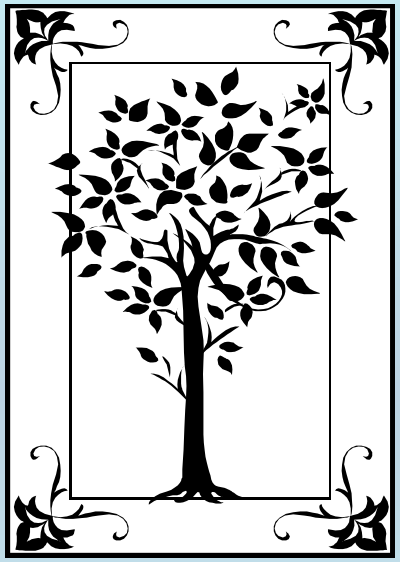
METADATA AND NUMERICAL DATA CAPTURE:
Densities ρ as f(*T*) with *p* = const.
(1 – Component)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Densities ρ as f(*T*) with *p* = const.**
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 2001, *46*, 1149−1152

Densities and Viscosities of Binary Mixtures of 1,4-Dioxane with 1-Propanol and 2-Propanol at (25, 30, 35, and 40) °C

Martín Contreras S.[†]

Facultad de Ciencias Químicas y Farmacéuticas, Universidad de Chile, Casilla 233, Santiago 1, Chile

Densities and viscosities for 1,4-dioxane with 1-propanol and 2-propanol mixtures have been measured as a function of mole fraction at atmospheric pressure at (25, 30, 35, and 40) °C. The calculated excess volumes (V^E) are positive over the whole range of composition in both systems. The V^E data were fitted by means of a Redlich−Kister type equation. Furthermore, McAllister's three-body-interaction model was used to correlate the kinematic viscosities of these systems.

Densities for 1 component as f(T) with p constrained
dioxane

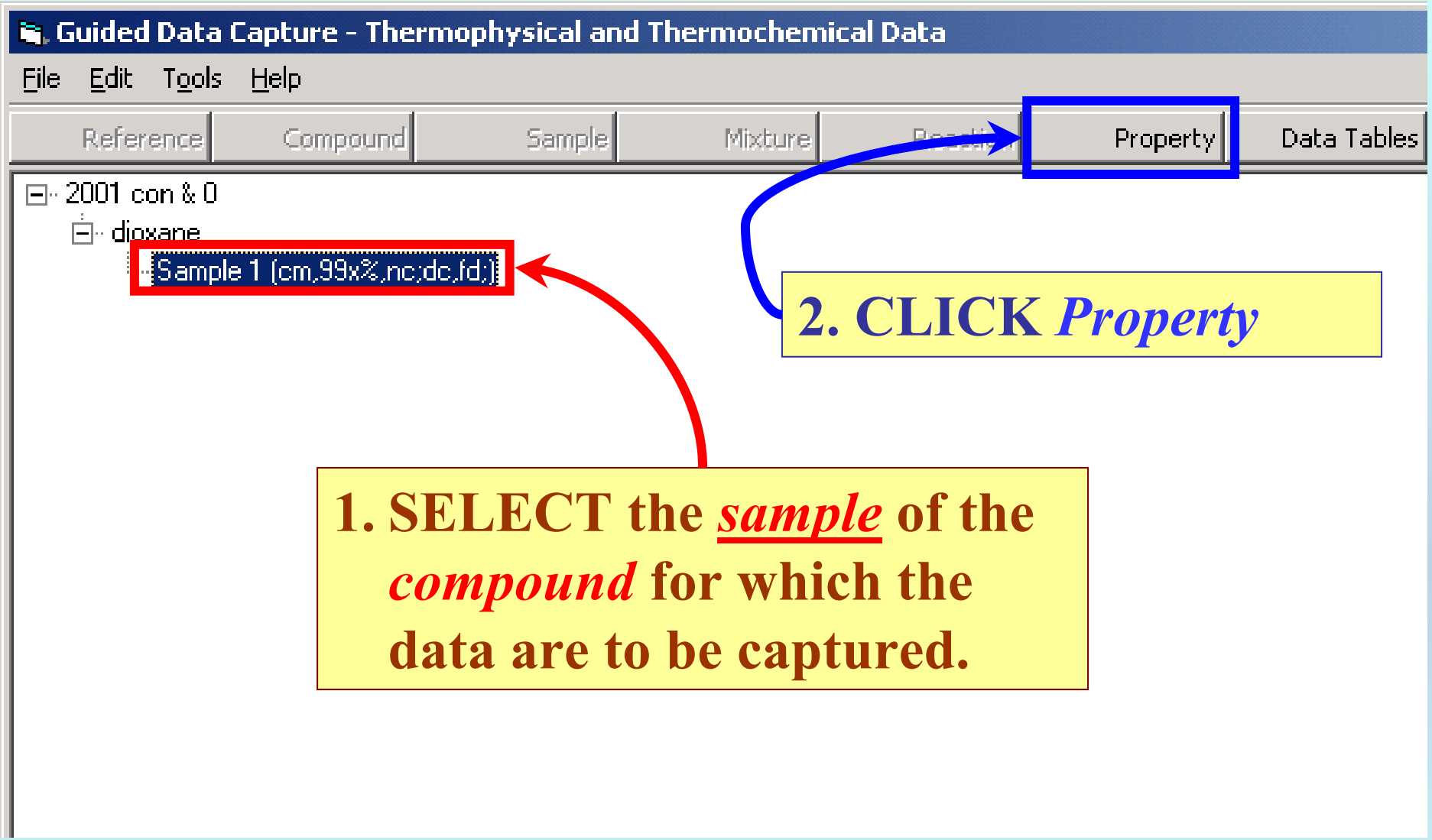
Table 1. Densities and Viscosities for the Pure Liquids at Different Temperatures

