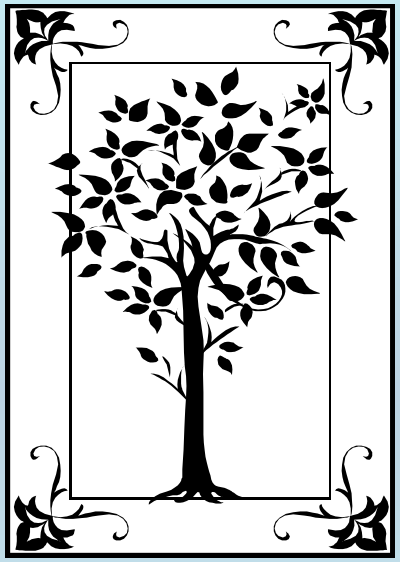
METADATA AND NUMERICAL DATA CAPTURE:
HENRY'S LAW CONSTANTS as f(*T*)
(2 – Components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components**
HENRY'S LAW CONSTANTS as f(*T*)
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:

1140 *J. Chem. Eng. Data* 2002, *47*, 1140−1144

Henry's Law Constant Measurements of $CHClF_2$, CH_2F_2, C_2HF_5, CH_2FCF_3, and CH_3CHF_2 in Ethanol and Methanol with Headspace Gas Chromatography

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Henry's law constants of hydrofluorocarbons in alcohols were measured with headspace gas chromatography. Isothermal vapor−liquid equilibria for 10 fluorocarbon + alcohol systems ranging from 303 to 323 K were also measured. The experimental data of chlorodifluoromethane ($CHClF_2$, HCFC22), difluoromethane (CH_2F_2, HFC32), pentafluoroethane (C_2HF_5, HFC125), 1,1,1,2-tetrafluoroethane (CH_2FCF_3, HFC134a), and 1,1-difluoroethane (CH_3CHF_2, HFC152a) in either methanol or ethanol were correlated as a function of temperature with the Valentiner equation.

HENRY'S LAW CONSTANT f(*T*)

(2 ñ Components)

Chlorodifluoromethane in Methanol

Table 2. Experimental Vapor–Liquid Equilibrium Data

T/K	*P*/kPa	liquid-phase mole fraction x_1	vapor-phase mole fraction y_1	Henry's law constant, *H*/MPa	*T*/K	*P*/kPa	liquid-phase mole fraction x_1	vapor-phase mole fraction y_1	Henry's law constant, *H*/MPa
Chlorodifluoromethane (HCFC22) + Methanol									
303.0	42.6	0.011 5	0.449	1.66	318.0	72.1	0.011 1	0.375	2.45
	37.8	0.008 80	0.383			72.9	0.011 0	0.373	
308.0	50.7	0.011 2	0.422	1.93	323.0	86.7	0.010 0	0.347	2.99
	50.6	0.011 1	0.423			86.5	0.010 2	0.349	
	45.6	0.008 50	0.362			79.8	0.008 10	0.305	
	44.3	0.008 00	0.353			80.8	0.008 20	0.304	
313.0	64.5	0.010 9	0.395	2.35					
	58.6	0.008 40	0.343						
	59.0	0.008 70	0.340						

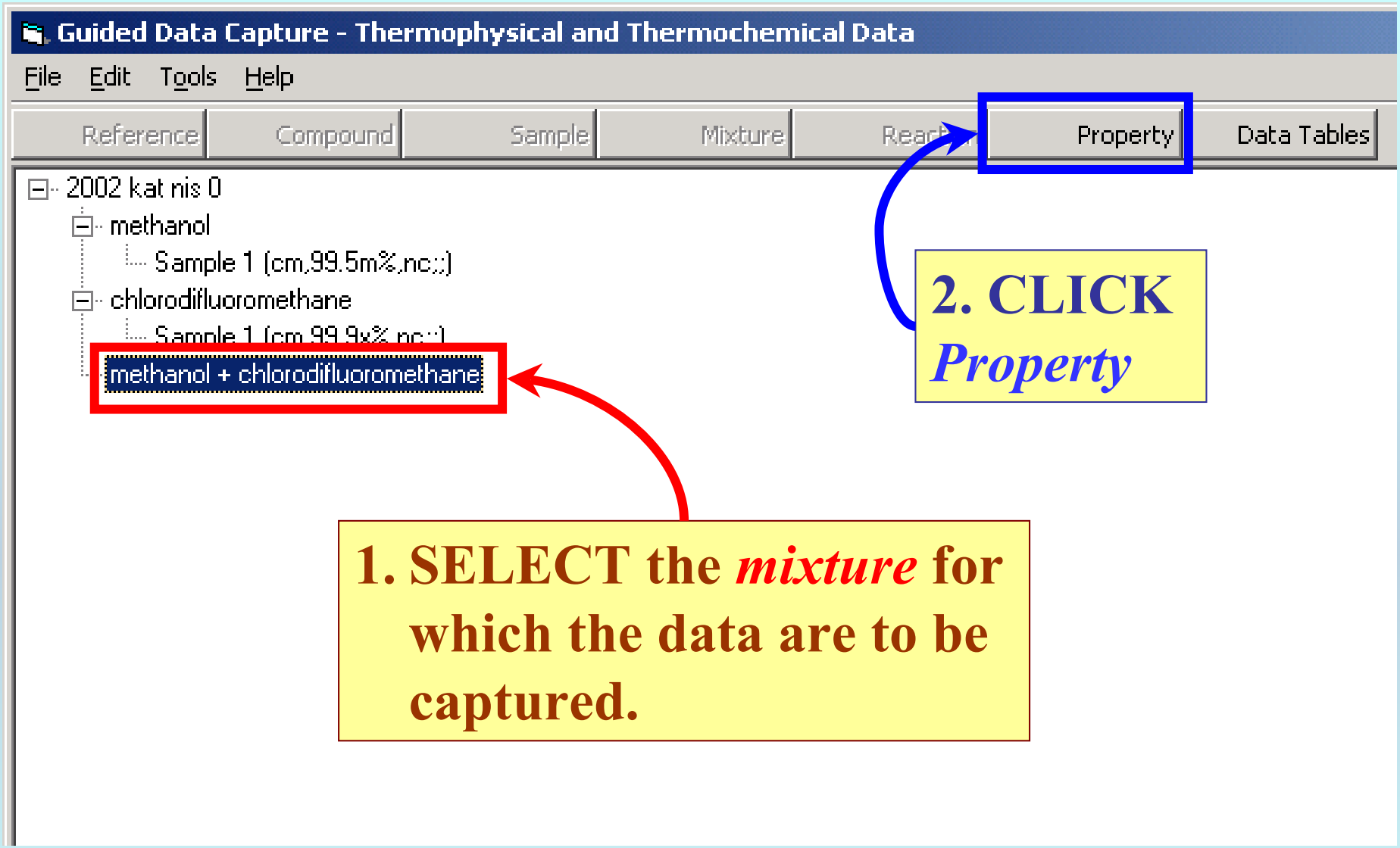
This data set is considered here.

