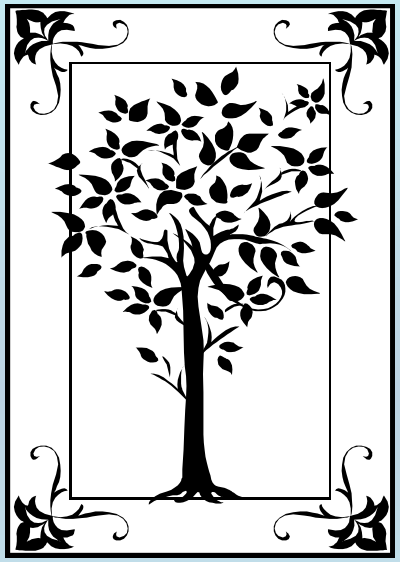
# METADATA AND NUMERICAL DATA CAPTURE:
# Densities ρ as f(*T*,*p*)
## (1 – Component)

**Guided Data Capture (GDC)**



**This tutorial describes**
**METADATA AND NUMERICAL DATA CAPTURE:**
for **Densities ρ as f(*T*, *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:

*J. Chem. Eng. Data* 2002, *47*, 233−238 

## High-Pressure Volumetric Behavior of *x* 1,1,1,2-Tetrafluoroethane + (1 − *x*) 2,5,8,11,14-Pentaoxapentadecane (TEGDME) Mixtures

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Laboratorio de Propiedades Termofísicas, Departamento de Física Aplicada, Facultad de Física, Universidad de Santiago de Compostela, E-15782 Santiago de Compostela, Spain, and Laboratoire des Fluides Complexes, Faculté des Sciences, BP 1155, F-64013 Pau Cedex, France

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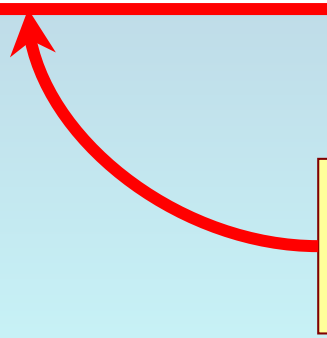
This paper reports 1017 new *pVT* measurements of the *x* 1,1,1,2-tetrafluoroethane (HFC-134a) + (1 − *x*) 2,5,8,11,14-pentaoxapentadecane (TEGDME) system for *x* = 0.0, 0.1114, 0.2896, 0.3648, 0.5702, 0.6931, 0.7288, 0.8727, 0.9290, and 1 between 10 and 60 MPa in the temperature range 293.15 K to 373.15 K at 5 MPa and 10 K intervals, respectively. In almost all the measurement range, the density of the pure compressed refrigerant is greater than that of the pure polyether. For temperatures higher than 343.15 K, the isocomposition curves for the mixtures show an intersection point. Similar behavior has been previously found for HFC-134a + triethylene glycol dimethyl ether, carbon dioxide + alkane or toluene systems, and mixtures of R-410A with polyolester lubricants. The excess molar volume is negative over the whole composition range at all temperatures and pressures.

# Densities for 1 component as f(T) with p constrained
## 2,5,8,11,14-pentaoxapentadecane (TEGDME)

Table 1. Experimental Values of Densities, $\rho$, for $x$ HFC-134a + $(1 - x)$ TEGDME at Different Temperatures, $T$, and Pressures, $p$