		ρ /(g·cm^{-3})		η /(mPa·s)	
liquid	t/°C	exptl	lit.	exptl	lit.
dioxane	25	1.027882	1.02812[a]	1.196	1.1944[a]
	30	1.022219	1.02223[a]	1.101	1.0937[a]
			1.02225[b]		
	35	1.016595	1.01689[a]	1.014	1.0112[a]
	40	1.011033	1.01157[b]	0.9425	–

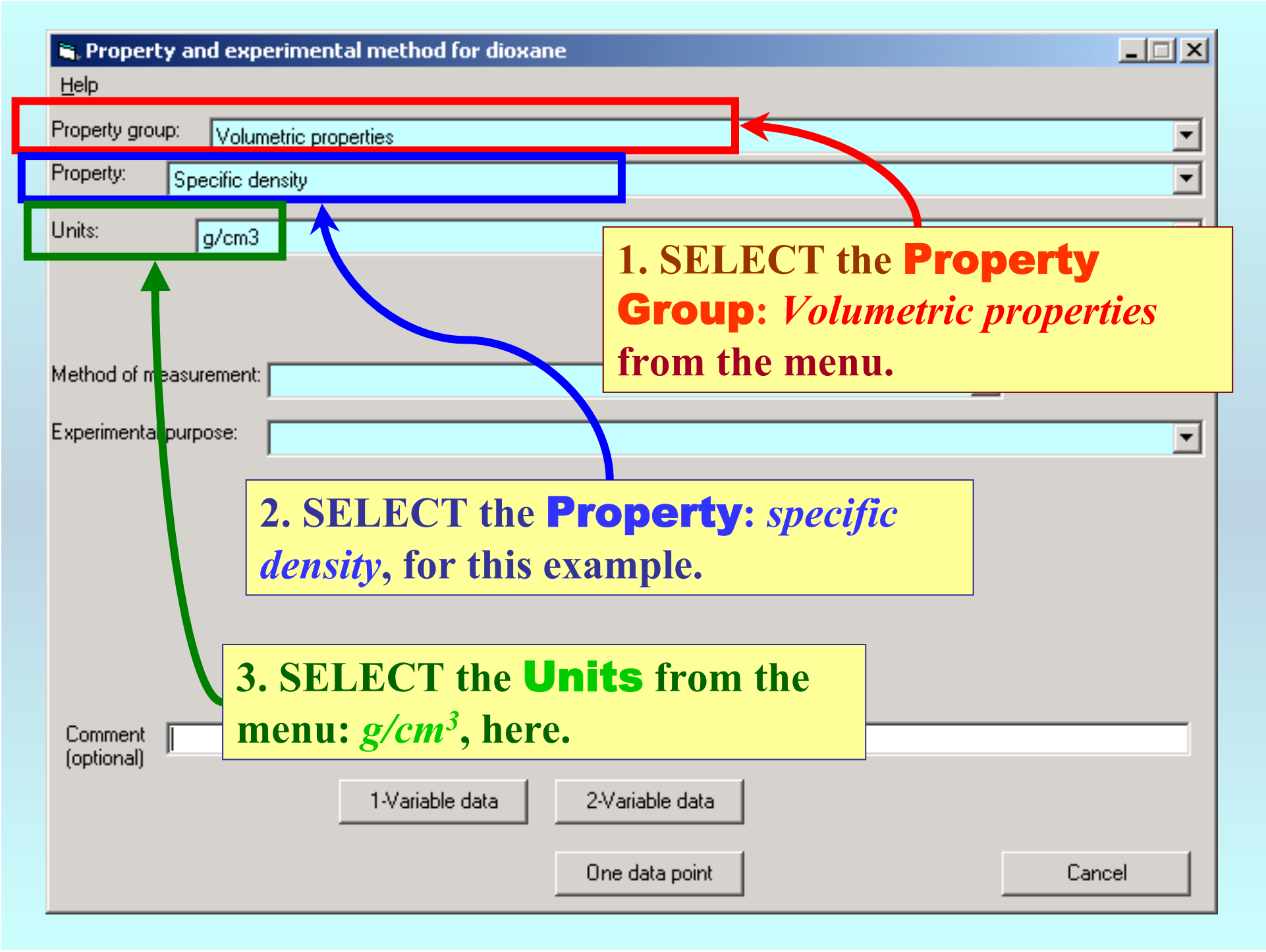
This data set is considered here.

