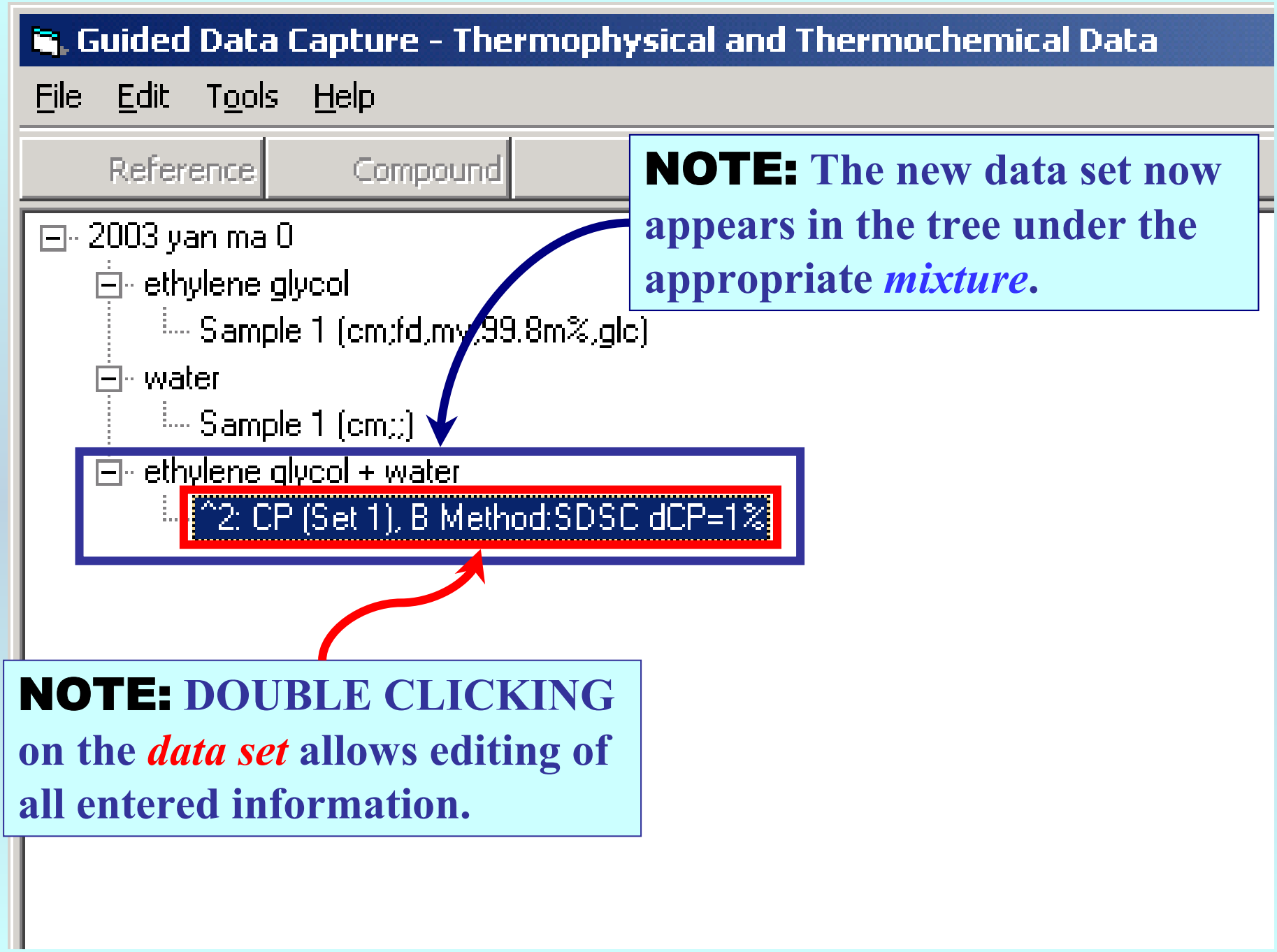
1. CLICK *View plot* to see a graphical representation of the data.



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

NOTE: The variable associated with the x-axis can be selected for best display.


Heat capacity at constant pressure Cp (J/K/g) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 293.15 0.0000 4.179
2 303.15 0.0000 4.184
3 313.15 0.0000 4.175
4 323.15 0.0000 4.176
5 333.15 0.0000 4.175
6 343.15 0.0000 4.181
7 353.15 0.0000 4.190
8 293.15 0.0312 4.540
9 303.15 0.0312 4.533
10 313.15 0.0312 4.557
11 323.15 0.0312 4.571
12 333.15 0.0312 4.580
13 343.15 0.0312 4.584
14 353.15 0.0312 4.598
15 363.15 0.0312 4.603
16 293.15 0.0676 4.173
17 303.15 0.0676 4.183
18 313.15 0.0676 4.201
19 323.15 0.0676 4.220
20 333.15 0.0676 4.239
21 343.15 0.0676 4.244
22 353.15 0.0676 4.262
23 363.15 0.0676 4.268
24 293.15 0.1105 3.789
25 303.15 0.1105 3.804
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
2003 yan ma 0
ethylene glycol
Sample 1 (cm;fd,mv,99.8m%,glc)
water
Sample 1 (cm;;)
ethylene glycol + water
^2: CP (Set 1), B Method:SDSC dCP=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.**