Experimental Method Info:

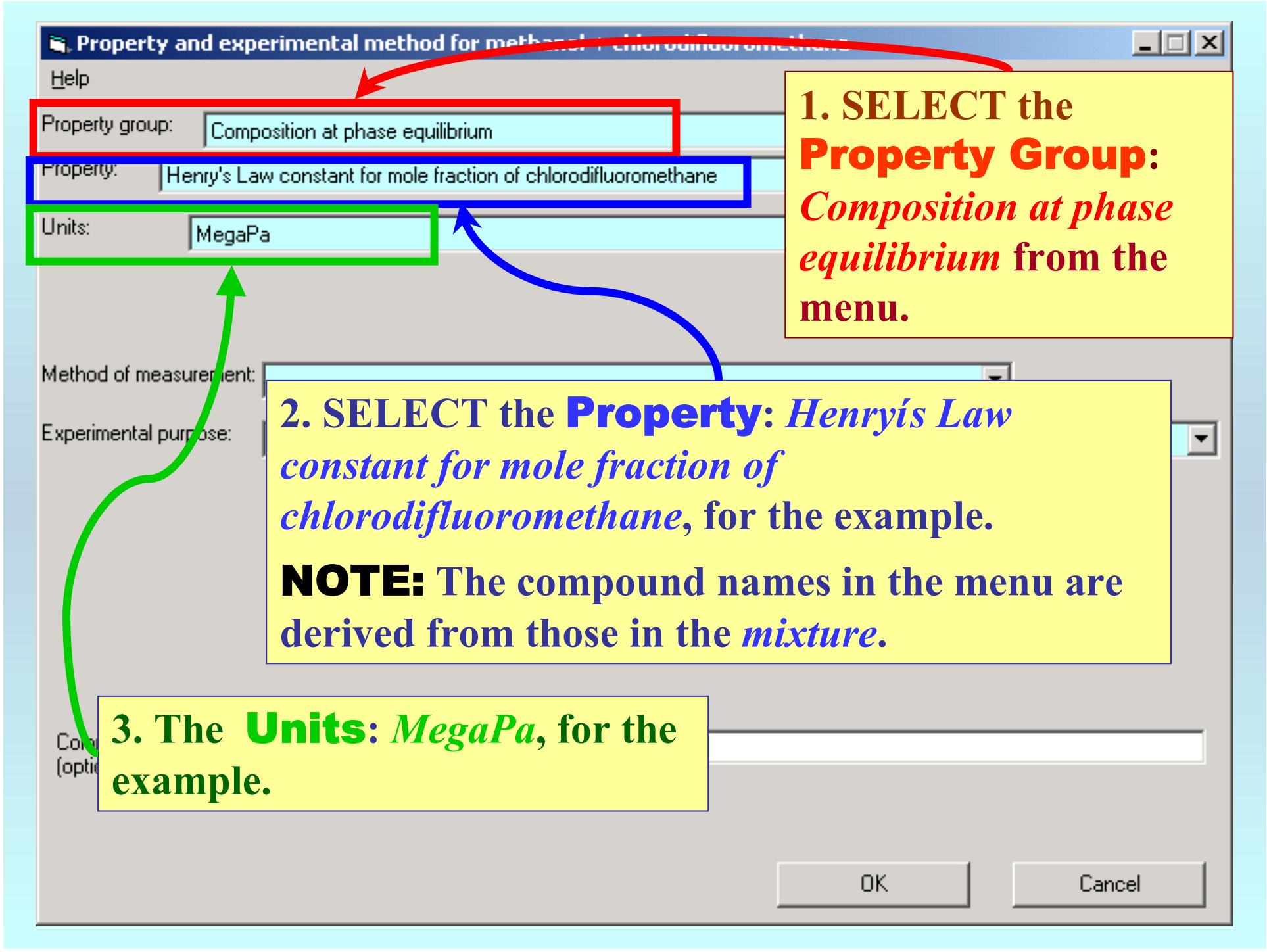
Method: Headspace Gas Chromatography

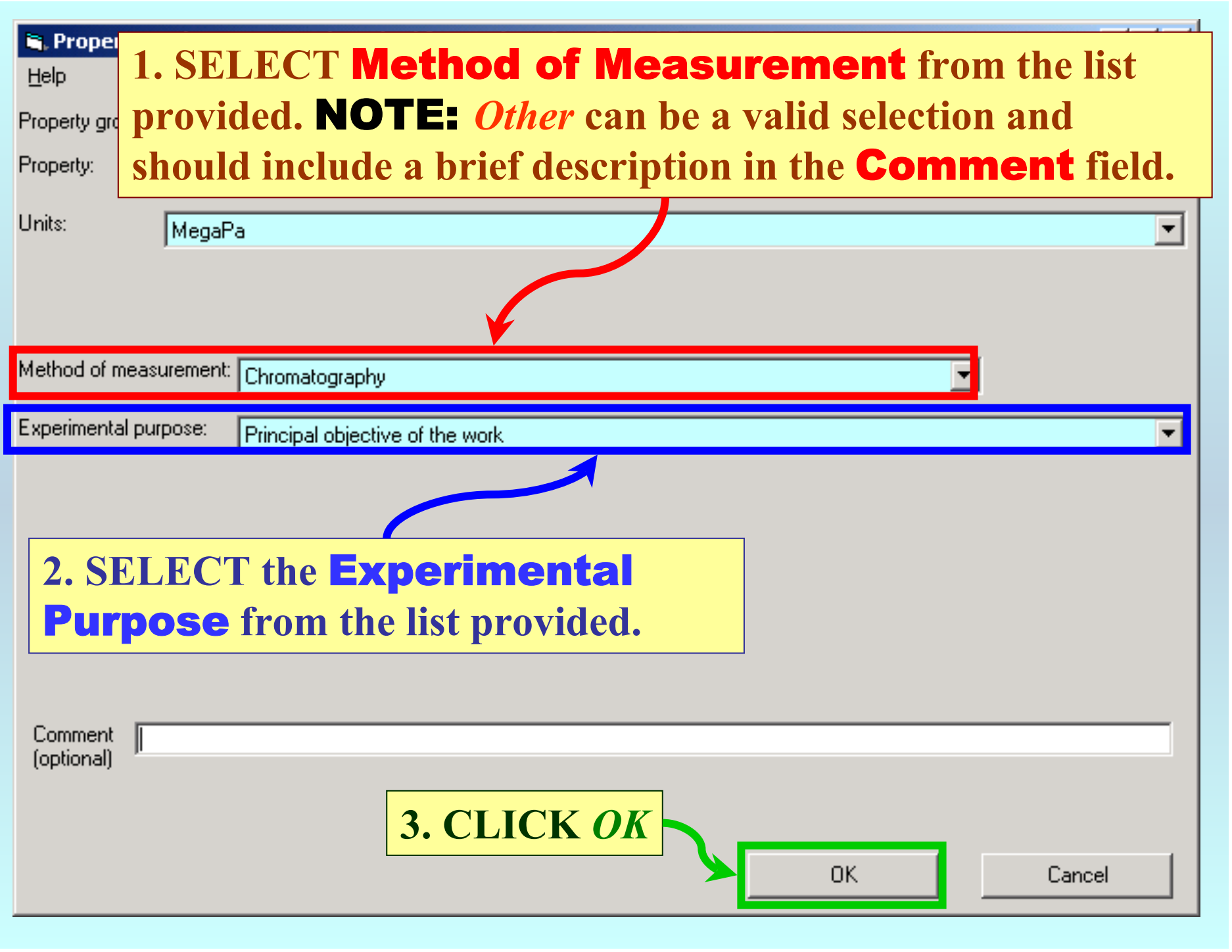
Uncertainties:

The Henry's law constants listed in Table 2 have estimated uncertainties of 4%.



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
Help
Property group:
Composition at phase equilibrium
Property:
Henry's Law constant for mole fraction of chlorodifluoromethane
Units:
MegaPa
Method of measurement:
Experimental purpose:
OK
Cancel
1. SELECT the Property Group: Composition at phase equilibrium from the menu.
2. SELECT the Property: Henryís Law constant for mole fraction of chlorodifluoromethane, for the example.
NOTE: The compound names in the menu are derived from those in the mixture.
3. The Units: MegaPa, for the example.