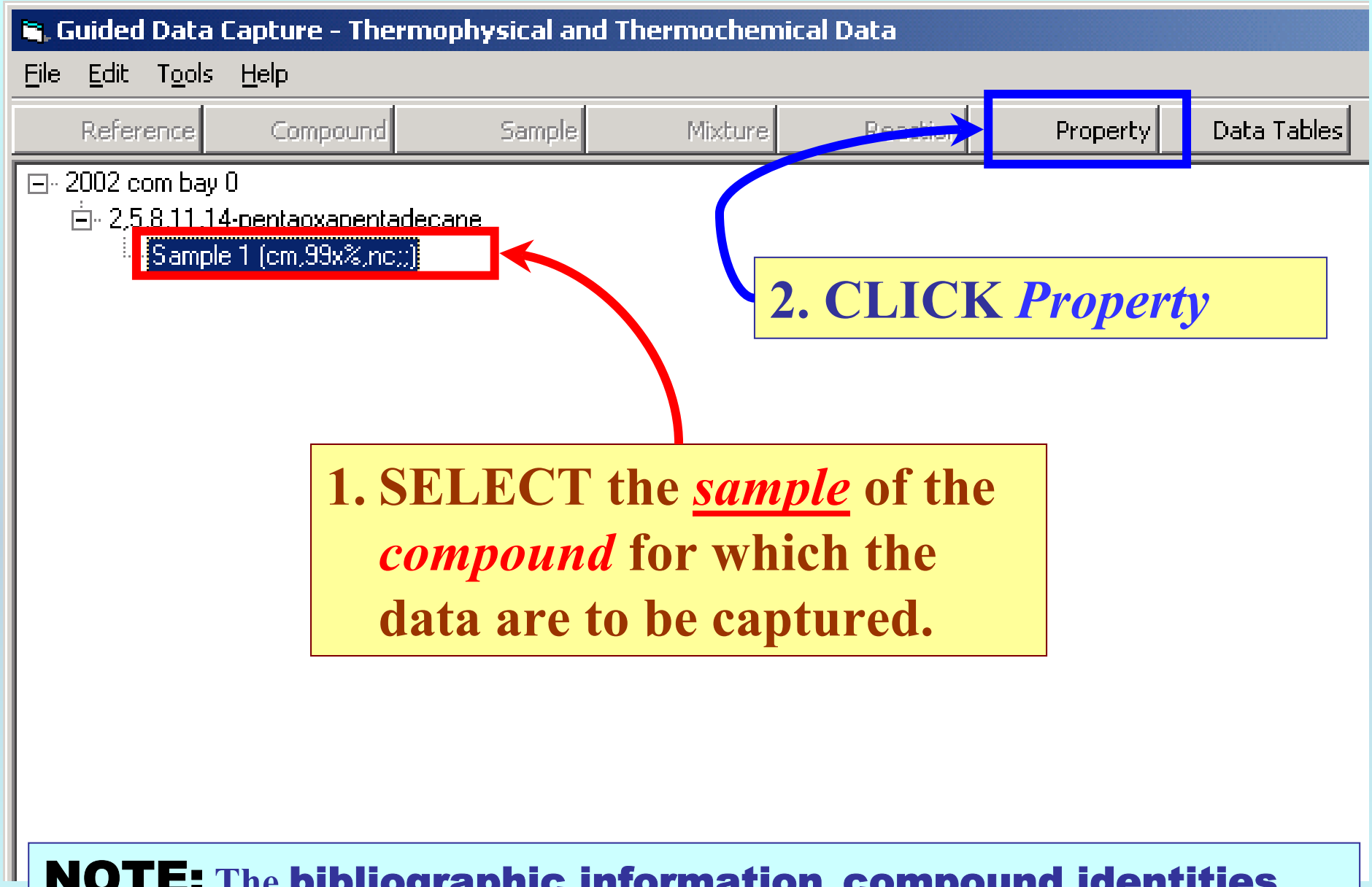
| | | $\rho$/(g·cm$^{-3}$) at the following values of $T$/K | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $x$ | $p$/MPa | 293.15 | 303.15 | 313.15 | 323.15 | 333.15 | 343.15 | 353.15 | 363.15 | 373.15 |
| 0 | 0.1 | 1.0112 | 1.0018 | 0.9925 | 0.9833 | 0.9740 | 0.9648 | 0.9556 | 0.9469 | 0.9375 |
| | 5 | 1.0142 | 1.0050 | 0.9959 | 0.9868 | 0.9778 | 0.9687 | 0.9598 | 0.9513 | 0.9423 |
| | 10 | 1.0172 | 1.0082 | 0.9992 | 0.9903 | 0.9814 | 0.9726 | 0.9639 | 0.9557 | 0.9468 |
| | 15 | 1.0201 | 1.0113 | 1.0025 | 0.9937 | 0.9850 | 0.9764 | 0.9679 | 0.9598 | 0.9511 |
| | 20 | 1.0229 | 1.0143 | 1.0055 | 0.9970 | 0.9883 | 0.9800 | 0.9716 | 0.9639 | 0.9552 |
| | 25 | 1.0257 | 1.0172 | 1.0086 | 1.0001 | 0.9917 | 0.9835 | 0.9752 | 0.9675 | 0.9593 |
| | 30 | 1.0284 | 1.0200 | 1.0116 | 1.0032 | 0.9950 | 0.9869 | 0.9788 | 0.9712 | 0.9631 |
| | 35 | 1.0310 | 1.0227 | 1.0144 | 1.0063 | 0.9982 | 0.9901 | 0.9821 | 0.9748 | 0.9669 |
| | 40 | 1.0336 | 1.0254 | 1.0172 | 1.0091 | 1.0012 | 0.9932 | 0.9855 | 0.9783 | 0.9704 |
| | 45 | 1.0361 | 1.0281 | 1.0201 | 1.0121 | 1.0042 | 0.9963 | 0.9886 | 0.9815 | 0.9739 |
| | 50 | 1.0385 | 1.0306 | 1.0226 | 1.0147 | 1.0070 | 0.9993 | 0.9917 | 0.9846 | 0.9771 |
| | 55 | 1.0410 | 1.0332 | 1.0252 | 1.0175 | 1.0098 | 1.0023 | 0.9947 | 0.9880 | 0.9805 |
| | 60 | 1.0434 | 1.0355 | 1.0278 | 1.0202 | 1.0126 | 1.0050 | 0.9976 | 0.9910 | 0.9838 |