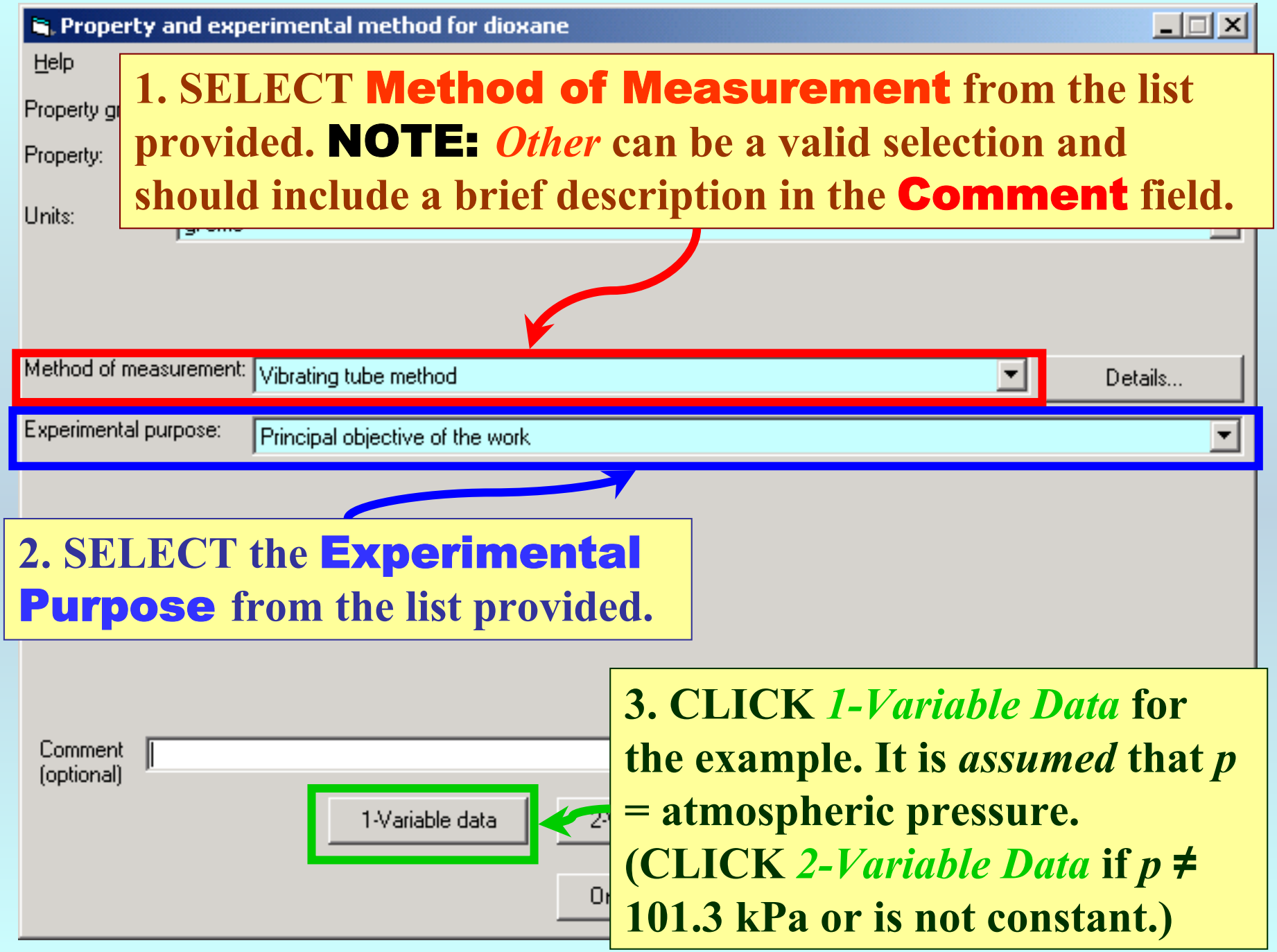
Experimental Method Info :

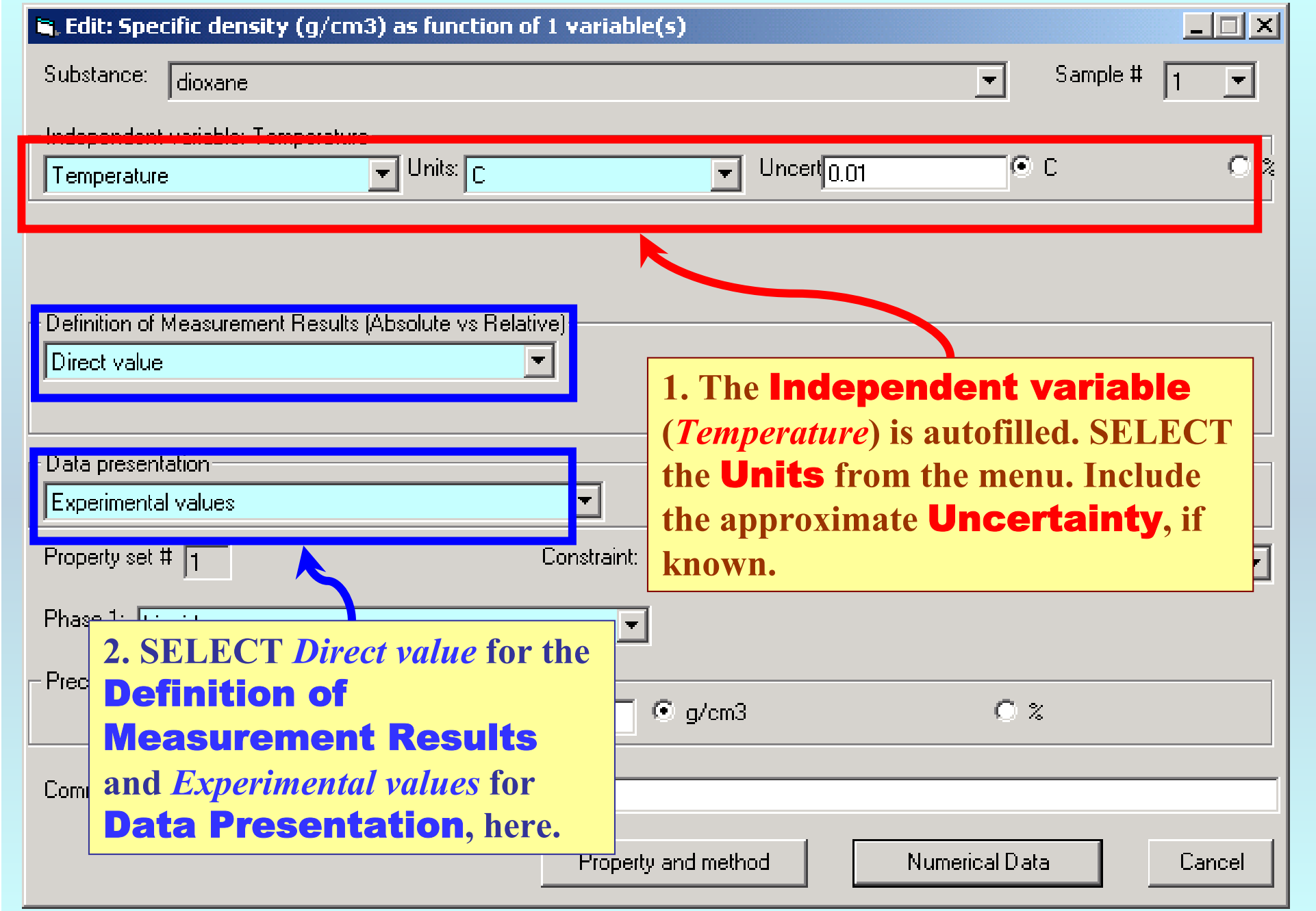
Apparatus and Procedure. The densities of the pure liquids and the mixtures were measured with an Anton Paar (DMA 602 + DMA 60) vibrating tube densimeter. It was calibrated with double-distilled water and air.[5,6] The temperatures were regulated using a circulating bath Heto DBT with a precision of ±0.01 K. The estimated uncertainty in density was $\pm 5 \times 10^{-6}$ g/cm^3.