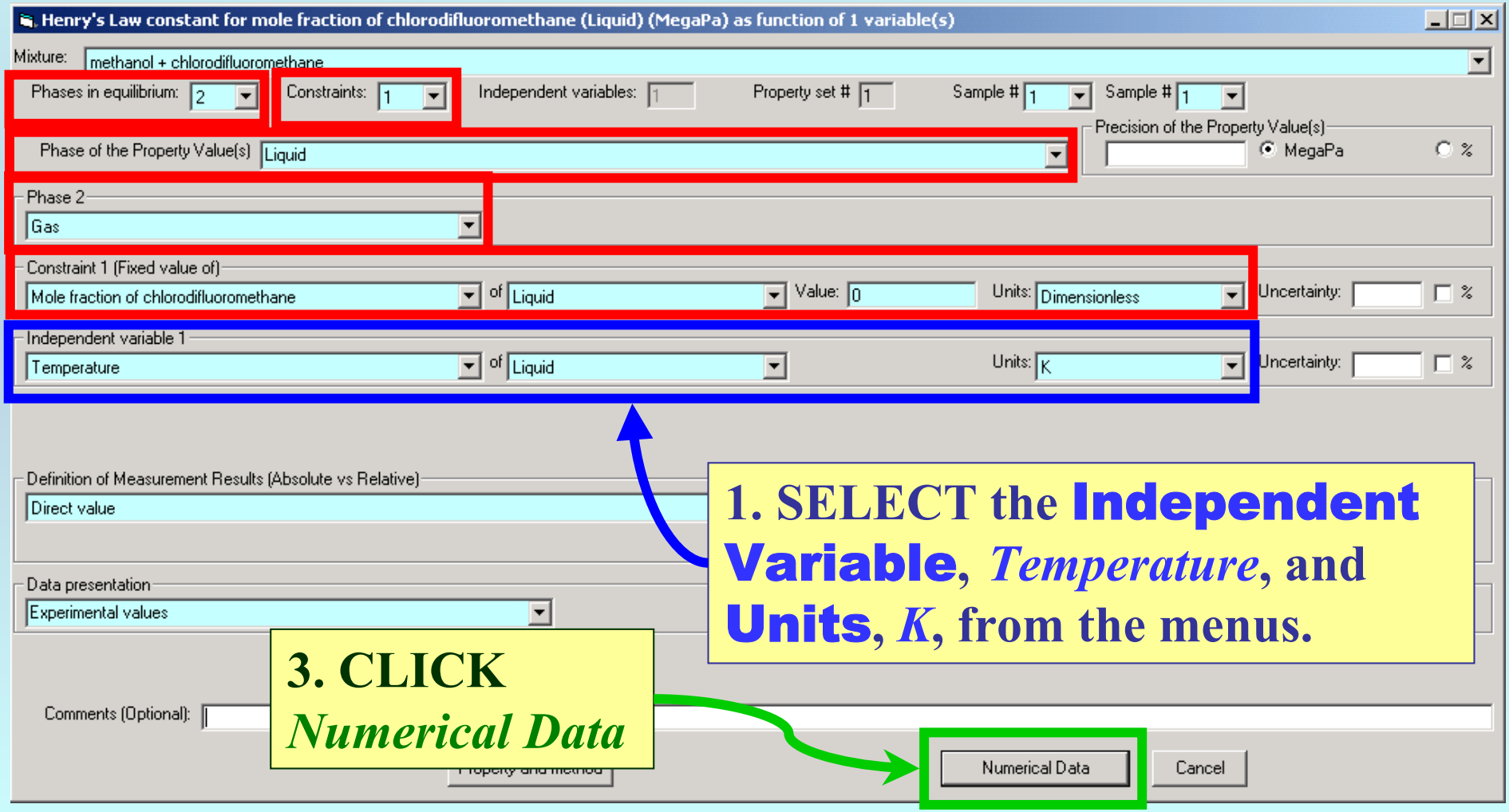


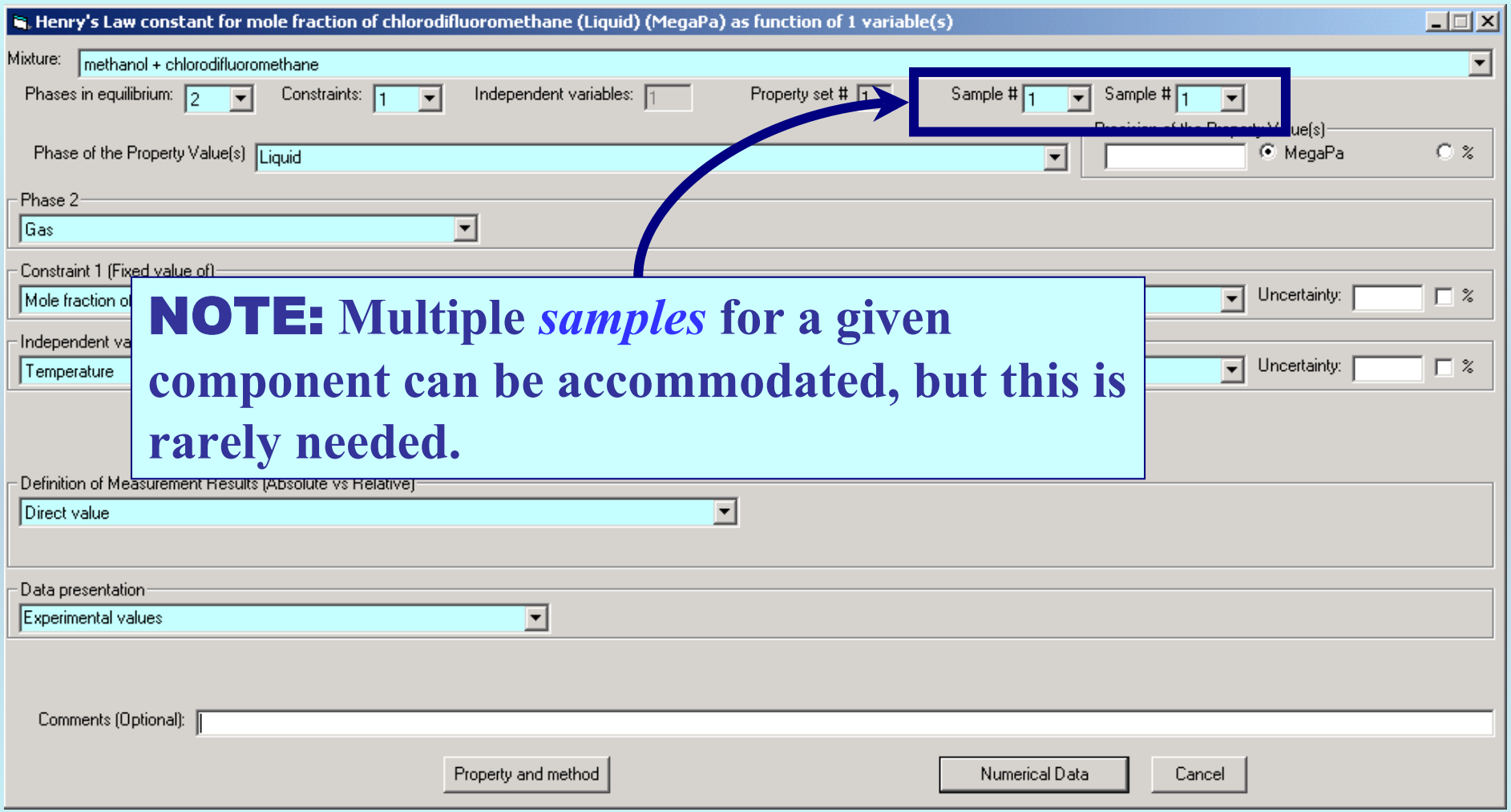
1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

