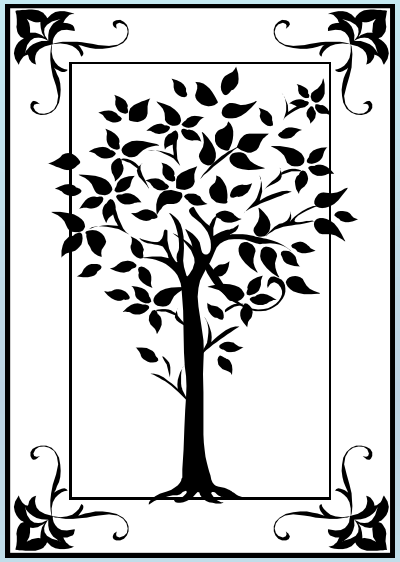
METADATA AND NUMERICAL DATA CAPTURE:
Heat Capacity: $C_{sat,m}$
(1 – Component)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **1-component**
HEAT CAPACITIES: $C_{sat,m}$
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 2000, *45*, 661−664

Measurement of Heat Capacities for Nine Organic Substances by Tian−Calvet Calorimetry

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Heat capacities for *n*-heptane, 2-methyl-1-propanol, toluene, and 1-propanol were measured with the "step by step" method and those for 2-methyl-1-propanol, 1-propanol, methylcyclohexane, toluene, 2,4-pentanedione, 1-bromooctane, dibenzyl ether, and benzoic acid with the "three-step" method using a Tian−Calvet batch calorimeter. The measurements of saturated liquid heat capacity have an approximate uncertainty of ±0.5% and cover temperatures within the range 288 K to 363 K.

Heat Capacity ($C_{sat,m}$) for 1 component
2-Methyl-1-propanol

Table 2. Experimental Saturated Liquid Heat Capacity Data c^s for 2-Methyl-1-propanol, 1-Propanol, Toluene, Methylcyclohexane, 2,4-Pentadione, 1-Bromooctane, and Dibenzyl Ether and Experimental Saturated Solid Heat Capacity Data for Benzoic Acid Measured Using the Three-Step Method

T/K	c^s/J mol^{-1} K^{-1}	T/K	c^s/J mol^{-1} K^{-1}	T/K	c^s/J mol^{-1} K^{-1}	T/K	c^s/J mol^{-1} K^{-1}
2-Methyl-1-propanol		1-Propanol		Toluene		Methylcyclohexane	
323.16	202.72	330.06	163.73	288.13	154.41	288.21	180.41
328.15	207.89	335.05	167.60	293.15	155.96	293.16	182.76
333.15	213.07	340.13	171.45	298.21	157.42	298.14	184.87
338.15	217.69	345.04	175.37	303.16	158.84	303.17	187.00
343.22	223.04	350.03	179.10	308.20	160.40	308.21	189.18
348.12	227.62	354.92	182.85	313.17	161.92	313.19	191.31
353.20	232.57			318.16	163.49	318.18	193.51
358.19	237.36			323.16	165.07	323.17	195.73
363.18	242.00			328.15	166.42	328.16	197.75
				333.15	168.14	333.16	199.99
				338.14	169.60	338.15	201.97
				343.13	171.06	343.23	204.74
				348.21	172.50	348.13	206.65
				353.20	174.13	353.21	208.98

This data set is considered here.

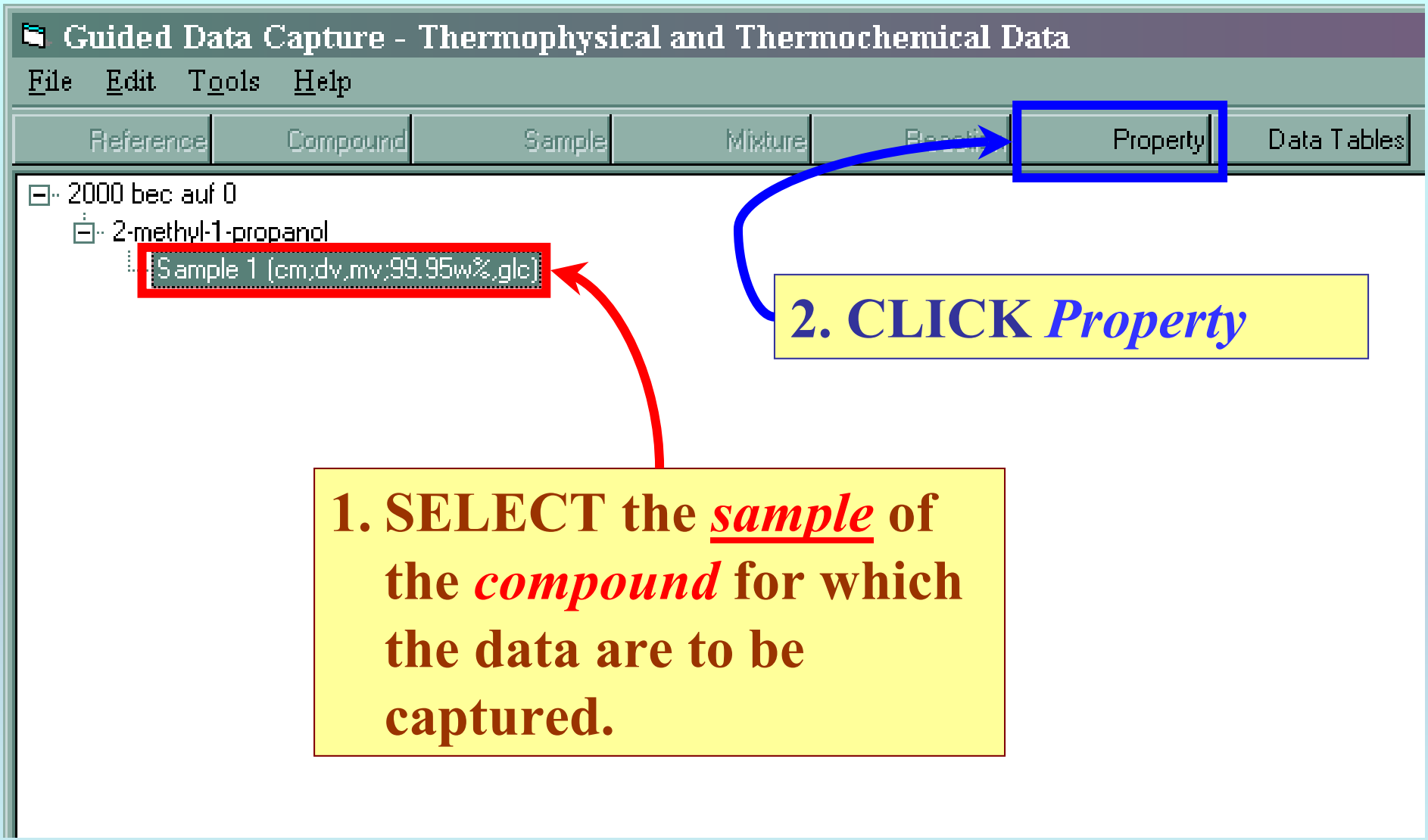
Experimental Method Info:

2. Experimental Section

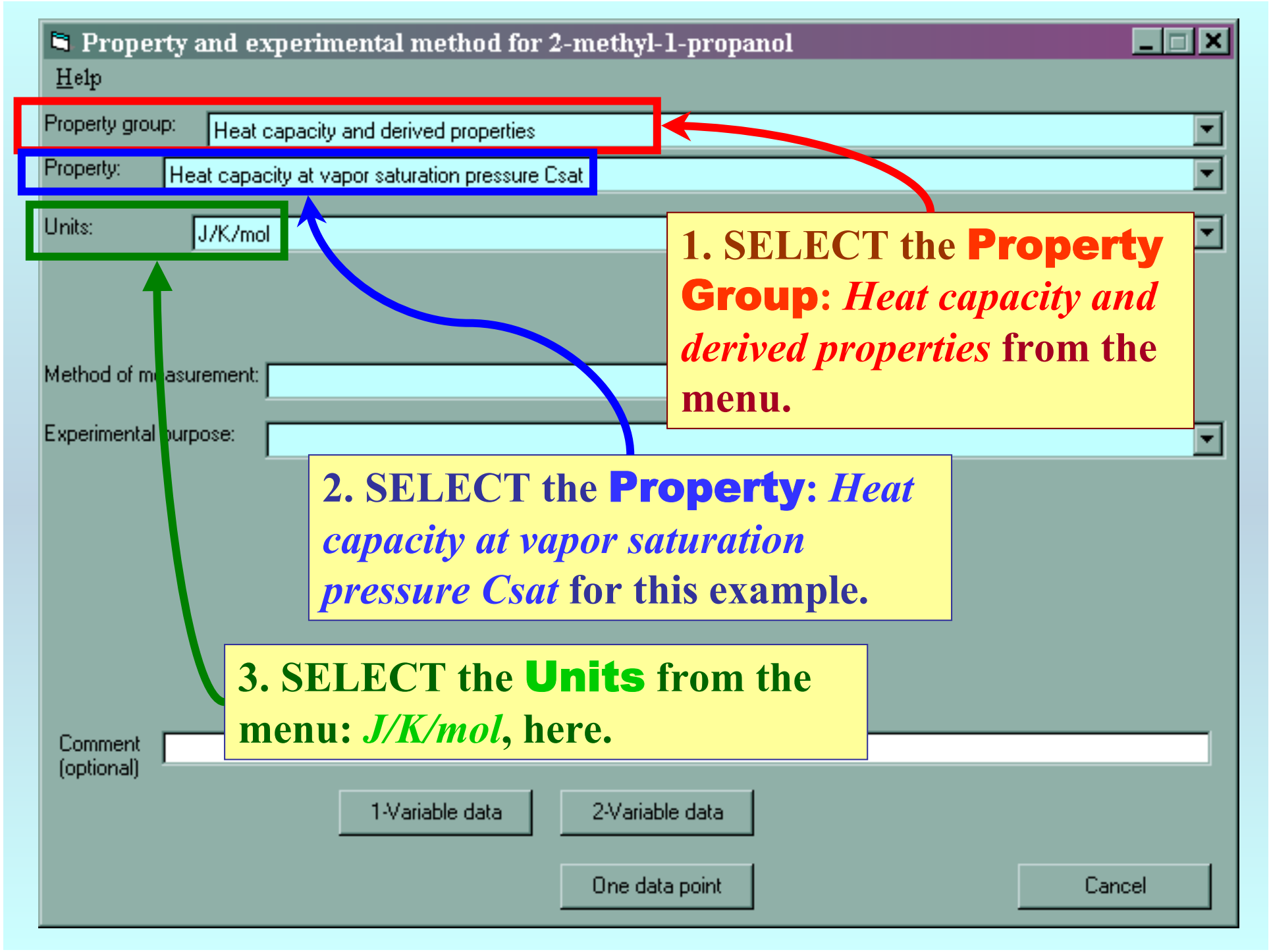
The measurements reported here were performed using a Tian–Calvet heat flow batch calorimeter from SETARAM, France (model BT2.15), with a temperature range from 77.15 K to 473.15 K.

