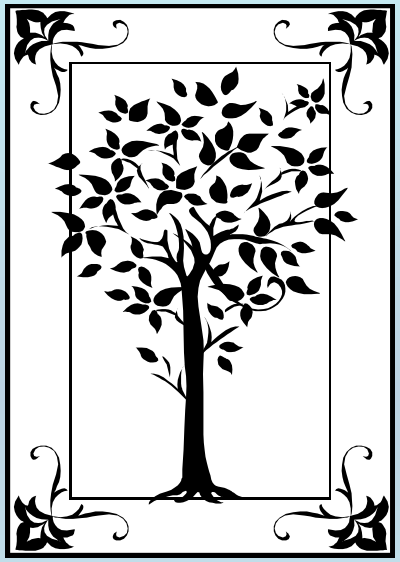
METADATA AND NUMERICAL DATA CAPTURE:
Surface Tension
(2 – Components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components**
Surface Tension
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:

216 *J. Chem. Eng. Data* 2002, *47*, 216−218

Densities, Viscosities, and Surface Tensions of the Trifluoroethanol + Quinoline System

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Densities, viscosities, and surface tensions of 2,2,2-trifluoroethanol (TFE) + quinoline were measured at various temperatures and concentrations. This system was chosen as it is a possible candidate for an organic working pair for an absorption heat pump. All results were correlated by a polynomial equation as a function of temperature and concentration, and the parameters of the regression equation were determined by a least-squares method. The average absolute deviations between the experimental and calculated values in the density, viscosity, and surface tension measurements were 0.12, 1.8, and 0.76%, respectively. The density values decreased with increasing temperature and quinoline mass fraction. As the temperature of the liquid mixture increased and the quinoline mass fraction decreased, the viscosity and surface tension values decreased.

Surface Tension (σ) for the binary system **2,2,2-trifluoroethanol + quinoline** at p = 101.3 kPa and various temperatures

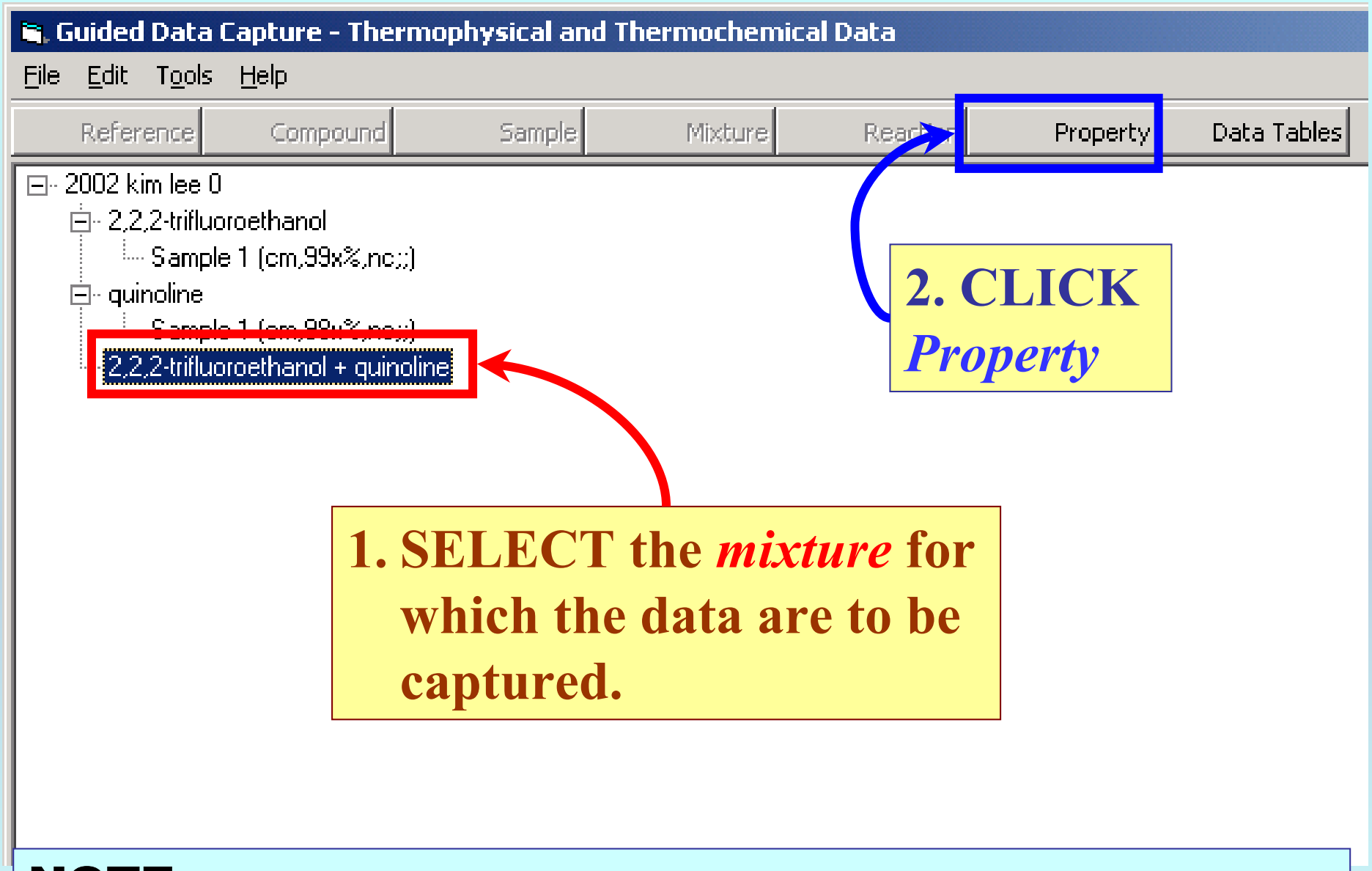
Table 3. Measured Surface Tensions (σ) for the 2,2,2-Trifluoroethanol ($1 - w$) + Quinoline (w) Mixtures