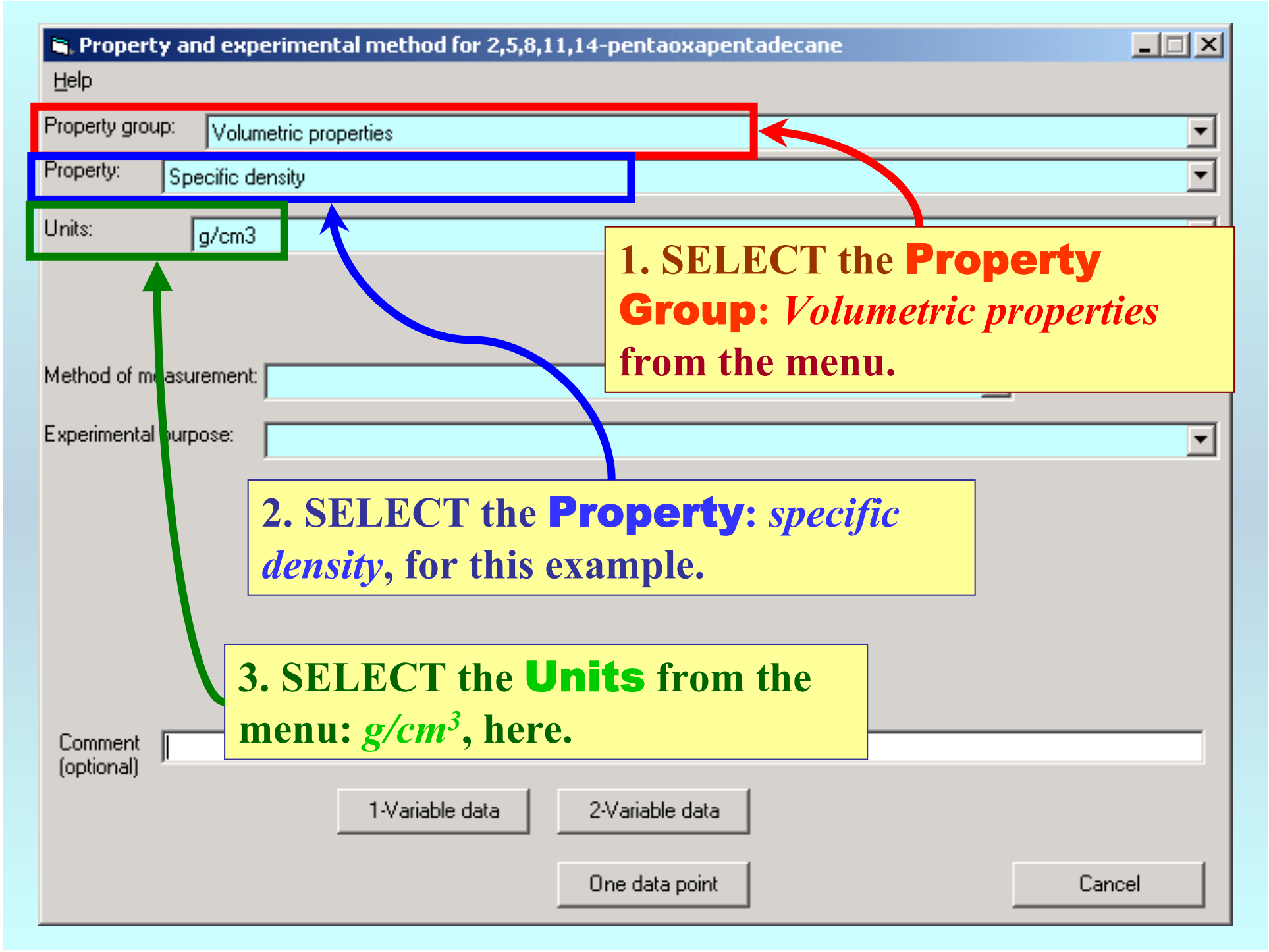
**This data set is considered here.**

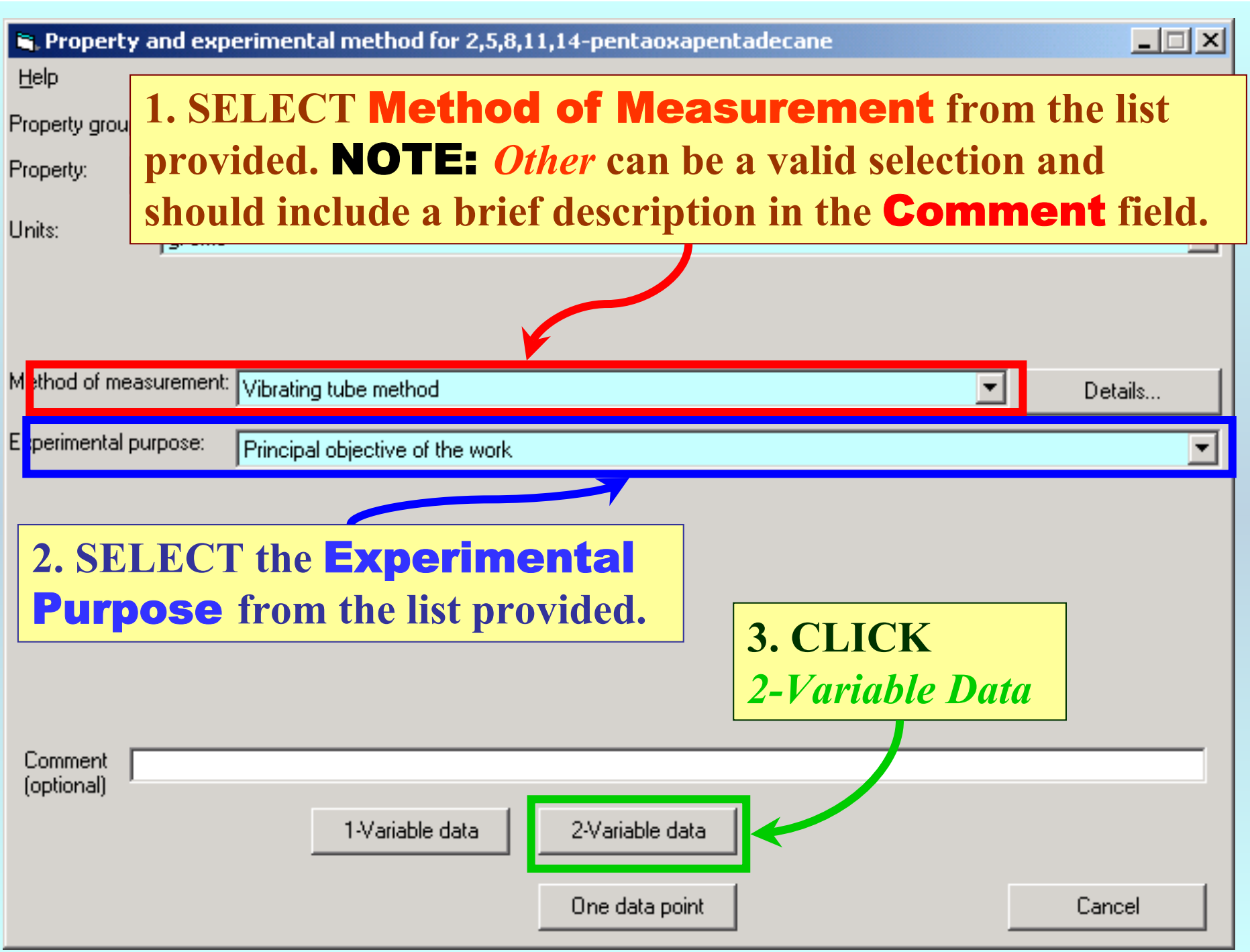
## Experimental Method Info :