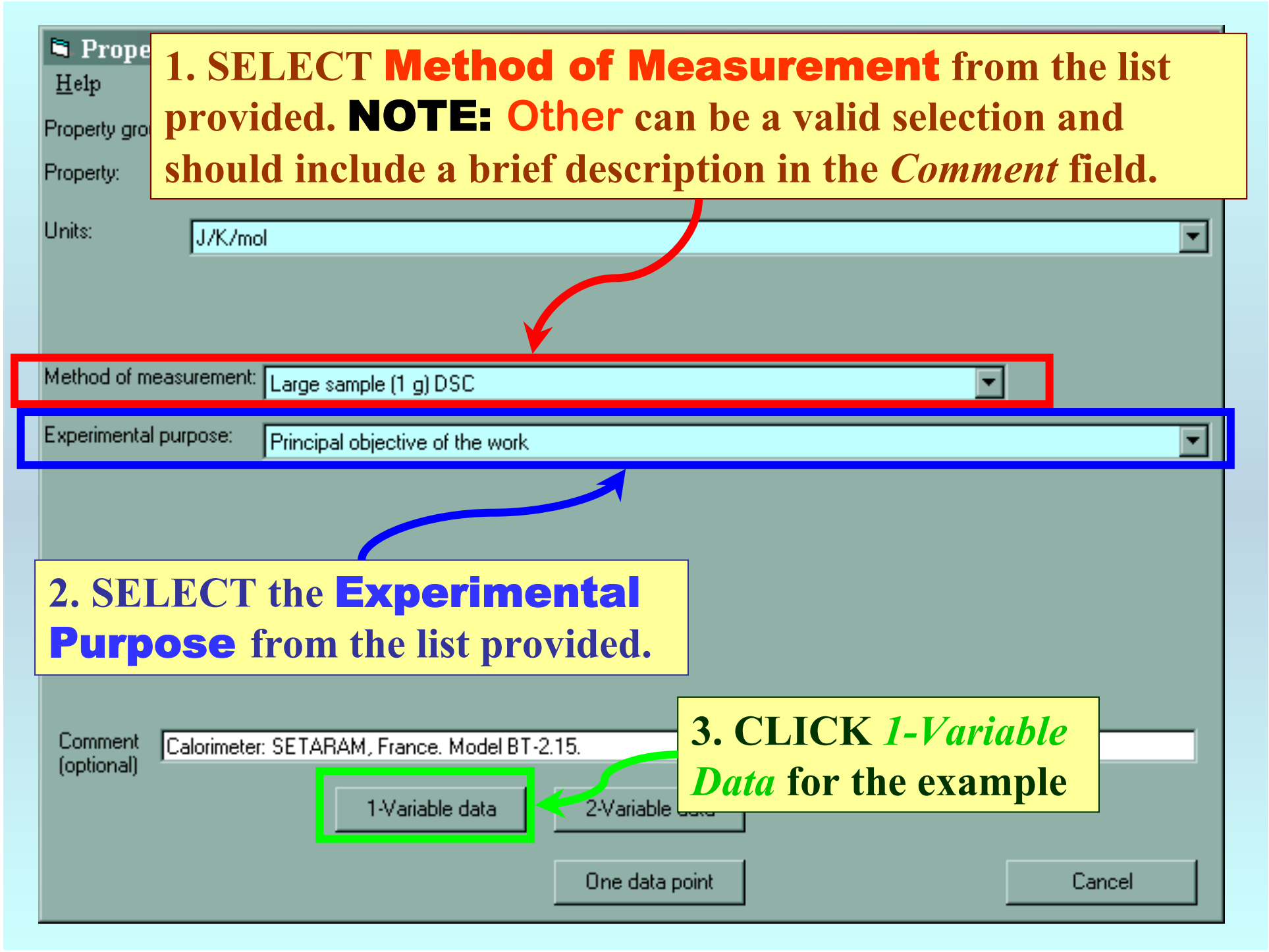
Uncertainty estimate:

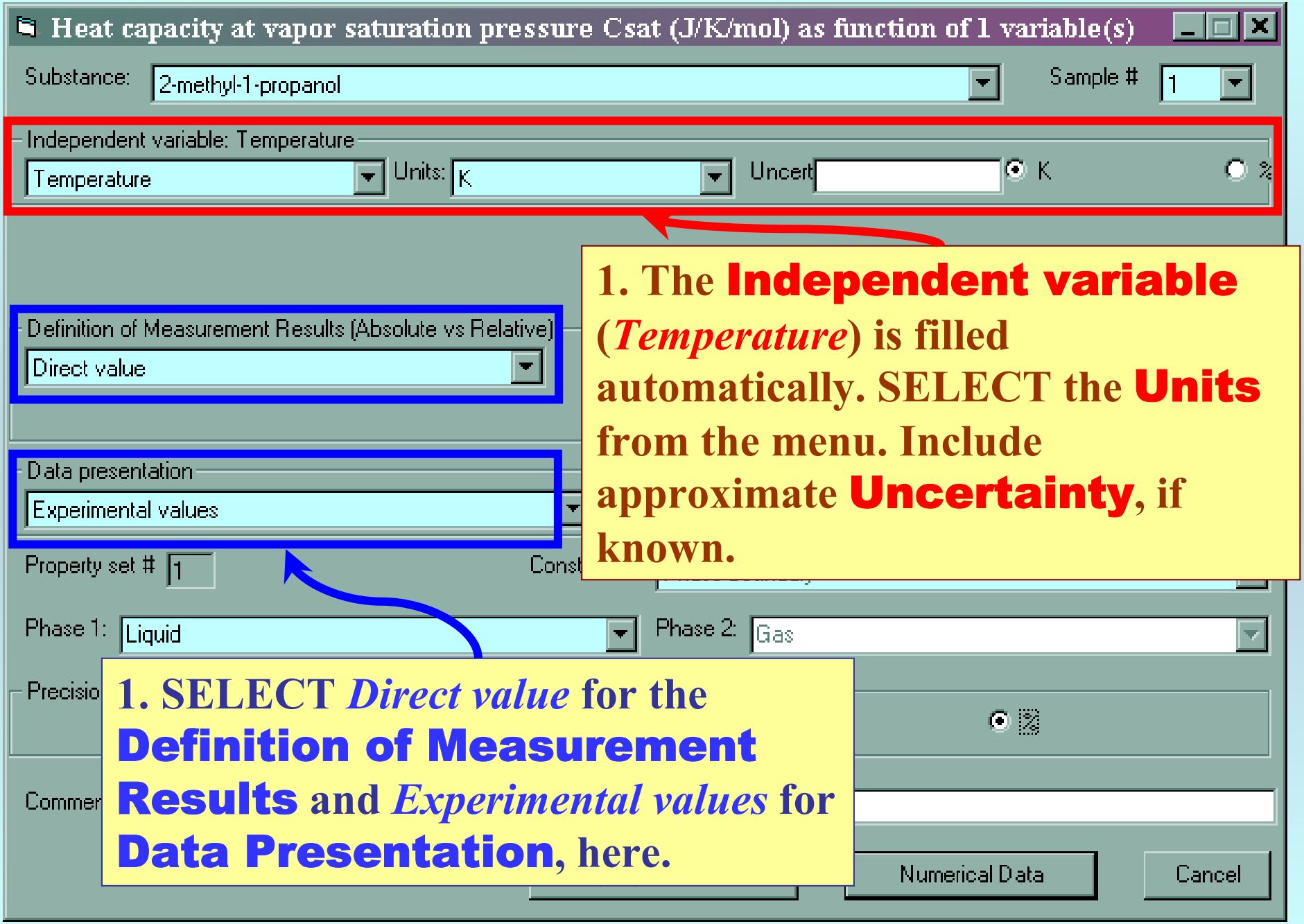
Calvet batch calorimeter. The measurements of saturated liquid heat capacity have an approximate uncertainty of ±0.5% and cover temperatures within the range 288 K to 363 K.