	σ/mN·m^{-1} at the following T/K			
w	293.15	303.15	313.15	323.15
0.00	21.11	20.31	19.44	18.58
0.20	24.78	23.07	21.87	20.86
0.40	28.62	26.98	25.84	25.00
0.60	32.57	31.53	30.56	29.34
0.80	37.23	36.02	35.07	33.77
1.00	43.27	42.10	41.05	39.84

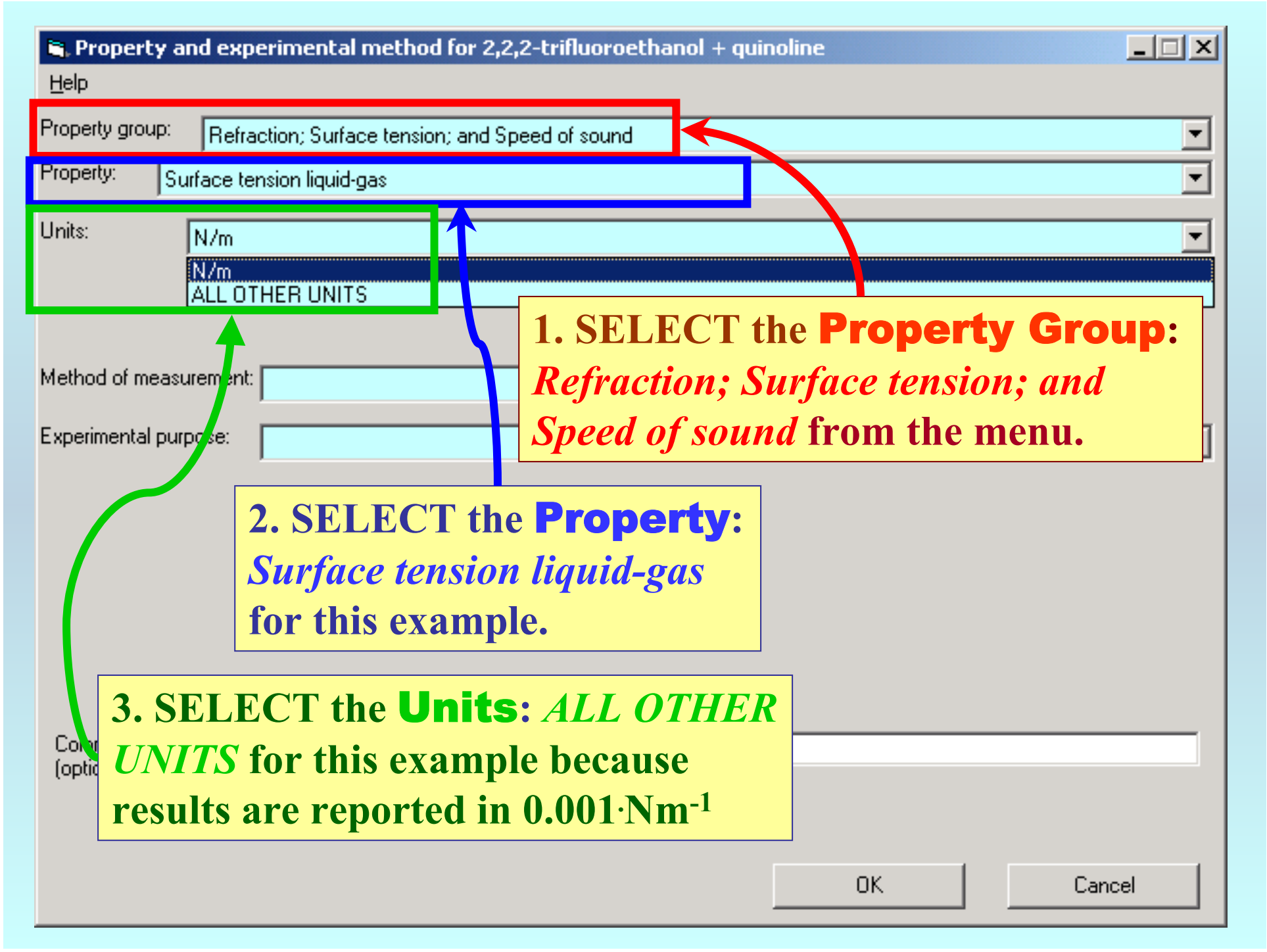
This data set is considered here.