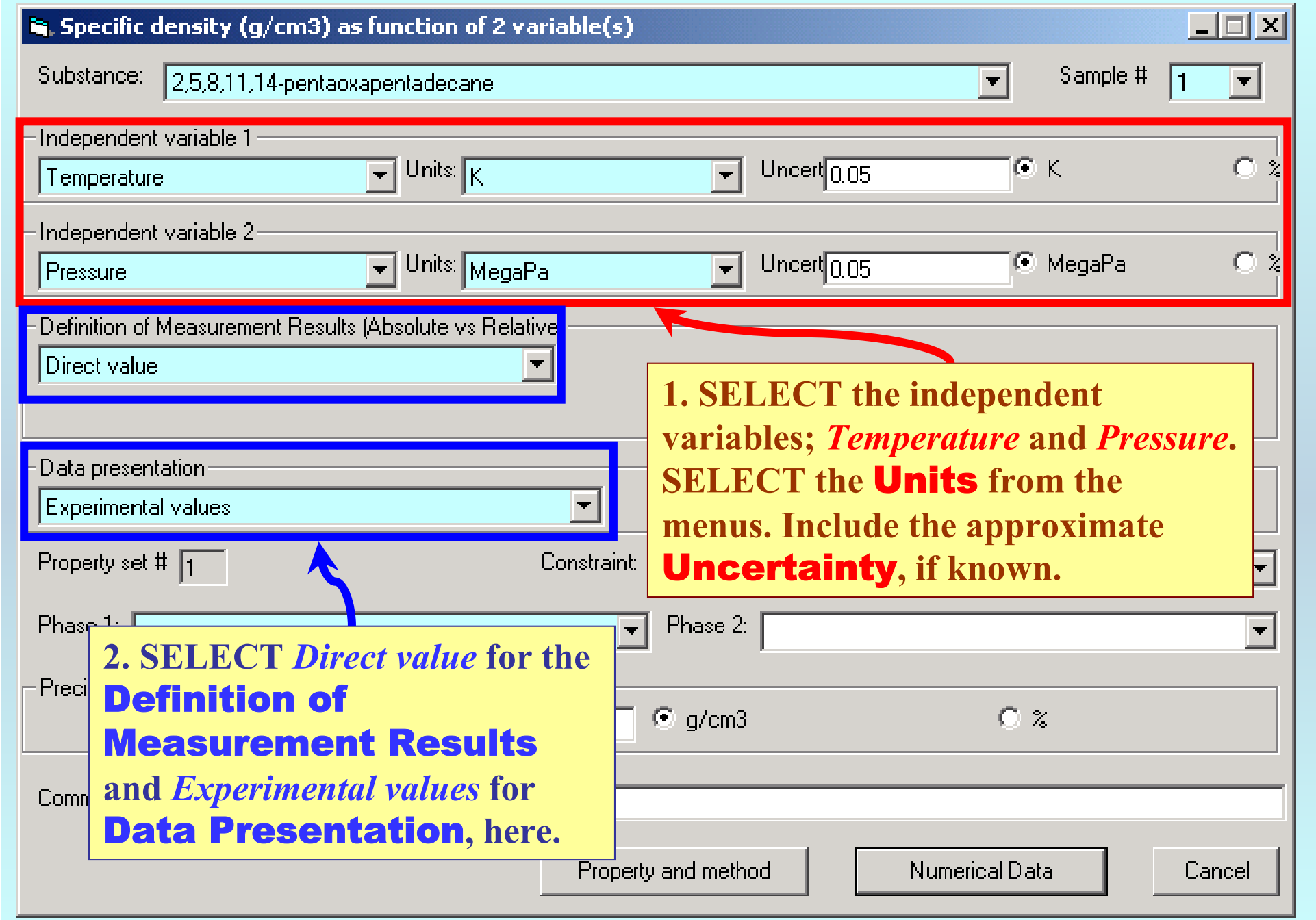
**Vibrating tube densimeter**

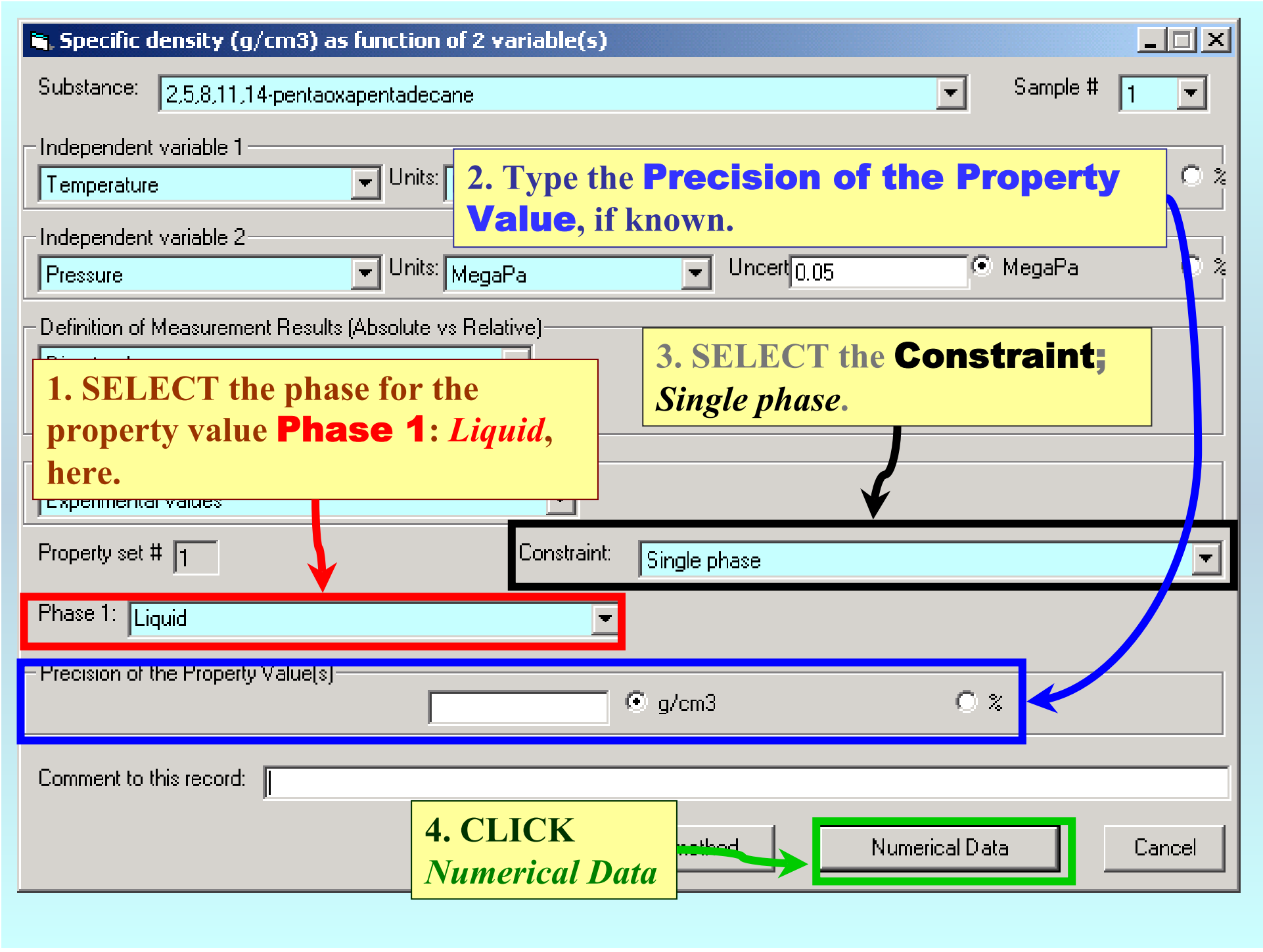



**NOTE:** The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for 2,5,8,11,14-pentaoxapentadecane
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 2,5,8,11,14-pentaoxapentadecane
Help
Property grou
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.
3. CLICK
2-Variable Data
Comment (optional)
1-Variable data
2-Variable data
One data point
Cancel