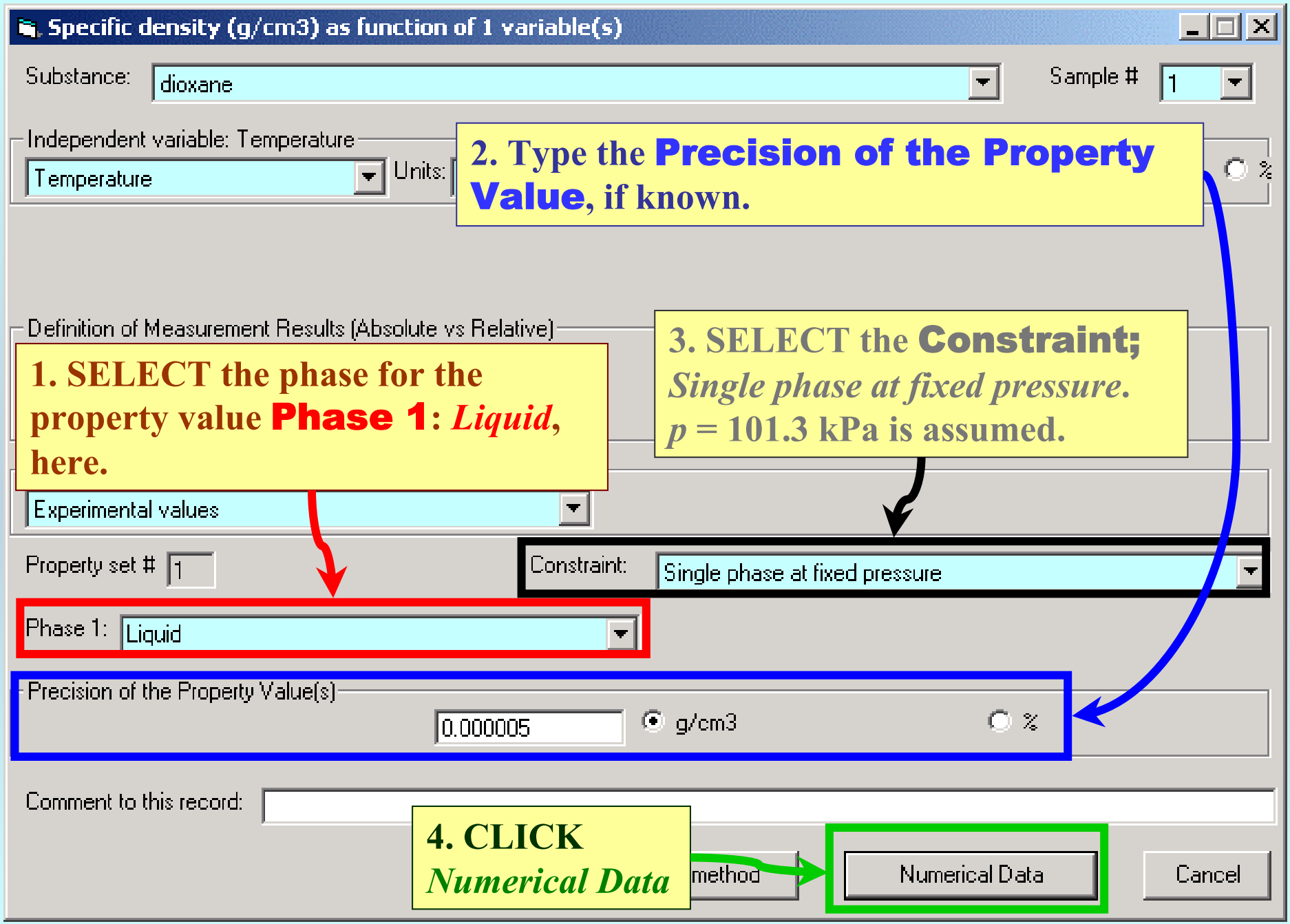


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for dioxane
Help
Property group:
Volumetric properties
Property:
Specific density
Units:
g/cm3
Method of measurement:
Experimental purpose:
Comment (optional)
1-Variable data
2-Variable data
One data point
Cancel
1. SELECT the Property Group: Volumetric properties from the menu.
2. SELECT the Property: specific density, for this example.
3. SELECT the Units from the menu: g/cm3, here.