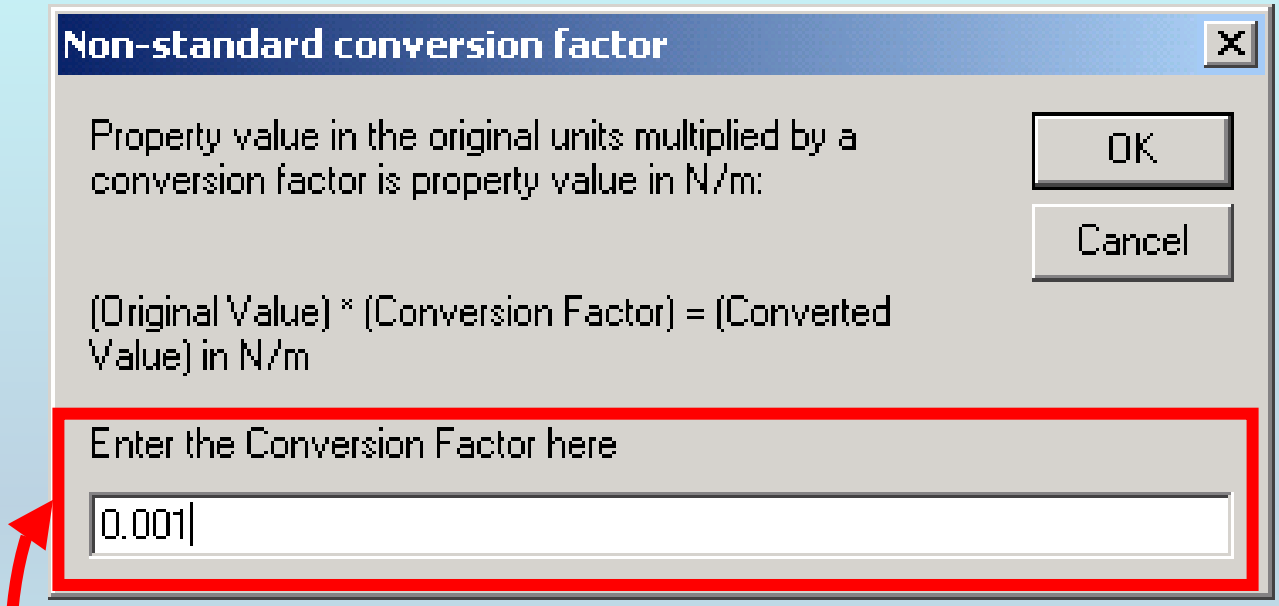
Experimental Method Info:

(iii) Surface Tension Measurement. The surface tensions of the binary system were measured by the plate (Wilhelmy) method using a dynamic contact angle analyzer (DCA) manufactured by Cahn Instruments. The plate was made of crystal clear−white glass with uniform surface quality, a precise squared edge, perfect flatness, and exact dimensions. Its size was 24 × 30 mm^2. The operation and analysis were automatically controlled by an external computer, which was connected to the DCA. To control the temperature of the sample within ±0.05 K, a bath circulator was used. The accuracy of the instrument is ±0.01 mN/m.