Specific density (g/cm3) as function of 2 variable(s)
Substance:
2,5,8,11,14-pentaoxapentadecane
Sample #
1
Independent variable 1
Temperature
Units:
K
Uncert
0.05
K
Independent variable 2
Pressure
Units:
MegaPa
Uncert
0.05
MegaPa
Definition of Measurement Results (Absolute vs Relative
Direct value
Data presentation
Experimental values
Property set #
1
Constraint:
Phase 1:
Phase 2:
g/cm3
Property and method
Numerical Data
Cancel
1. SELECT the independent variables; Temperature and Pressure. SELECT the Units from the menus. 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 2 variable(s)
Substance:
2,5,8,11,14-pentaoxapentadecane
Sample #
1
Independent variable 1
Temperature
Units:
Independent variable 2
Pressure
Units:
MegaPa
Uncert
0.05
MegaPa
Definition of Measurement Results (Absolute vs Relative)
2. Type the Precision of the Property Value, if known.
3. SELECT the Constraint; Single phase.
1. SELECT the phase for the property value Phase 1: Liquid, here.
Property set #
1
Constraint:
Single phase
Phase 1:
Liquid
Precision of the Property Value(s)
g/cm3
%
Comment to this record:
4. CLICK Numerical Data
Numerical Data
Cancel

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

***See next page...***

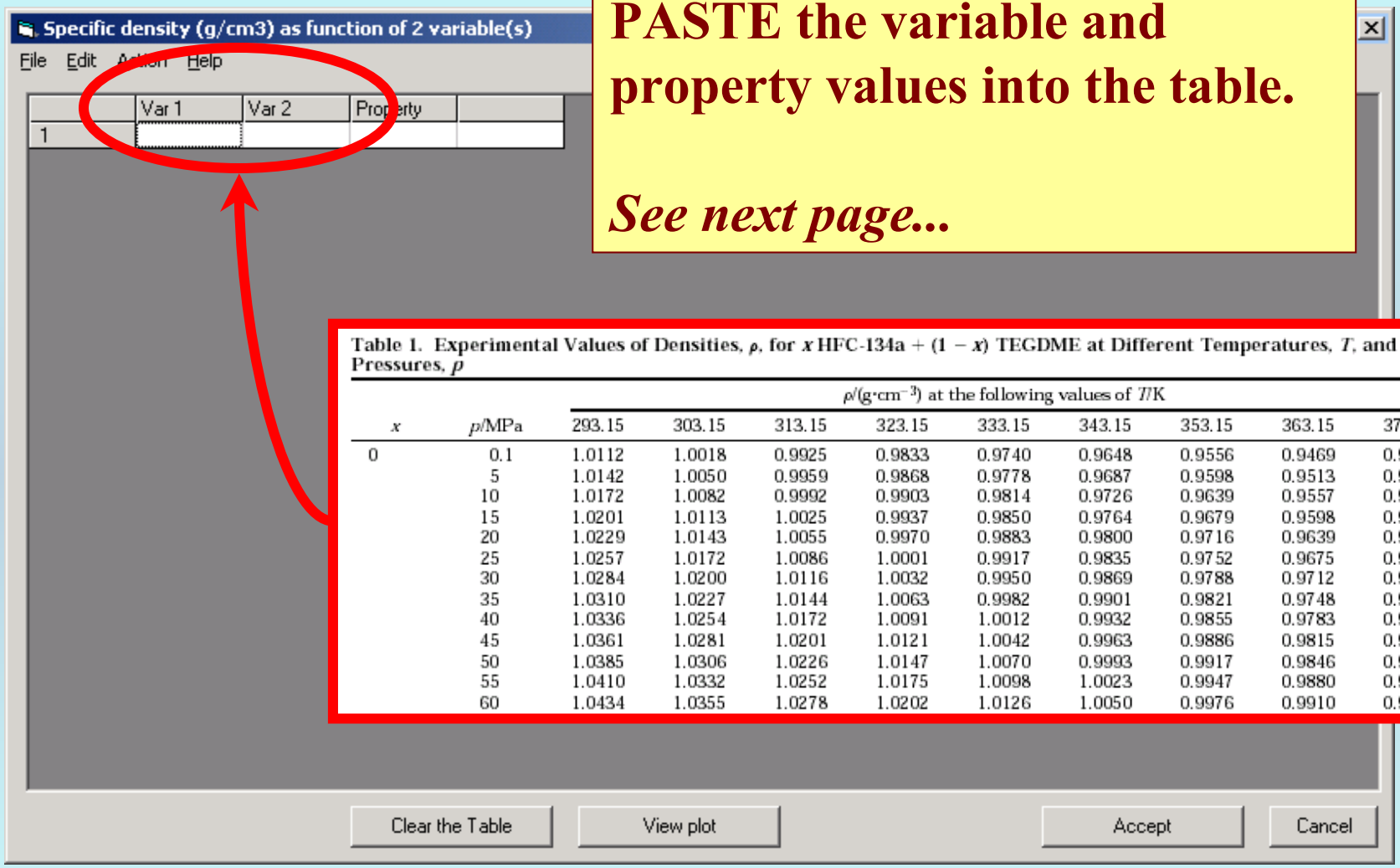



Table 1. Experimental Values of Densities, $\rho$, for $x$ HFC-134a + $(1 - x)$ TEGDME at Different Temperatures, $T$, and Pressures, $p$