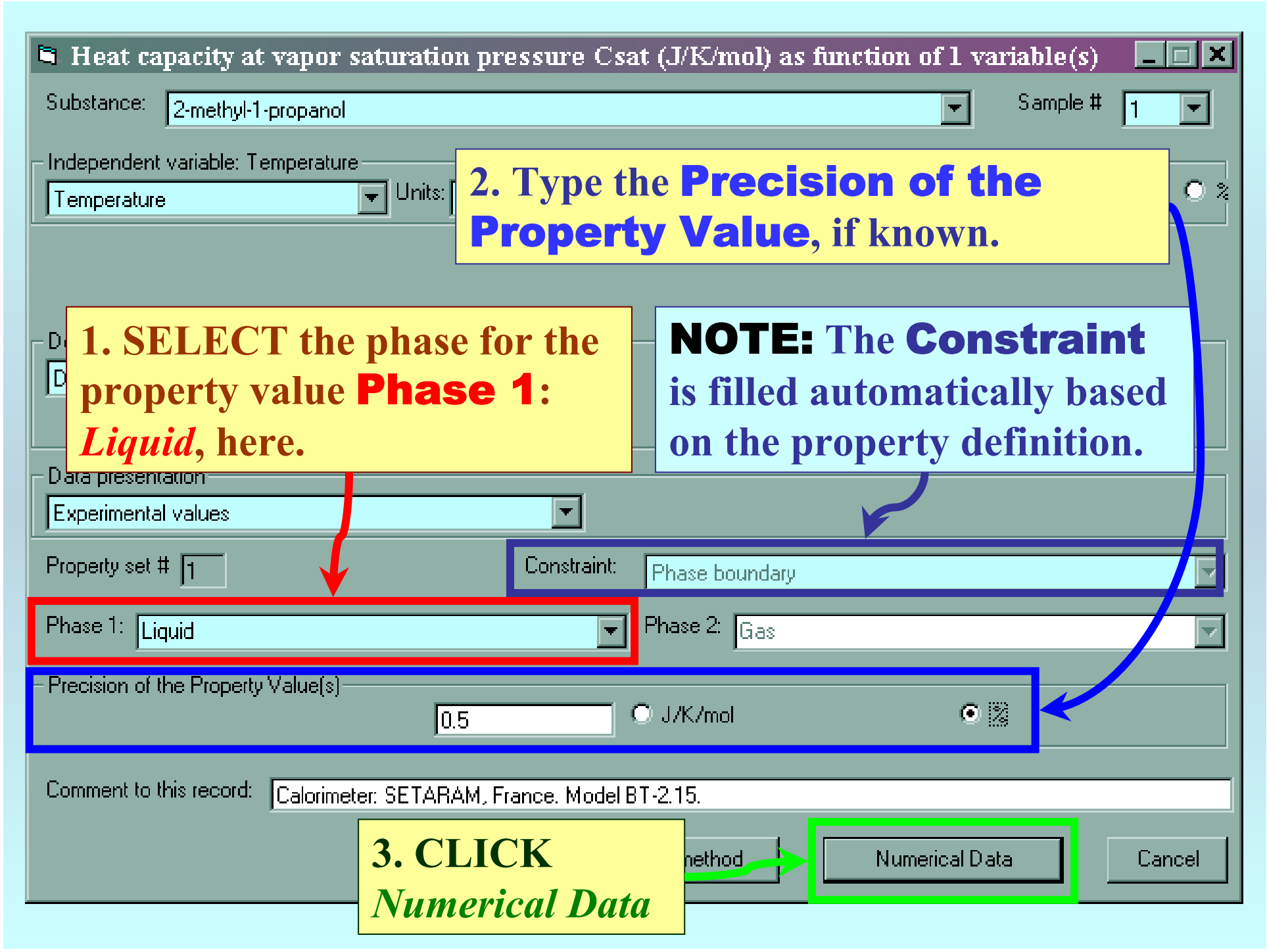


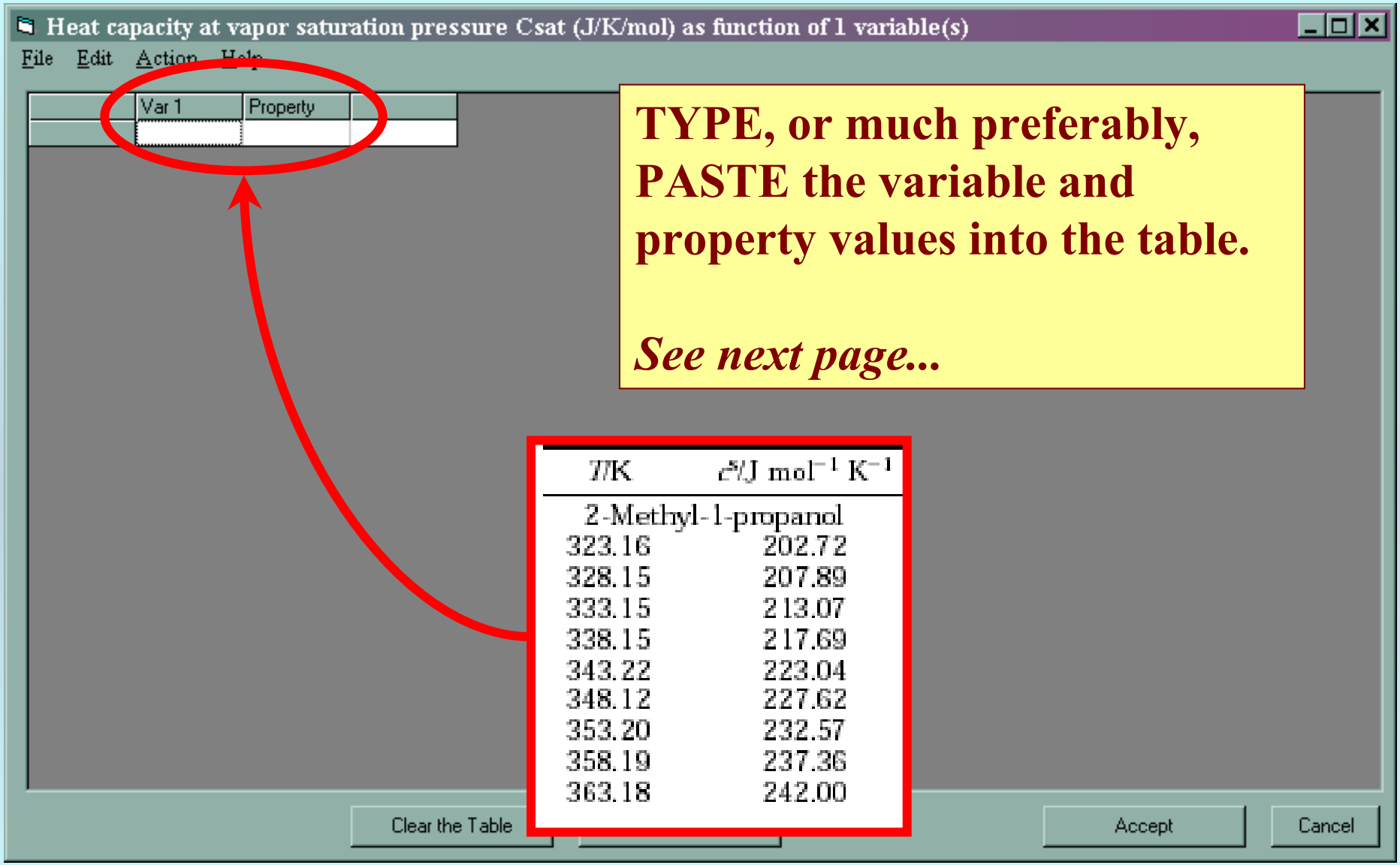
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