Property and experimental method for dioxane
Help
Property gr
Property:
Units:
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.
Method of measurement:
Vibrating tube method
Details...
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
1-Variable data
3. CLICK 1-Variable Data for the example. It is assumed that p = atmospheric pressure. (CLICK 2-Variable Data if p ≠ 101.3 kPa or is not constant.)


Edit: Specific density (g/cm3) as function of 1 variable(s)
Substance:
dioxane
Sample #
1
Temperature
Units:
C
Uncert
0.01
C
%
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Property set #
1
Constraint:
g/cm3
%
Property and method
Numerical Data
Cancel
1. The Independent variable (Temperature) is autofilled. SELECT the Units from the menu. Include the approximate Uncertainty, if known.
2. SELECT Direct value for the Definition of Measurement Results and Experimental values for Data Presentation, here.


Specific density (g/cm3) as function of 1 variable(s)
Substance:
dioxane
Sample #
1
Independent variable: Temperature
Temperature
Units:
%
2. Type the Precision of the Property Value, if known.
Definition of Measurement Results (Absolute vs Relative)
1. SELECT the phase for the property value Phase 1: Liquid, here.
3. SELECT the Constraint; Single phase at fixed pressure. p = 101.3 kPa is assumed.
Experimental values
Property set #
1
Constraint:
Single phase at fixed pressure
Phase 1:
Liquid
Precision of the Property Value(s)
0.000005
g/cm3
%
Comment to this record:
4. CLICK Numerical Data
method
Numerical Data
Cancel

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

See next page...