| | | $\rho$/(g·cm$^{-3}$) at the following values of $T$/K | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
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| | 5 | 1.0142 | 1.0050 | 0.9959 | 0.9868 | 0.9778 | 0.9687 | 0.9598 | 0.9513 | 0.9423 |
| | 10 | 1.0172 | 1.0082 | 0.9992 | 0.9903 | 0.9814 | 0.9726 | 0.9639 | 0.9557 | 0.9468 |
| | 15 | 1.0201 | 1.0113 | 1.0025 | 0.9937 | 0.9850 | 0.9764 | 0.9679 | 0.9598 | 0.9511 |
| | 20 | 1.0229 | 1.0143 | 1.0055 | 0.9970 | 0.9883 | 0.9800 | 0.9716 | 0.9639 | 0.9552 |
| | 25 | 1.0257 | 1.0172 | 1.0086 | 1.0001 | 0.9917 | 0.9835 | 0.9752 | 0.9675 | 0.9593 |
| | 30 | 1.0284 | 1.0200 | 1.0116 | 1.0032 | 0.9950 | 0.9869 | 0.9788 | 0.9712 | 0.9631 |
| | 35 | 1.0310 | 1.0227 | 1.0144 | 1.0063 | 0.9982 | 0.9901 | 0.9821 | 0.9748 | 0.9669 |
| | 40 | 1.0336 | 1.0254 | 1.0172 | 1.0091 | 1.0012 | 0.9932 | 0.9855 | 0.9783 | 0.9704 |
| | 45 | 1.0361 | 1.0281 | 1.0201 | 1.0121 | 1.0042 | 0.9963 | 0.9886 | 0.9815 | 0.9739 |
| | 50 | 1.0385 | 1.0306 | 1.0226 | 1.0147 | 1.0070 | 0.9993 | 0.9917 | 0.9846 | 0.9771 |
| | 55 | 1.0410 | 1.0332 | 1.0252 | 1.0175 | 1.0098 | 1.0023 | 0.9947 | 0.9880 | 0.9805 |
| | 60 | 1.0434 | 1.0355 | 1.0278 | 1.0202 | 1.0126 | 1.0050 | 0.9976 | 0.9910 | 0.9838 |

Specific density (g/cm3) as function of 2 variable(s)

File Edit Action Help

| | Var 1 | Var 2 | Property |
|---|---|---|---|
| 1 | 293.15 | 0.10 | 1.0112 |
| 2 | 293.15 | 5.00 | 1.0142 |
| 3 | 293.15 | 10.00 | 1.0172 |
| 4 | 293.15 | 15.00 | 1.0201 |
| 5 | 293.15 | 20.00 | 1.0229 |
| 6 | 293.15 | 25.00 | 1.0257 |
| 7 | 293.15 | 30.00 | 1.0284 |
| 8 | 293.15 | 35.00 | 1.0310 |
| 9 | 293.15 | 40.00 | 1.0336 |
| 10 | 293.15 | 45.00 | 1.0361 |
| 11 | 293.15 | 50.00 | |
| 12 | 293.15 | 55.00 | |
| 13 | 293.15 | 60.00 | |
| 14 | 303.15 | 0.10 | |
| 15 | 303.15 | 5.00 | |
| 16 | 303.15 | 10.00 | 1.0082 |
| 17 | 303.15 | 15.00 | 1.0113 |
| 18 | 303.15 | 20.00 | 1.0143 |
| 19 | 303.15 | 25.00 | 1.0172 |
| 20 | 303.15 | 30.00 | 1.0200 |
| 21 | 303.15 | 35.00 | 1.0227 |
| 22 | 303.15 | 40.00 | 1.0254 |
| 23 | 303.15 | 45.00 | 1.0281 |
| 24 | 303.15 | 50.00 | 1.0306 |
| 25 | 303.15 | 55.00 | 1.0332 |

Table 1. Experimental Values of Densities, $\rho$, for $x$ HFC-134a + $(1 - x)$ TEGDME at Different Temperatures, $T$, and Pressures, $p$