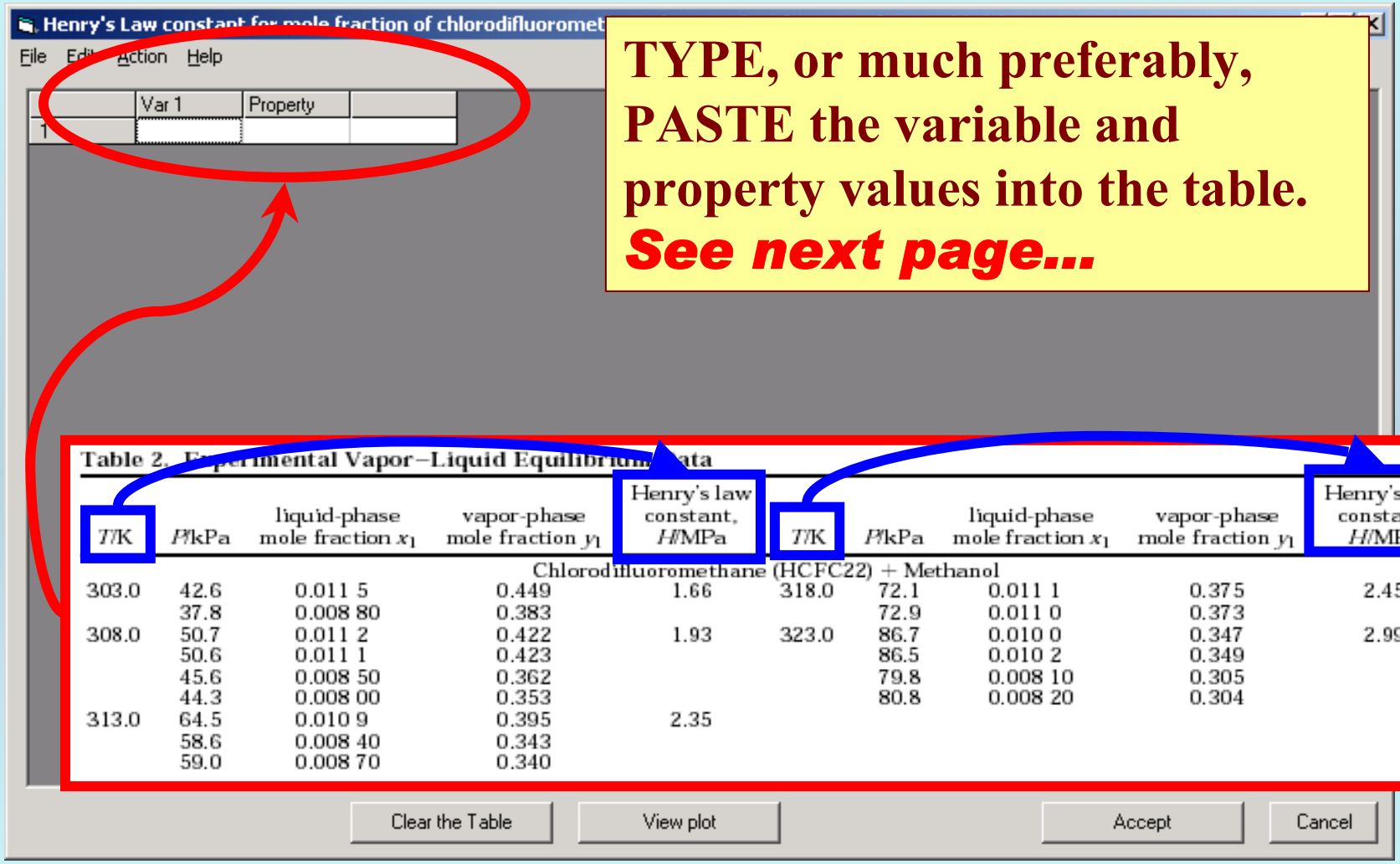
2. SELECT the **Experimental Purpose** from the list provided.