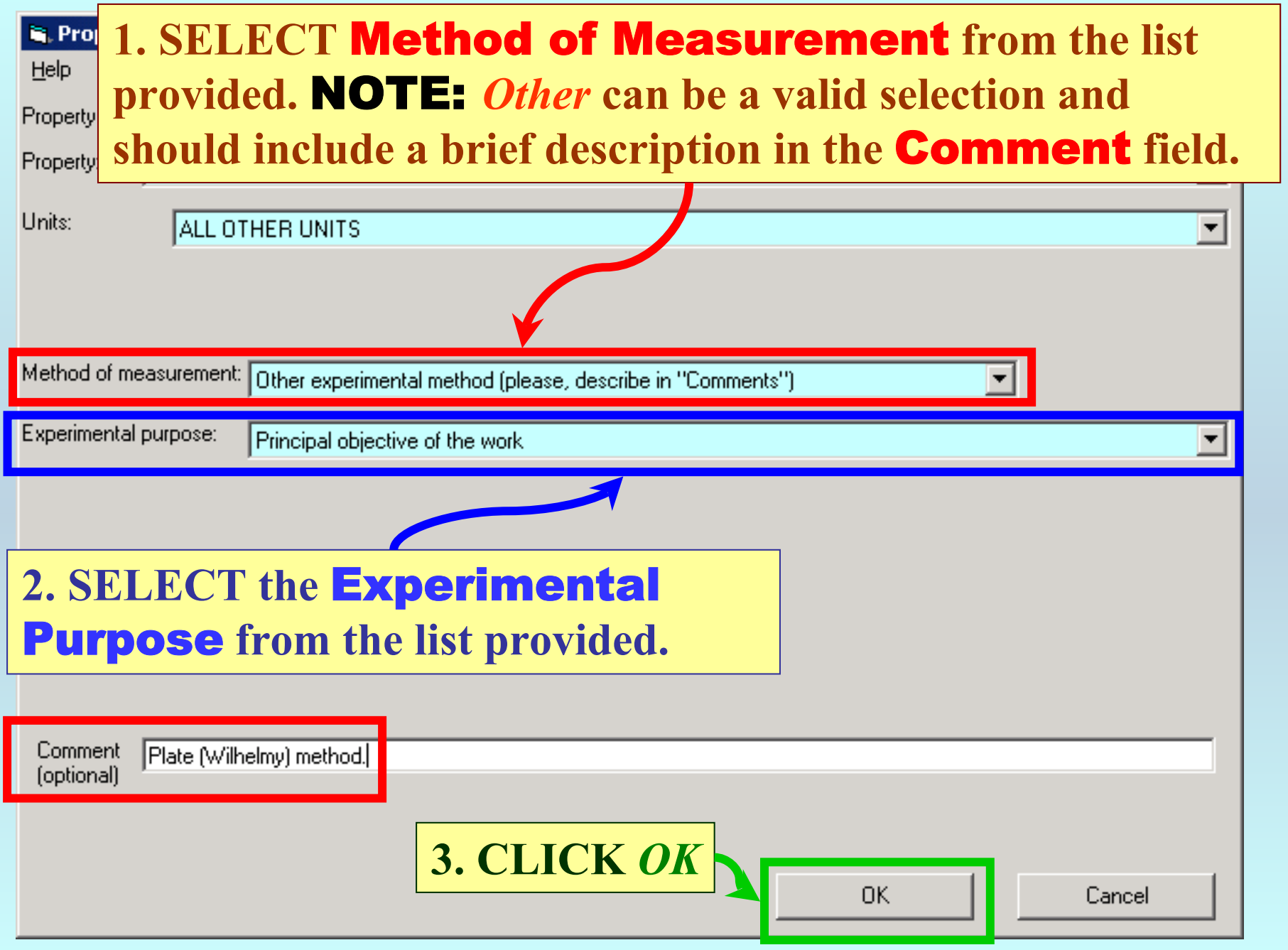


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

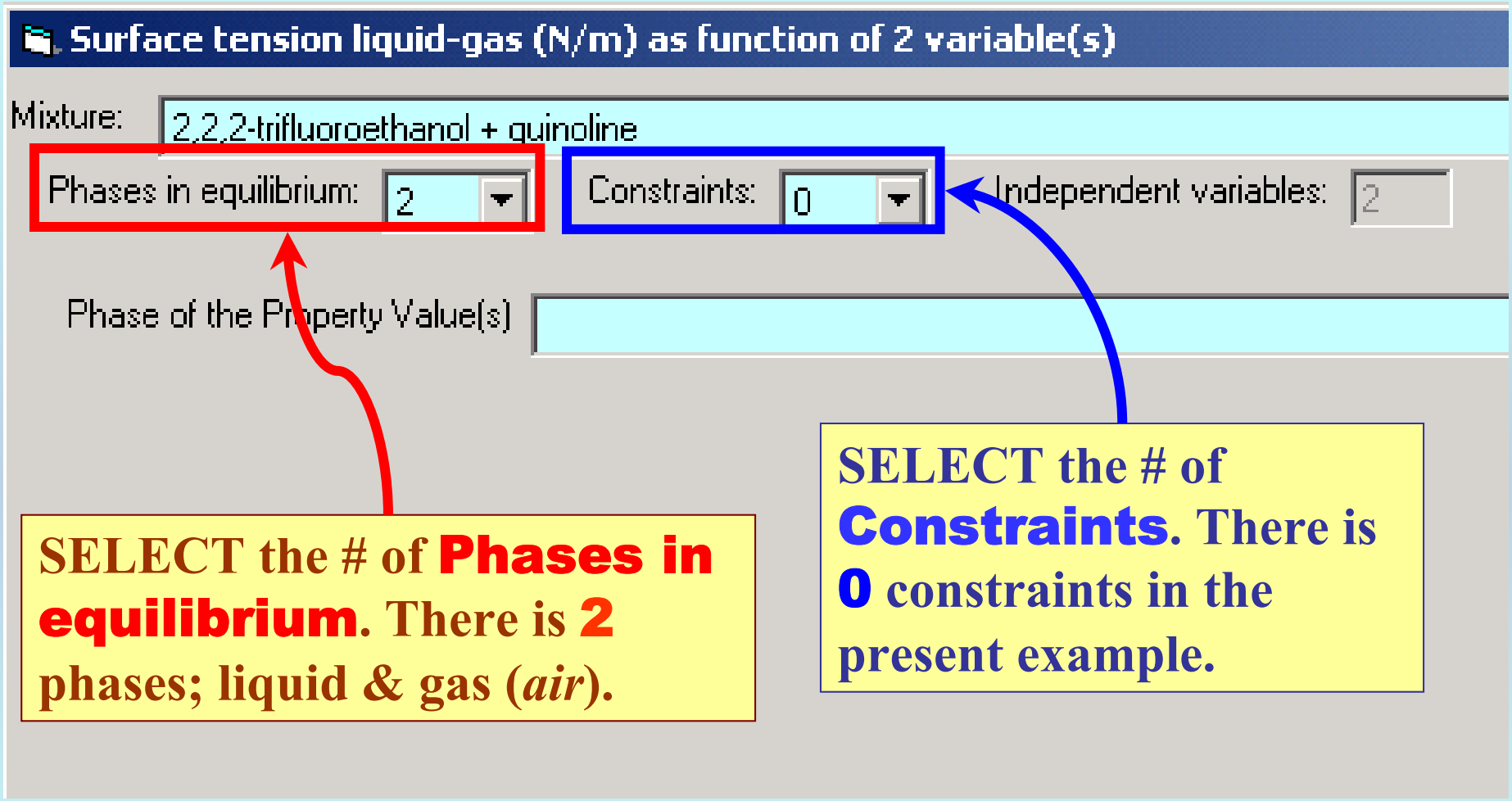

Property and experimental method for 2,2,2-trifluoroethanol + quinoline
Help
Property group:
Refraction; Surface tension; and Speed of sound
Property:
Surface tension liquid-gas
Units:
N/m
N/m
ALL OTHER UNITS
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Refraction; Surface tension; and Speed of sound from the menu.
2. SELECT the Property: Surface tension liquid-gas for this example.
3. SELECT the Units: ALL OTHER UNITS for this example because results are reported in 0.001·Nm-1
OK
Cancel