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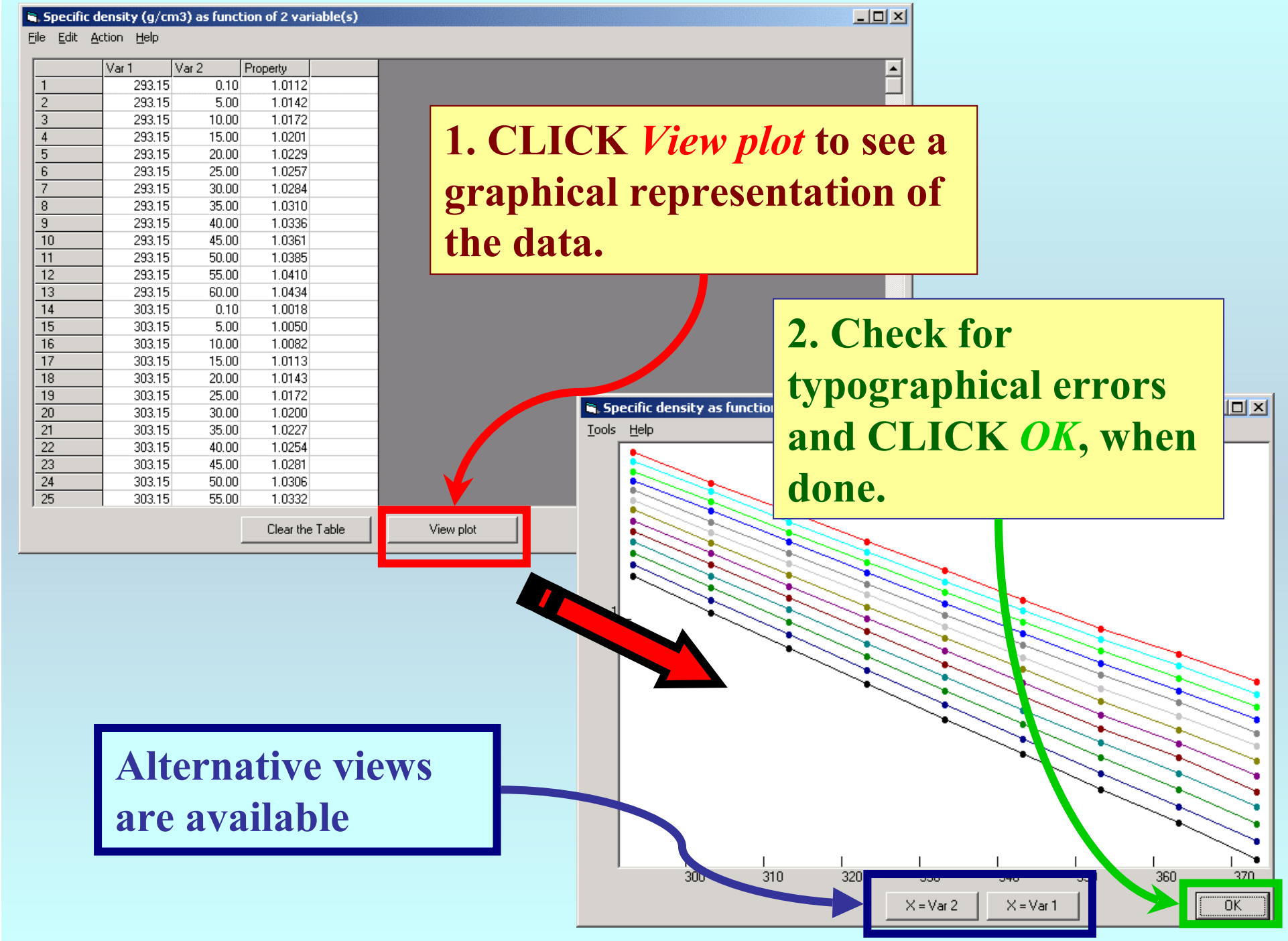
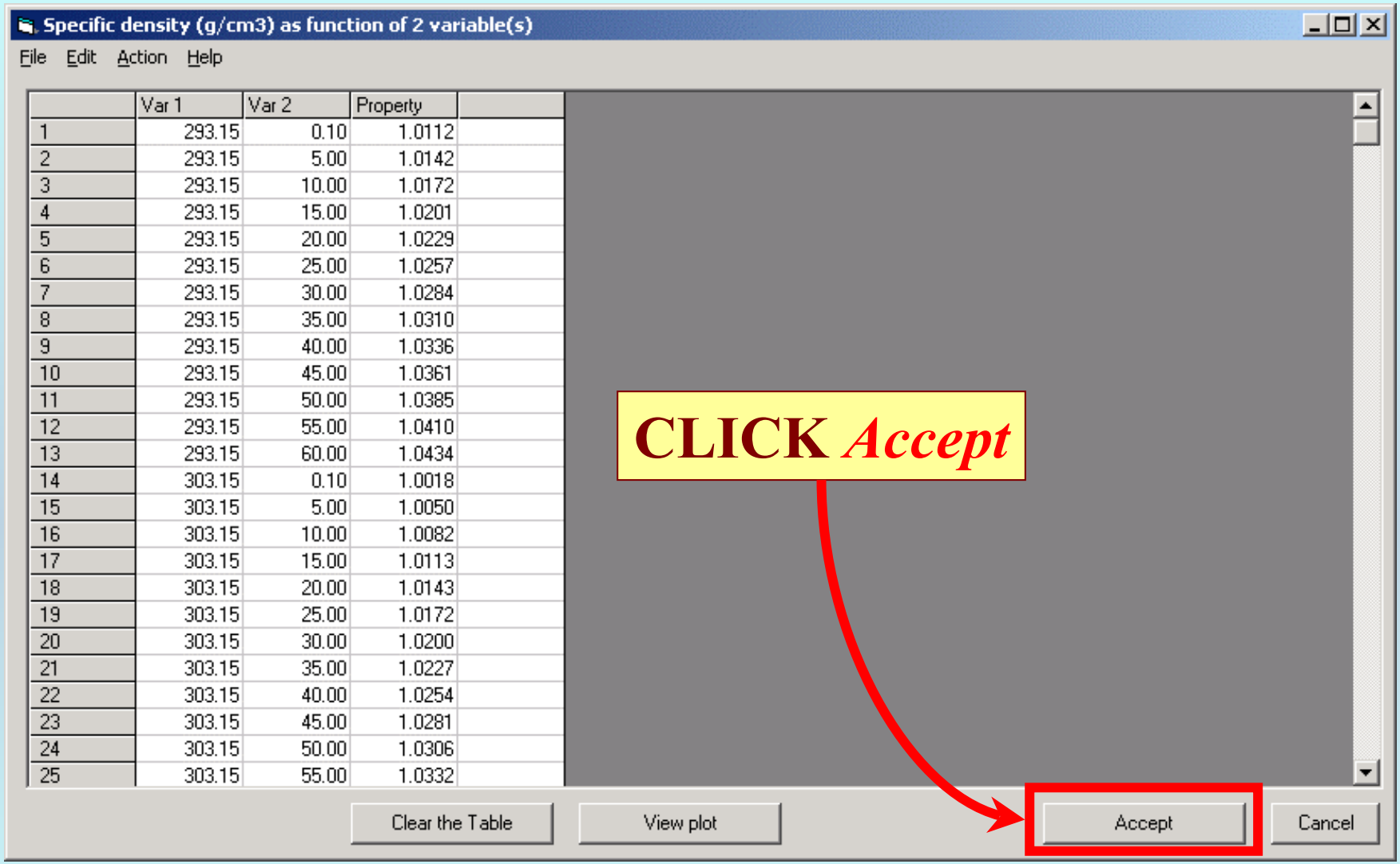
| | 30 | 1.0284 | 1.0200 | 1.0116 | 1.0032 | 0.9950 | 0.9869 | 0.9788 | 0.9712 | 0.9631 |
| | 35 | 1.0310 | 1.0227 | 1.0144 | 1.0063 | 0.9982 | 0.9901 | 0.9821 | 0.9748 | 0.9669 |
| | 40 | 1.0336 | 1.0254 | 1.0172 | 1.0091 | 1.0012 | 0.9932 | 0.9855 | 0.9783 | 0.9704 |
| | 45 | 1.0361 | 1.0281 | 1.0201 | 1.0121 | 1.0042 | 0.9963 | 0.9886 | 0.9815 | 0.9739 |
| | 50 | 1.0385 | 1.0306 | 1.0226 | 1.0147 | 1.0070 | 0.9993 | 0.9917 | 0.9846 | 0.9771 |
| | 55 | 1.0410 | 1.0332 | 1.0252 | 1.0175 | 1.0098 | 1.0023 | 0.9947 | 0.9880 | 0.9805 |
| | 60 | 1.0434 | 1.0355 | 1.0278 | 1.0202 | 1.0126 | 1.0050 | 0.9976 | 0.9910 | 0.9838 |

Clear the Table | View plot | 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.)