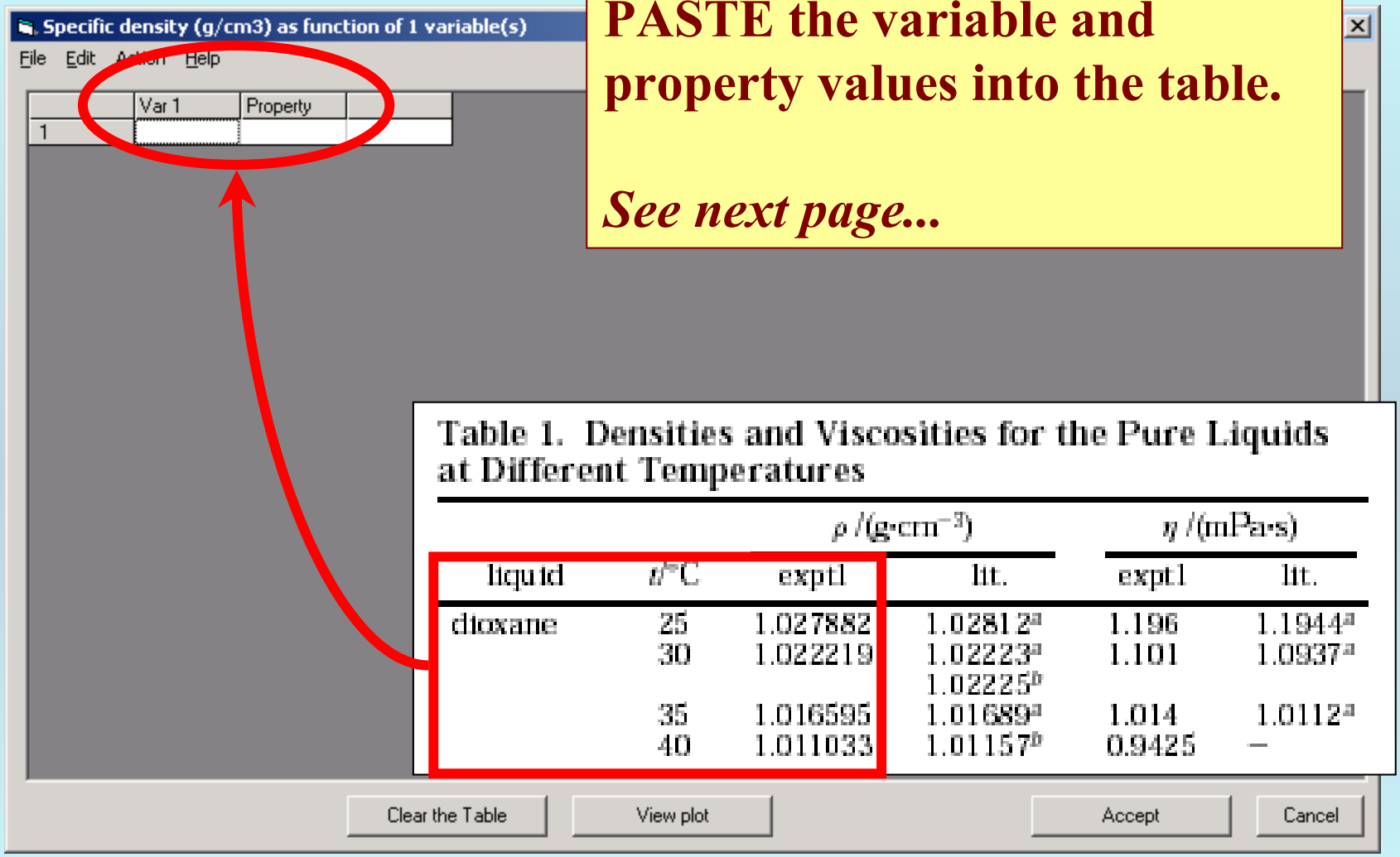
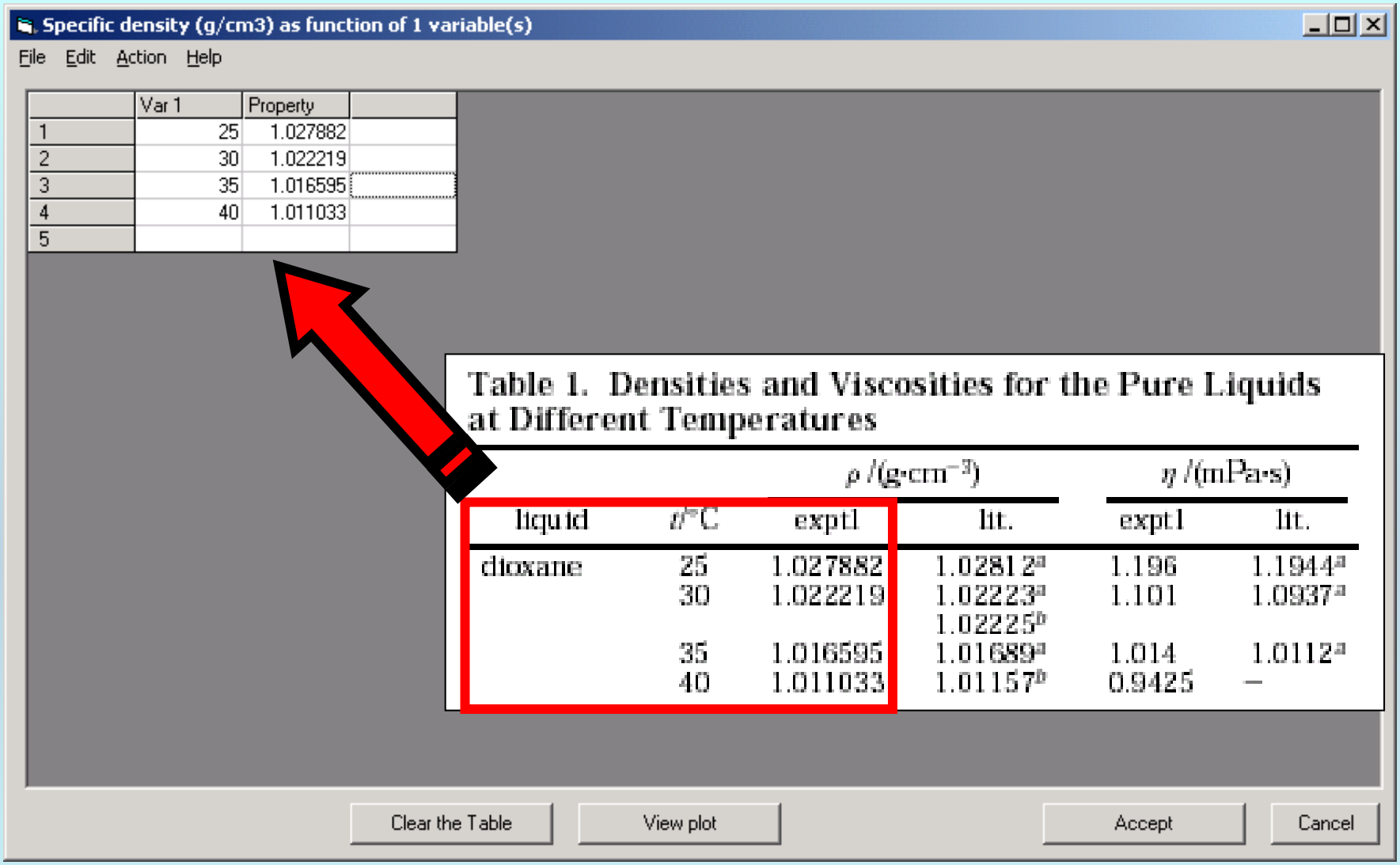
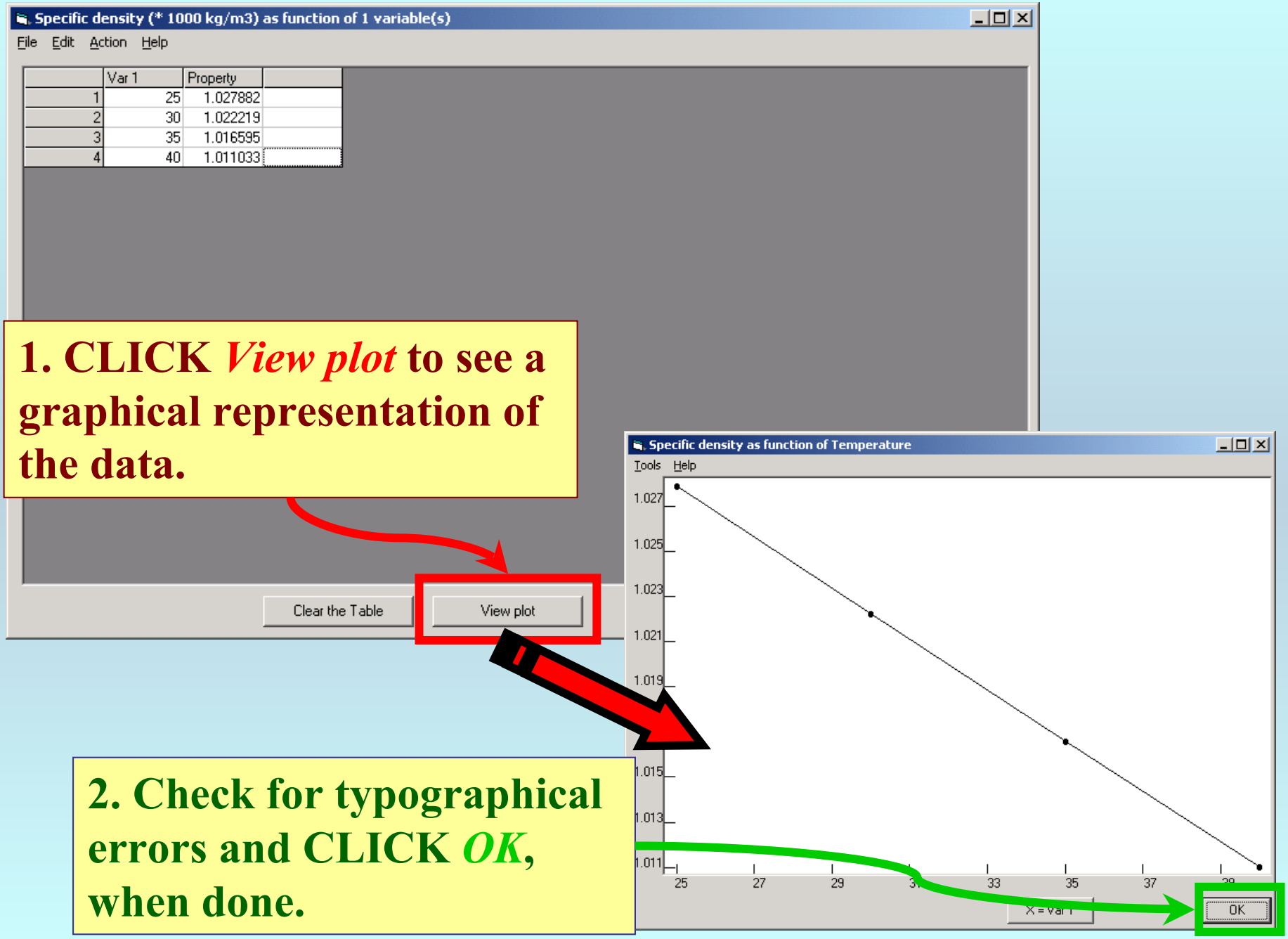