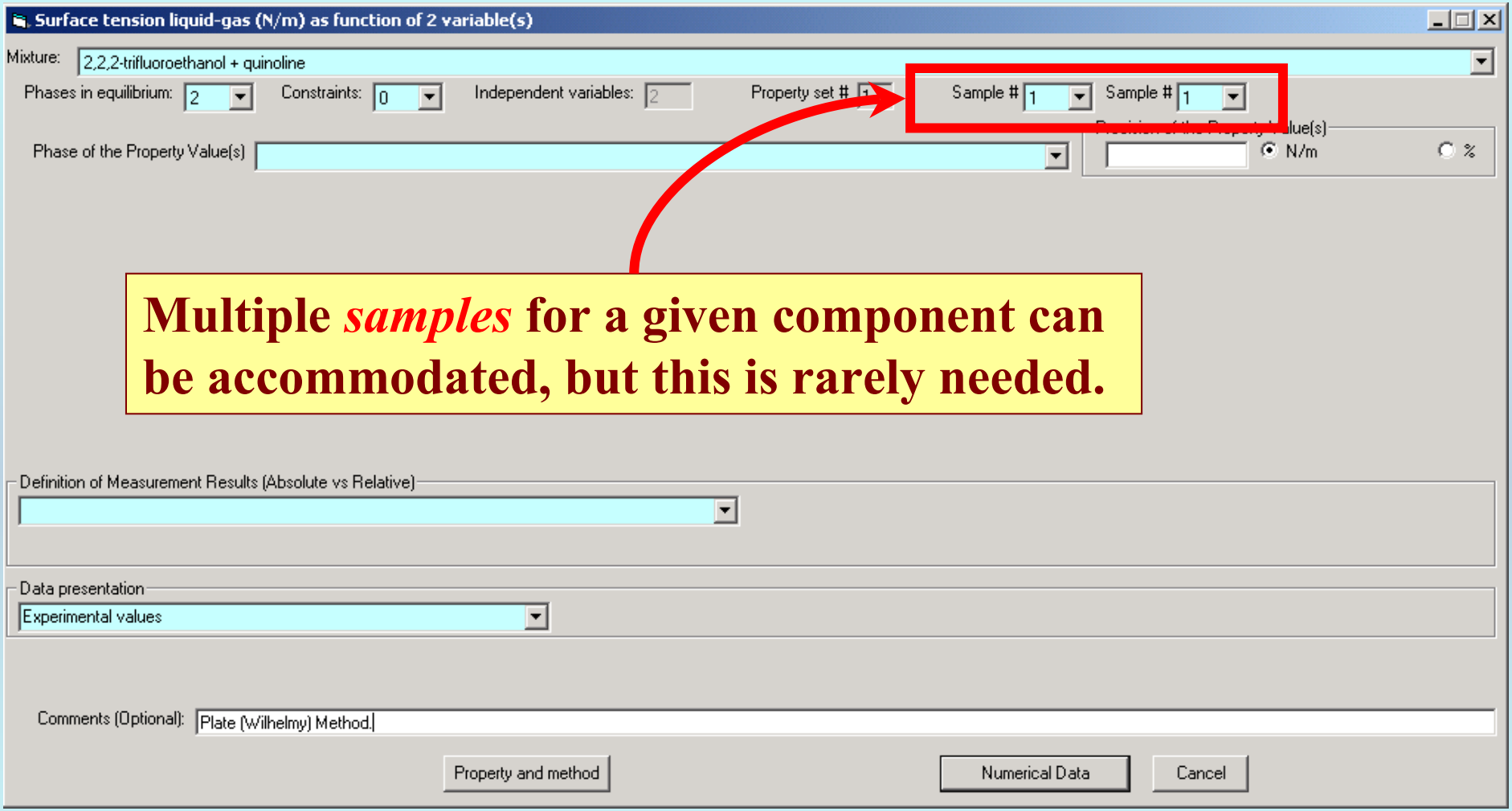


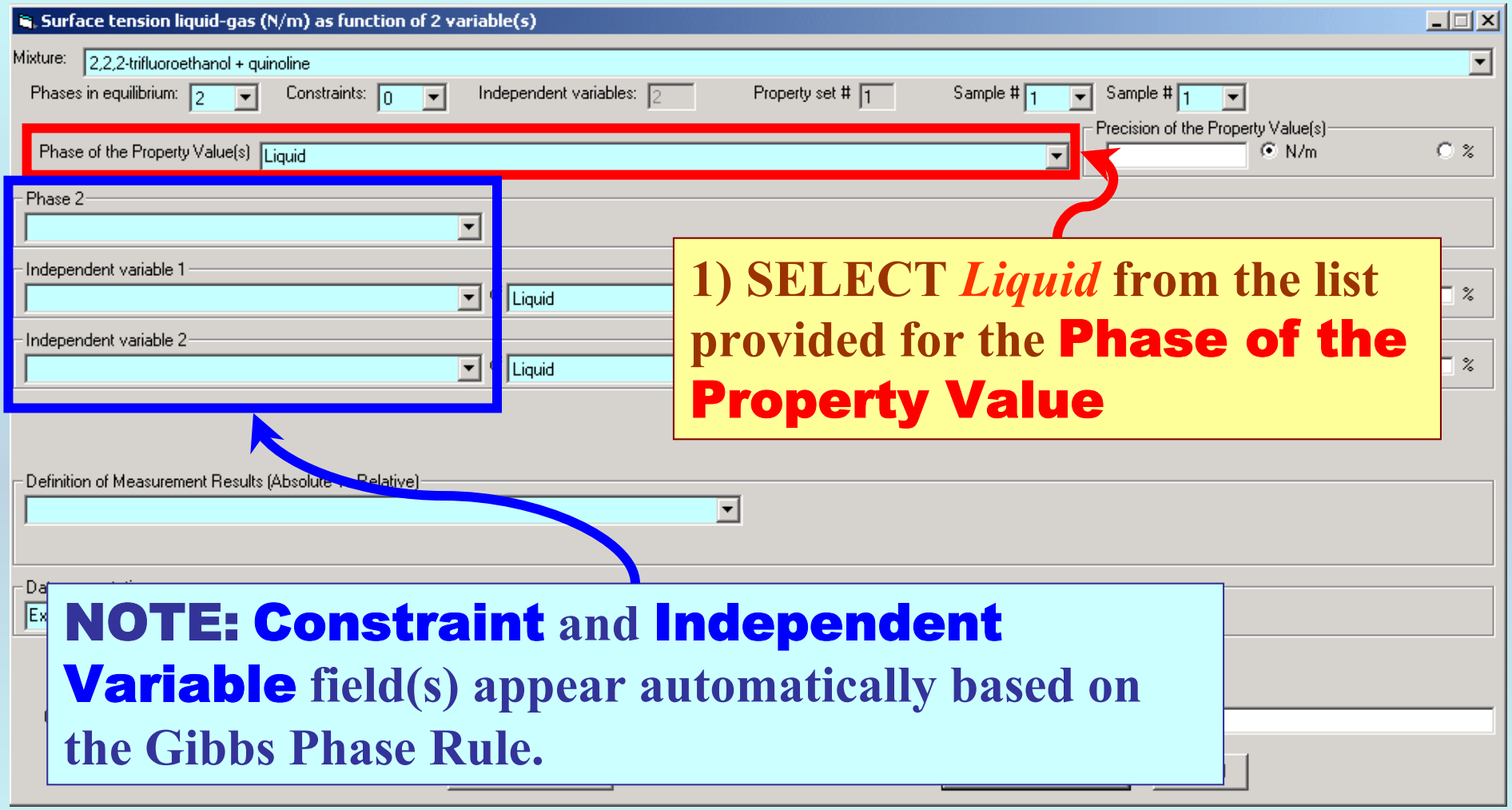
ENTER the *Conversion Factor* to obtain (1/K). Here, it is 0.001.