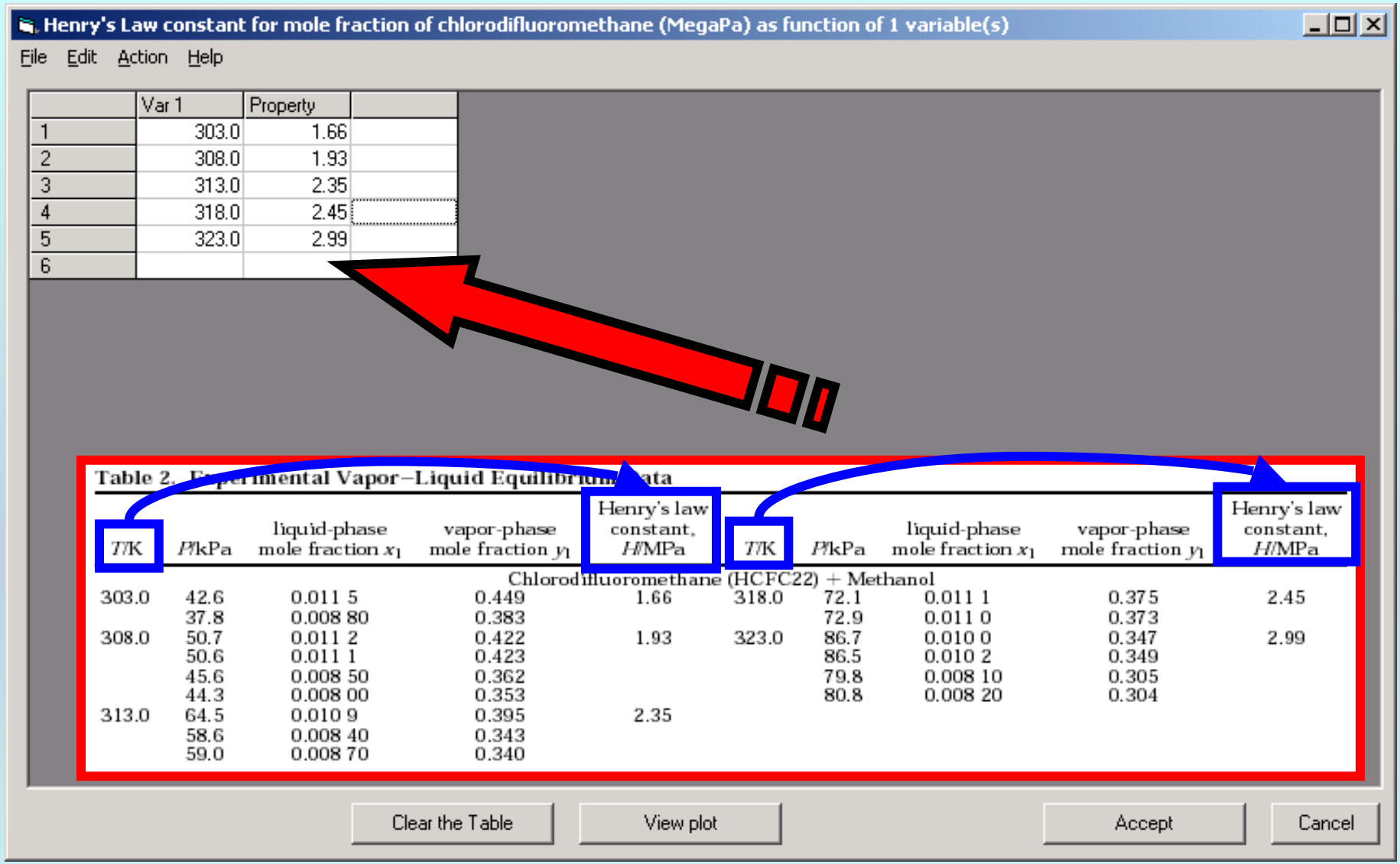
3. CLICK *OK*

NOTE: The # of **Phases in equilibrium**, # of **Constraints**, the **Phase of the Property Value(s)**, **Phase 2**, and **Constraint 1** are filled automatically based upon the property definition.