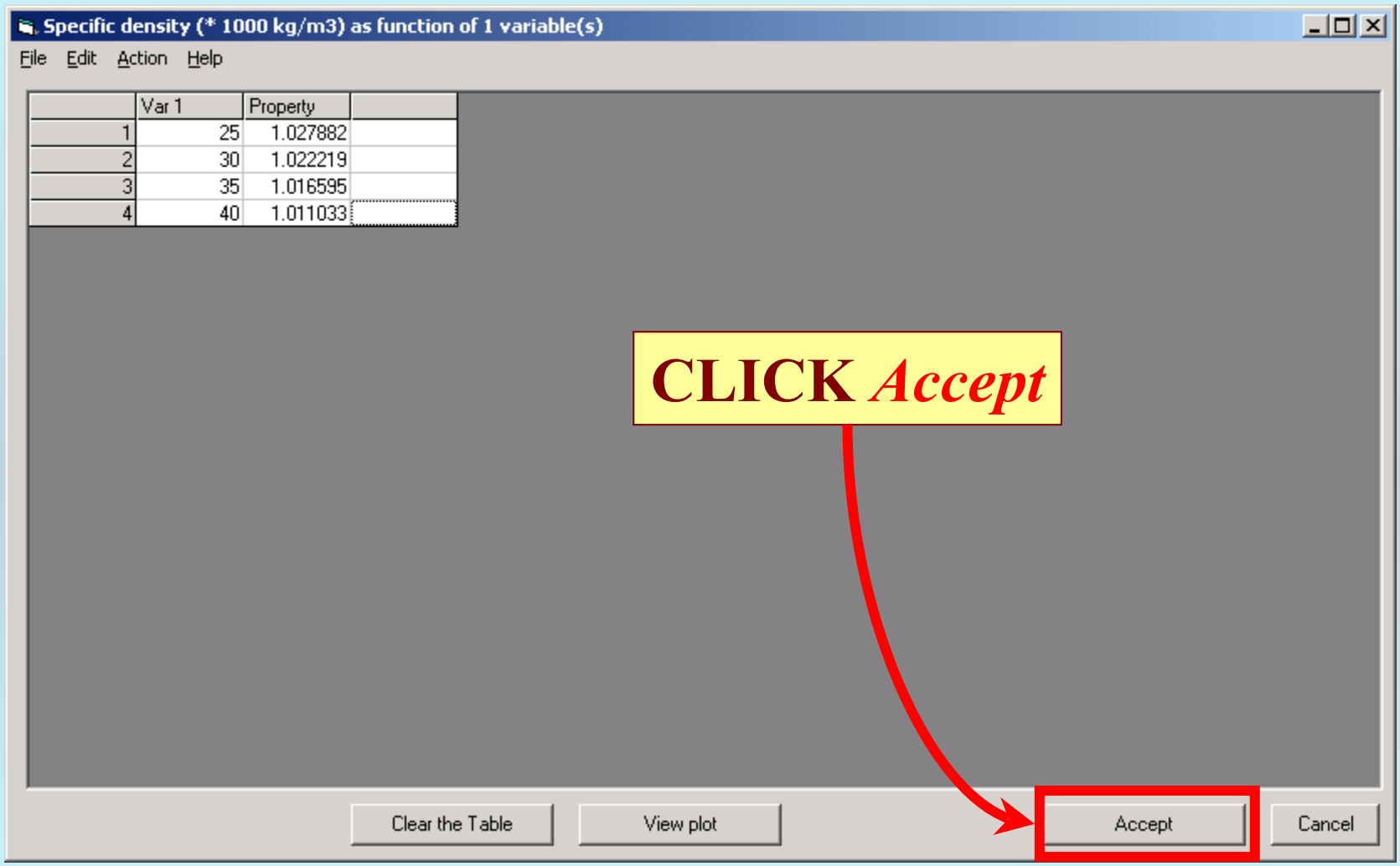
Table 1. Densities and Viscosities for the Pure Liquids at Different Temperatures