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
Property
Units:
ALL OTHER UNITS
Method of measurement:
Other experimental method (please, describe in "Comments")
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
Plate (Wilhelmy) method.
3. CLICK OK
OK
Cancel

SELECTION of # of Phases in Equilibrium and # of Constraints

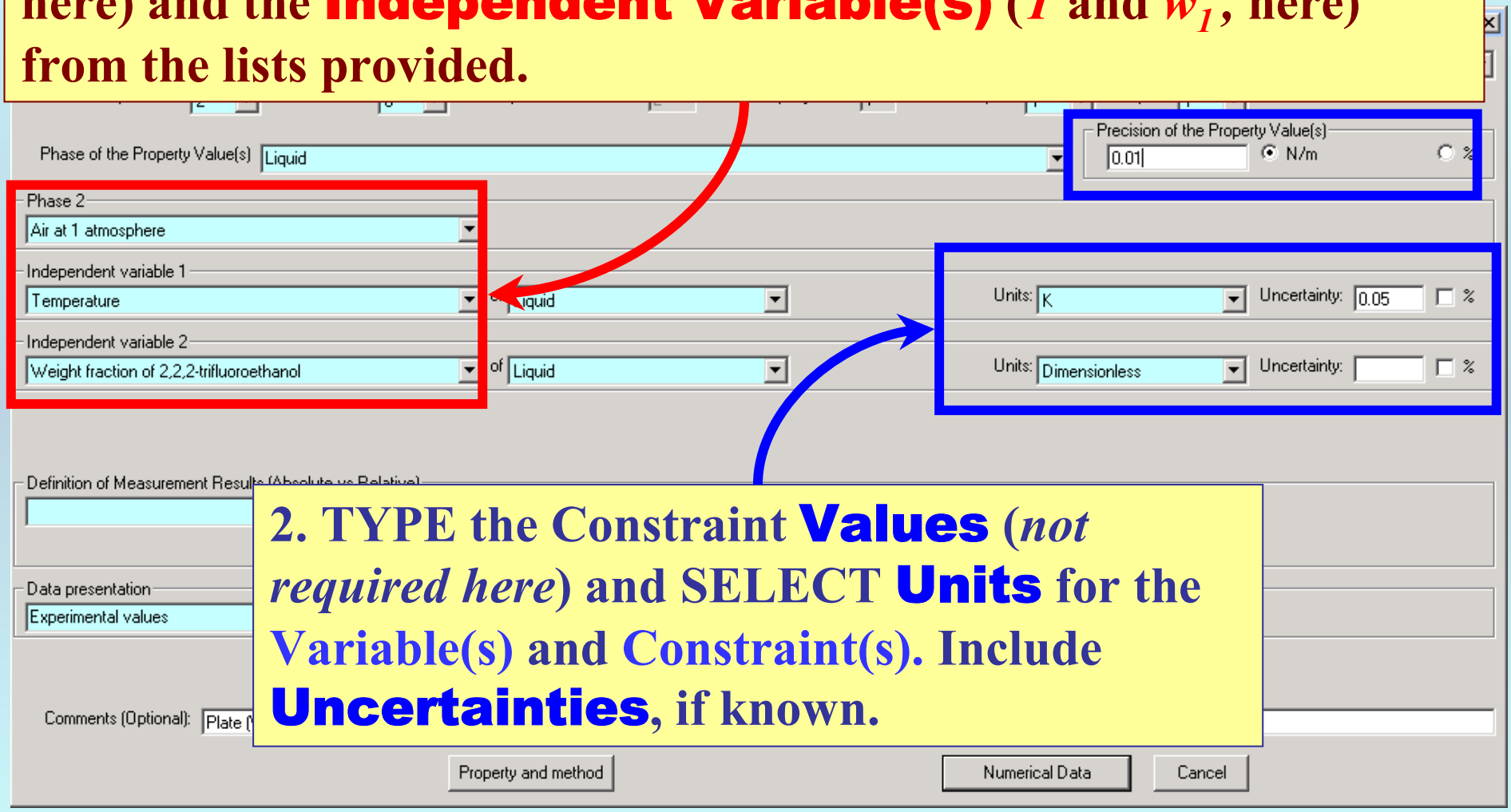



Surface tension liquid-gas (N/m) as function of 2 variable(s)
Mixture:
2,2,2-trifluoroethanol + quinoline
Phases in equilibrium:
2
Constraints:
0
Independent variables:
2
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
N/m
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Plate (Wilhelmy) Method.
Property and method
Numerical Data
Cancel


Surface tension liquid-gas (N/m) as function of 2 variable(s)
Mixture:
2,2,2-trifluoroethanol + quinoline
Phases in equilibrium:
2
Constraints:
0
Independent variables:
2
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
N/m
%
Phase 2
Independent variable 1
Liquid
Independent variable 2
Liquid
Definition of Measurement Results (Absolute
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.