Specific density (g/cm3) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 293.15 0.10 1.0112
2 293.15 5.00 1.0142
3 293.15 10.00 1.0172
4 293.15 15.00 1.0201
5 293.15 20.00 1.0229
6 293.15 25.00 1.0257
7 293.15 30.00 1.0284
8 293.15 35.00 1.0310
9 293.15 40.00 1.0336
10 293.15 45.00 1.0361
11 293.15 50.00 1.0385
12 293.15 55.00 1.0410
13 293.15 60.00 1.0434
14 303.15 0.10 1.0018
15 303.15 5.00 1.0050
16 303.15 10.00 1.0082
17 303.15 15.00 1.0113
18 303.15 20.00 1.0143
19 303.15 25.00 1.0172
20 303.15 30.00 1.0200
21 303.15 35.00 1.0227
22 303.15 40.00 1.0254
23 303.15 45.00 1.0281
24 303.15 50.00 1.0306
25 303.15 55.00 1.0332
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
2. Check for typographical errors and CLICK OK, when done.
Specific density as functio
Tools Help
300 310 320 360 370
X = Var 2
X = Var 1
OK
Alternative views are available


Specific density (g/cm3) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 293.15 0.10 1.0112
2 293.15 5.00 1.0142
3 293.15 10.00 1.0172
4 293.15 15.00 1.0201
5 293.15 20.00 1.0229
6 293.15 25.00 1.0257
7 293.15 30.00 1.0284
8 293.15 35.00 1.0310
9 293.15 40.00 1.0336
10 293.15 45.00 1.0361
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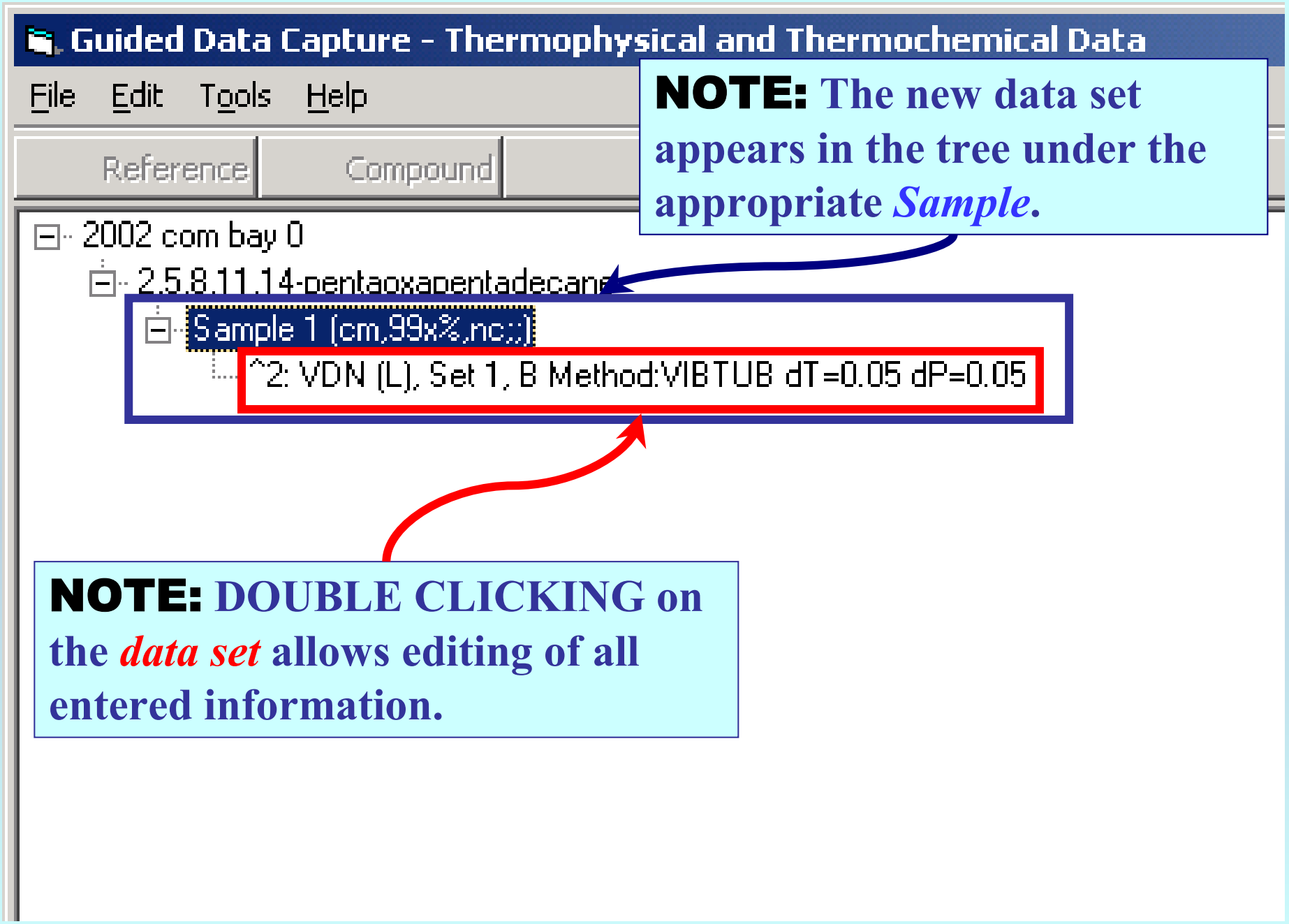
12 293.15 55.00 1.0410
13 293.15 60.00 1.0434
14 303.15 0.10 1.0018
15 303.15 5.00 1.0050
16 303.15 10.00 1.0082
17 303.15 15.00 1.0113
18 303.15 20.00 1.0143
19 303.15 25.00 1.0172
20 303.15 30.00 1.0200
21 303.15 35.00 1.0227
22 303.15 40.00 1.0254
23 303.15 45.00 1.0281
24 303.15 50.00 1.0306
25 303.15 55.00 1.0332
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
2002 com bay 0
2,5,8,11,14-pentaoxapentadecane
Sample 1 (cm,99x%,nc;;)
^2: VDN (L), Set 1, B Method:VIBTUB dT=0.05 dP=0.05
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.**