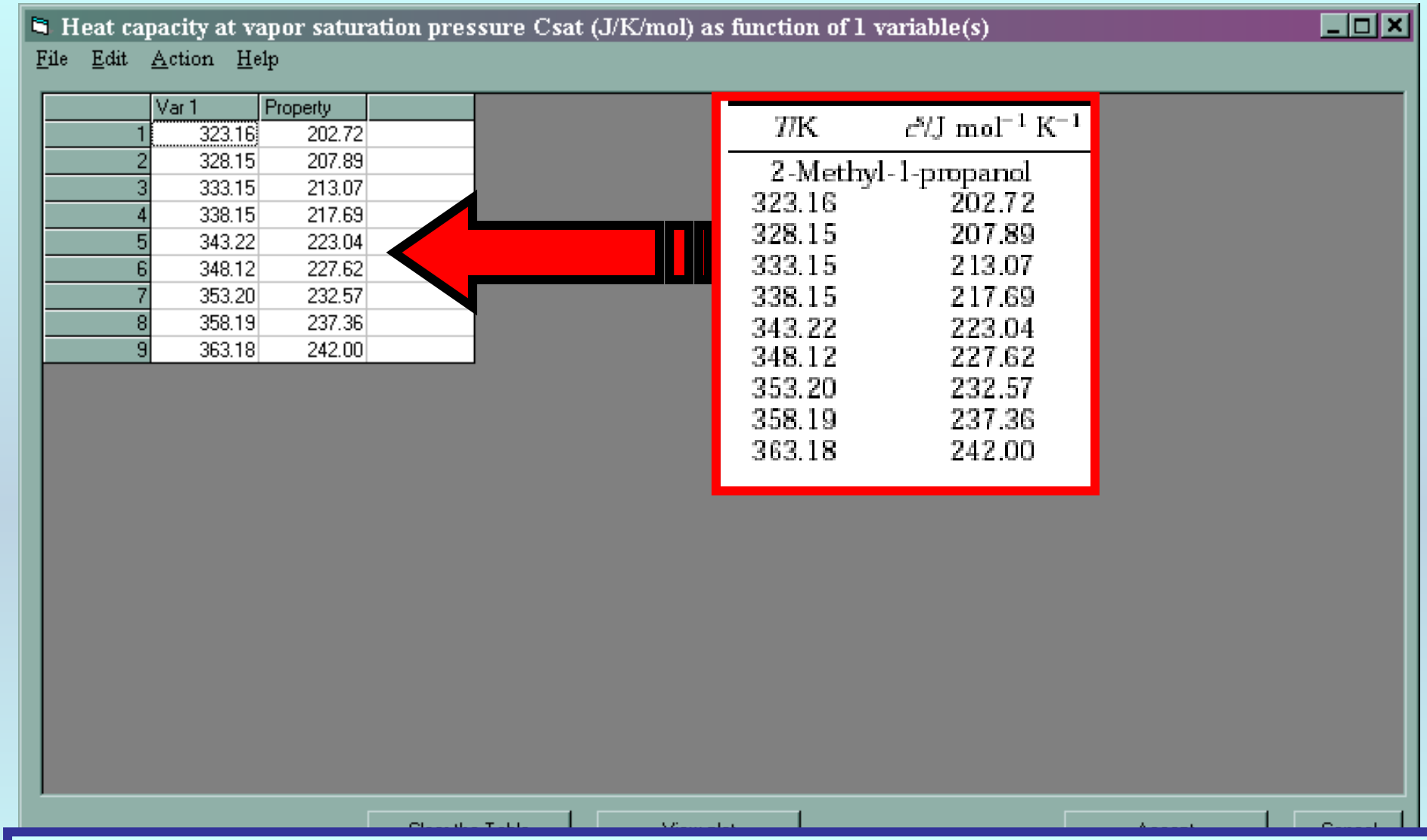

Property and experimental method for 2-methyl-1-propanol
Help
Property group:
Heat capacity and derived properties
Property:
Heat capacity at vapor saturation pressure Csat
Units:
J/K/mol
Method of measurement:
Experimental purpose:
Comment (optional)
1-Variable data
2-Variable data
One data point
Cancel
1. SELECT the Property Group: Heat capacity and derived properties from the menu.
2. SELECT the Property: Heat capacity at vapor saturation pressure Csat for this example.
3. SELECT the Units from the menu: J/K/mol, here.


Prope
Help
Property gro
Property:
Units:
J/K/mol
Method of measurement:
Large sample (1 g) DSC
Experimental purpose:
Principal objective of the work
Comment (optional)
Calorimeter: SETARAM, France. Model BT-2.15.
1-Variable data
2-Variable
One data point
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.
2. SELECT the Experimental Purpose from the list provided.
3. CLICK 1-Variable Data for the example