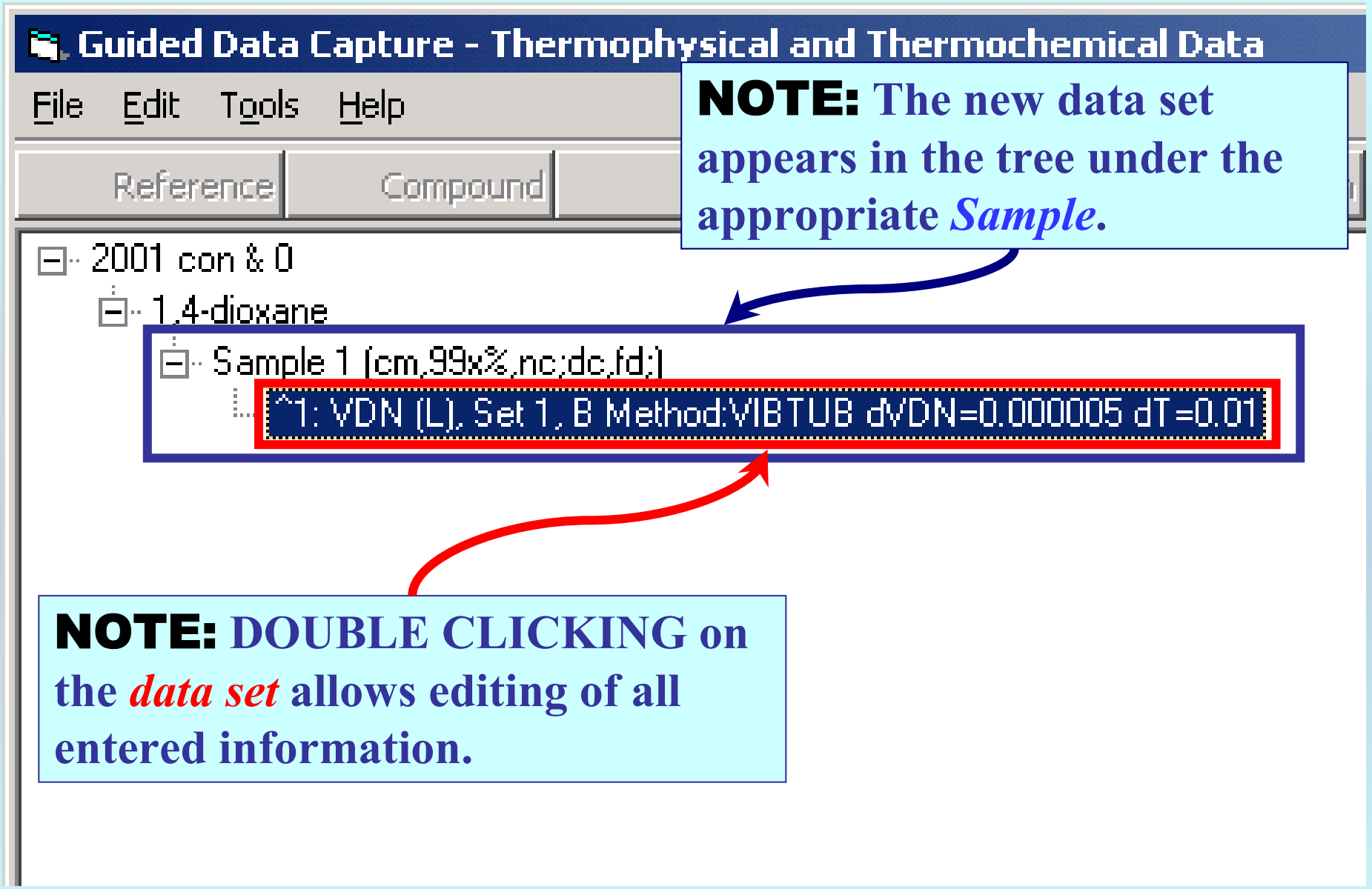
		ρ /(g·cm^{-3})		η /(mPa·s)	
liquid	t/°C	exptl	lit.	exptl	lit.
dioxane	25	1.027882	1.02812[a]	1.196	1.1944[a]
	30	1.022219	1.02223[a]	1.101	1.0937[a]
			1.02225[b]		
	35	1.016595	1.01689[a]	1.014	1.0112[a]
	40	1.011033	1.01157[b]	0.9425	–



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.)


Specific density (* 1000 kg/m3) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 25 1.027882
2 30 1.022219
3 35 1.016595
4 40 1.011033
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
Specific density as function of Temperature
Tools Help
1.027
1.025
1.023
1.021
1.019
1.015
1.013
1.011
25 27 29 33 35 37
X = Var 1
OK
2. Check for typographical errors and CLICK OK, when done.


Specific density (* 1000 kg/m3) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 25 1.027882
2 30 1.022219
3 35 1.016595
4 40 1.011033
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound
2001 con & 0
1,4-dioxane
Sample 1 [cm,99x%,nc;dc,fd;]
^1: VDN (L), Set 1, B Method:VIBTUB dVDN=0.000005 dT=0.01
NOTE: The new data set 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.**