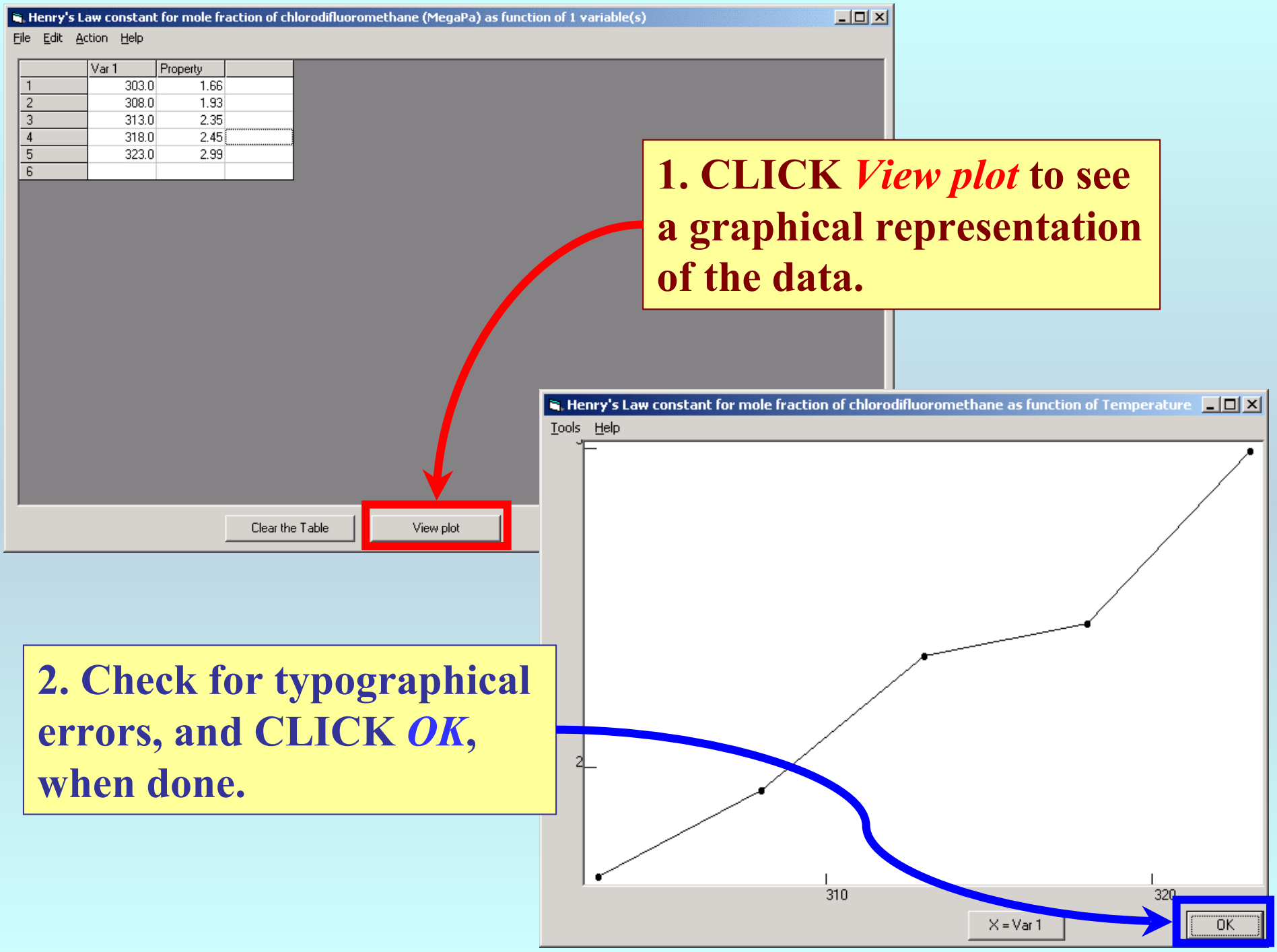


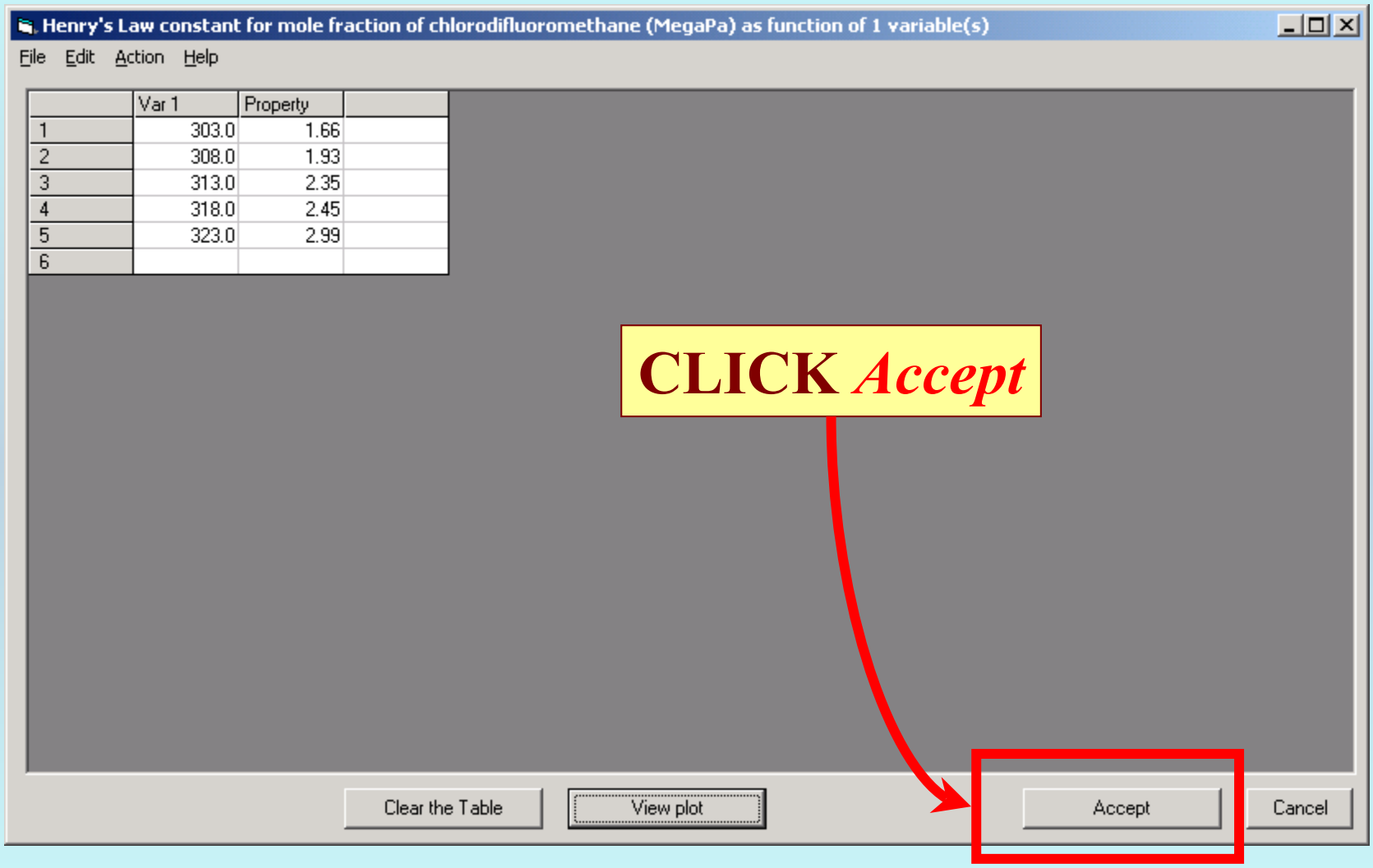

Henry's Law constant for mole fraction of chlorodifluoromethane (Liquid) (MegaPa) as function of 1 variable(s)
Mixture:
methanol + chlorodifluoromethane
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Liquid
MegaPa
%
Phase 2
Gas
Constraint 1 (Fixed value of)
Mole fraction o
Uncertainty:
%
Independent va
Temperature
Uncertainty:
%
NOTE: Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel