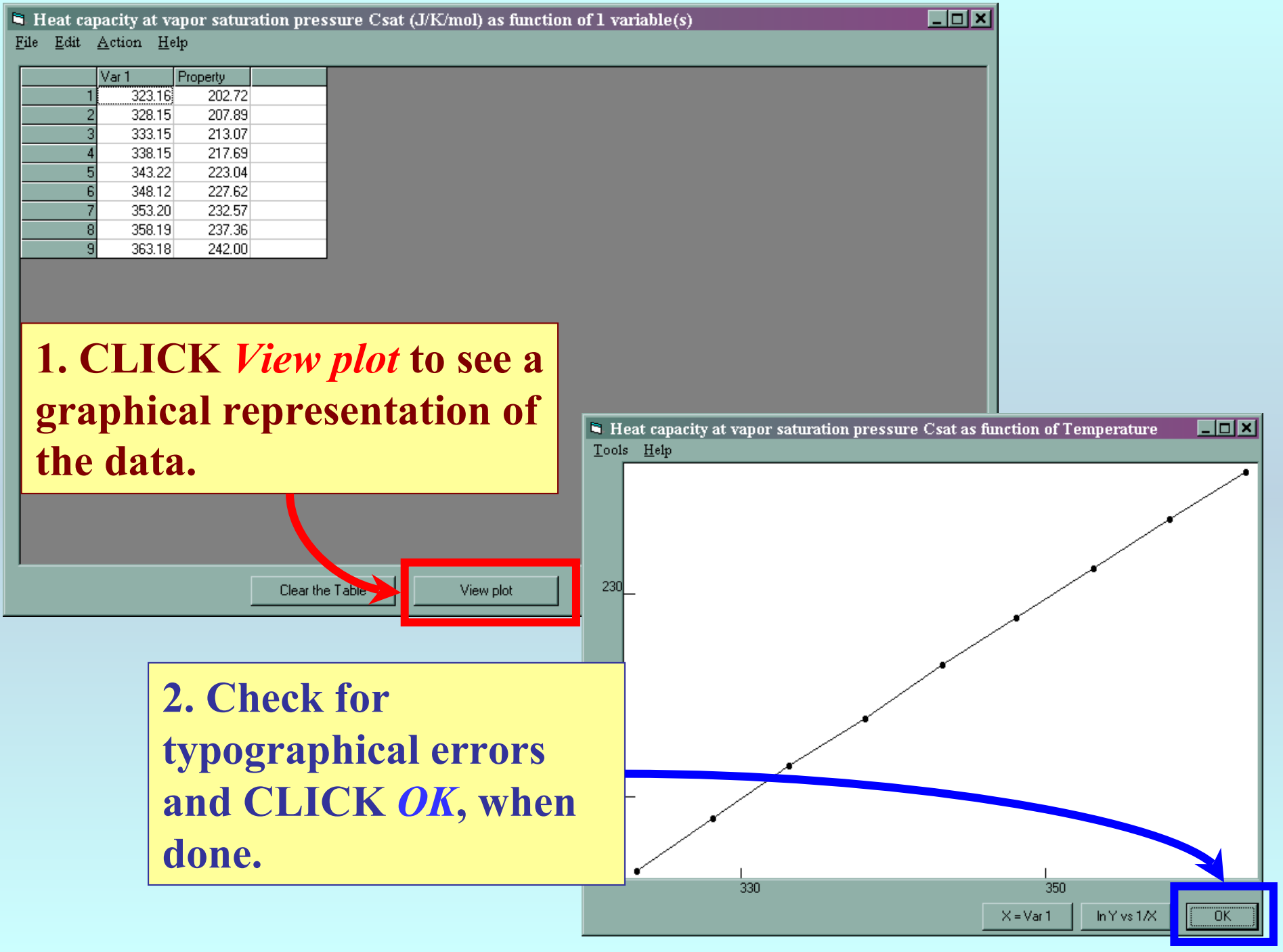

Heat capacity at vapor saturation pressure Csat (J/K/mol) as function of 1 variable(s)
Substance:
2-methyl-1-propanol
Sample #
1
Independent variable: Temperature
Temperature
Units:
K
Uncert
K
%
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Property set #
1
Phase 1:
Liquid
Phase 2:
Gas
Precisio
Commer
Numerical Data
Cancel
1. The Independent variable (Temperature) is filled automatically. SELECT the Units from the menu. Include approximate Uncertainty, if known.
1. SELECT Direct value for the Definition of Measurement Results and Experimental values for Data Presentation, here.

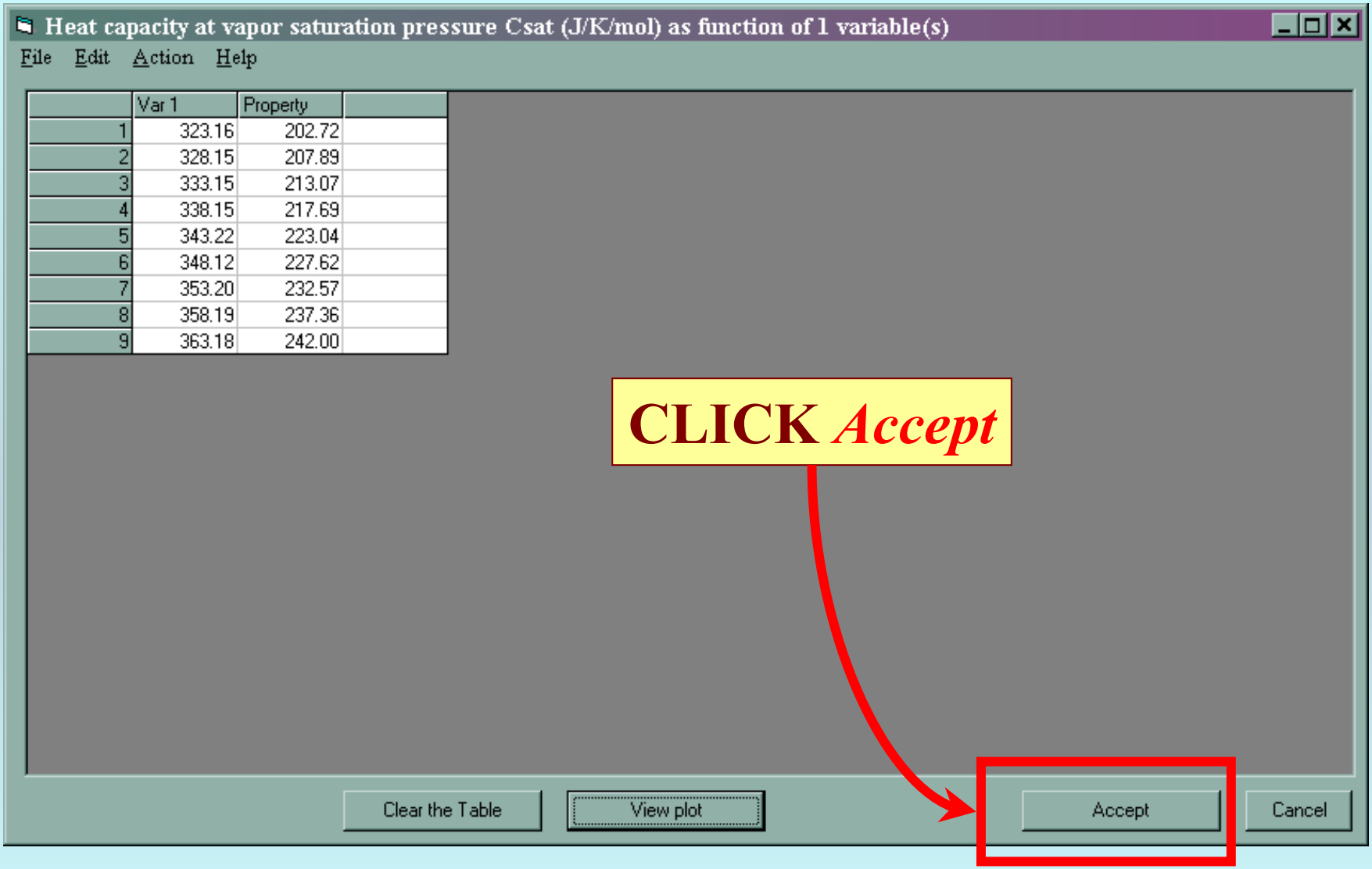

Heat capacity at vapor saturation pressure Csat (J/K/mol) as function of 1 variable(s)
Substance:
2-methyl-1-propanol
Sample #
1
Independent variable: Temperature
Temperature
Units:
2. Type the Precision of the Property Value, if known.
1. SELECT the phase for the property value Phase 1: Liquid, here.
NOTE: The Constraint is filled automatically based on the property definition.
Data presentation
Experimental values
Property set #
1
Constraint:
Phase boundary
Phase 1:
Liquid
Phase 2:
Gas
Precision of the Property Value(s)
0.5
J/K/mol
Comment to this record:
Calorimeter: SETARAM, France. Model BT-2.15.
3. CLICK Numerical Data
Numerical Data
Cancel