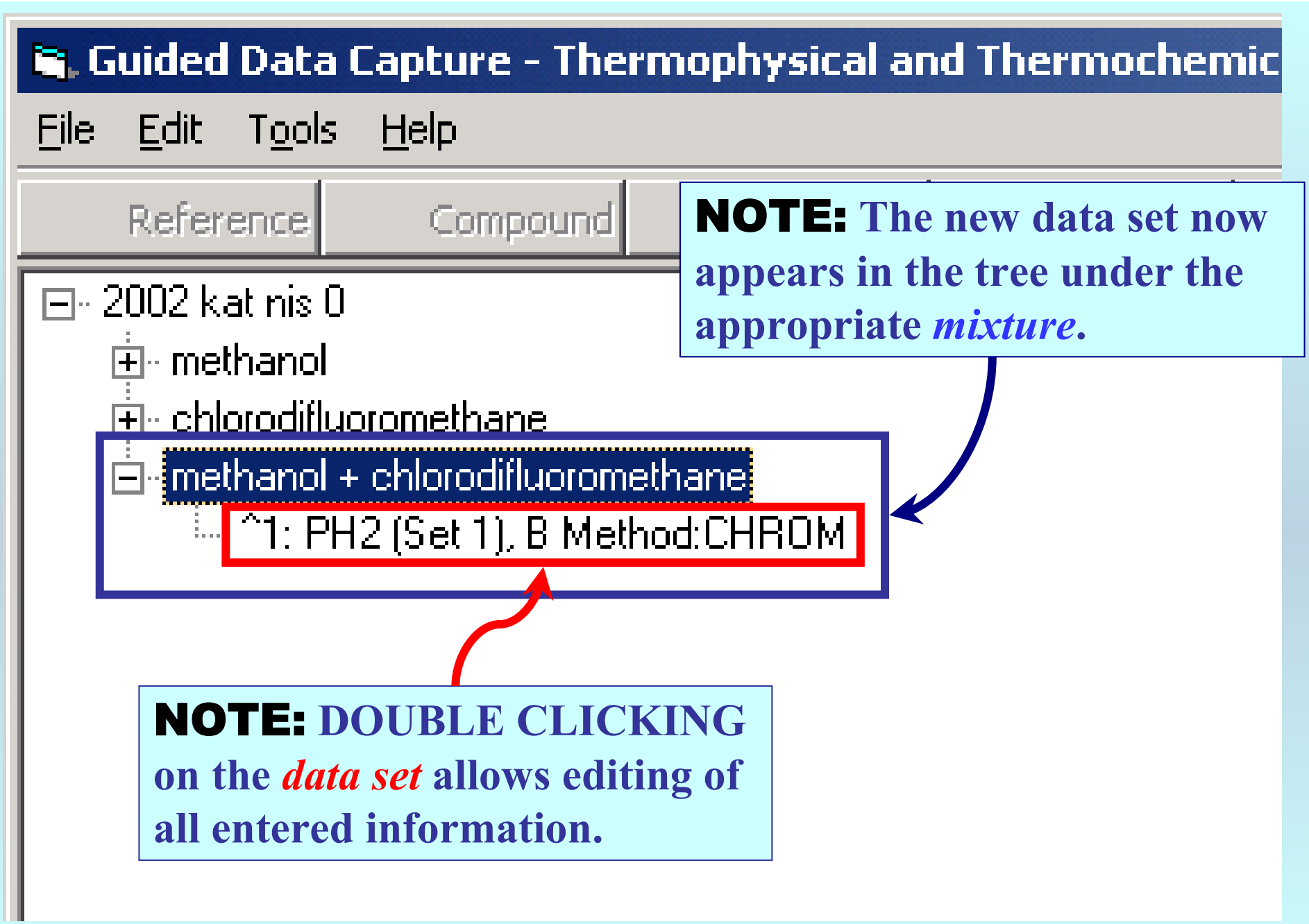

Henry's Law constant for mole fraction of chlorodifluoromet
File Edit Action Help
Var 1
Property
1
TYPE, or much preferably, PASTE the variable and property values into the table.
See next page...
Table 2. Experimental Vapor–Liquid Equilibrium Data
T/K
P/kPa
liquid-phase mole fraction x_1
vapor-phase mole fraction y_1
Henry's law constant, H/MPa
Chlorodifluoromethane (HCFC22) + Methanol
303.0 42.6 0.011 5 0.449 1.66
37.8 0.008 80 0.383
308.0 50.7 0.011 2 0.422 1.93
50.6 0.011 1 0.423
45.6 0.008 50 0.362
44.3 0.008 00 0.353
313.0 64.5 0.010 9 0.395 2.35
58.6 0.008 40 0.343
59.0 0.008 70 0.340
318.0 72.1 0.011 1 0.375 2.45
72.9 0.011 0 0.373
323.0 86.7 0.010 0 0.347 2.99
86.5 0.010 2 0.349
79.8 0.008 10 0.305
80.8 0.008 20 0.304
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.)


Henry's Law constant for mole fraction of chlorodifluoromethane (MegaPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 303.0 1.66
2 308.0 1.93
3 313.0 2.35
4 318.0 2.45
5 323.0 2.99
6
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
Henry's Law constant for mole fraction of chlorodifluoromethane as function of Temperature
Tools Help
2
310
320
X = Var 1
OK
2. Check for typographical errors, and CLICK OK, when done.


Henry's Law constant for mole fraction of chlorodifluoromethane (MegaPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 303.0 1.66
2 308.0 1.93
3 313.0 2.35
4 318.0 2.45
5 323.0 2.99
6
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemic
File Edit Tools Help
Reference
Compound
2002 kat nis 0
methanol
chlorodifluoromethane
methanol + chlorodifluoromethane
^1: PH2 (Set 1), B Method:CHROM
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.**