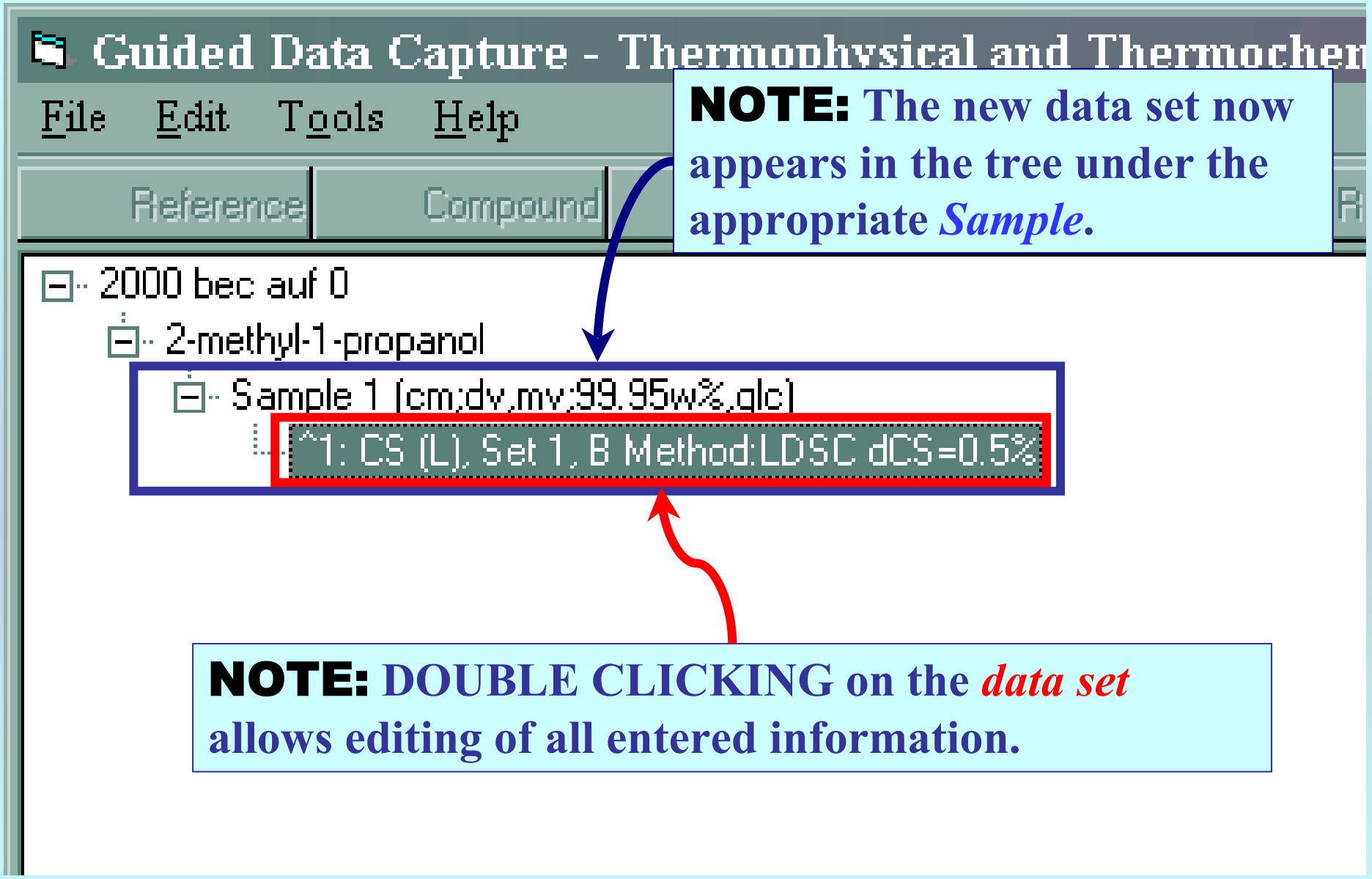

Heat capacity at vapor saturation pressure Csat (J/K/mol) as function of 1 variable(s)
File
Edit
Action
Help
Var 1
Property
TYPE, or much preferably, PASTE the variable and property values into the table.
See next page...
T/K
c_p^s/J mol^{-1} K^{-1}
2-Methyl-1-propanol
323.16 202.72
328.15 207.89
333.15 213.07
338.15 217.69
343.22 223.04
348.12 227.62
353.20 232.57
358.19 237.36
363.18 242.00
Clear the Table
Accept
Cancel



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.)


Heat capacity at vapor saturation pressure Csat (J/K/mol) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 323.16 202.72
2 328.15 207.89
3 333.15 213.07
4 338.15 217.69
5 343.22 223.04
6 348.12 227.62
7 353.20 232.57
8 358.19 237.36
9 363.18 242.00
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
Heat capacity at vapor saturation pressure Csat as function of Temperature
Tools Help
230
330
350
X = Var 1
ln Y vs 1/X
OK
2. Check for typographical errors and CLICK OK, when done.


Heat capacity at vapor saturation pressure Csat (J/K/mol) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 323.16 202.72
2 328.15 207.89
3 333.15 213.07
4 338.15 217.69
5 343.22 223.04
6 348.12 227.62
7 353.20 232.57
8 358.19 237.36
9 363.18 242.00
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochen
File Edit Tools Help
Reference
Compound
2000 bec auf 0
2-methyl-1-propanol
Sample 1 [cm;dv,mv;99.95w%,glc]
^1: CS (L), Set 1, B Method:LDSC dCS=0.5%
NOTE: The new data set now appears in the tree under the appropriate Sample.
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.**