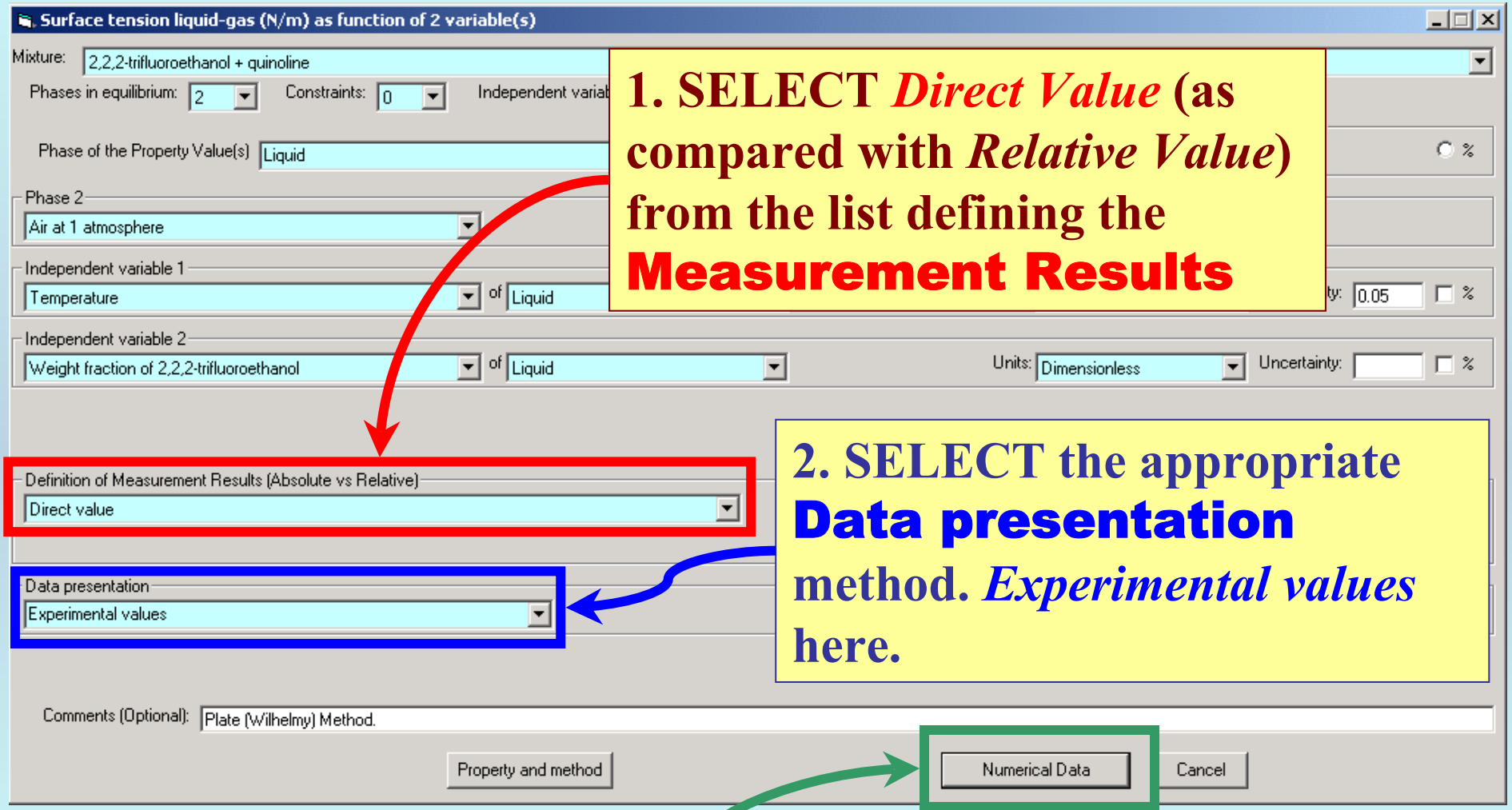
Specification of constraints, constraint values, and constraint units

1. SELECT the Phase 2 (*Air at 1 atm*), Constraint(s) (*none* here) and the Independent Variable(s) (*T* and w_1, here) from the lists provided.



2. TYPE the Constraint Values (*not required here*) and SELECT Units for the Variable(s) and Constraint(s). Include Uncertainties, if known.

Measurement definition and Data presentation



1. SELECT *Direct Value* (as compared with *Relative Value*) from the list defining the **Measurement Results**

2. SELECT the appropriate **Data presentation** method. *Experimental values* here.

3. CLICK *Numerical Data*

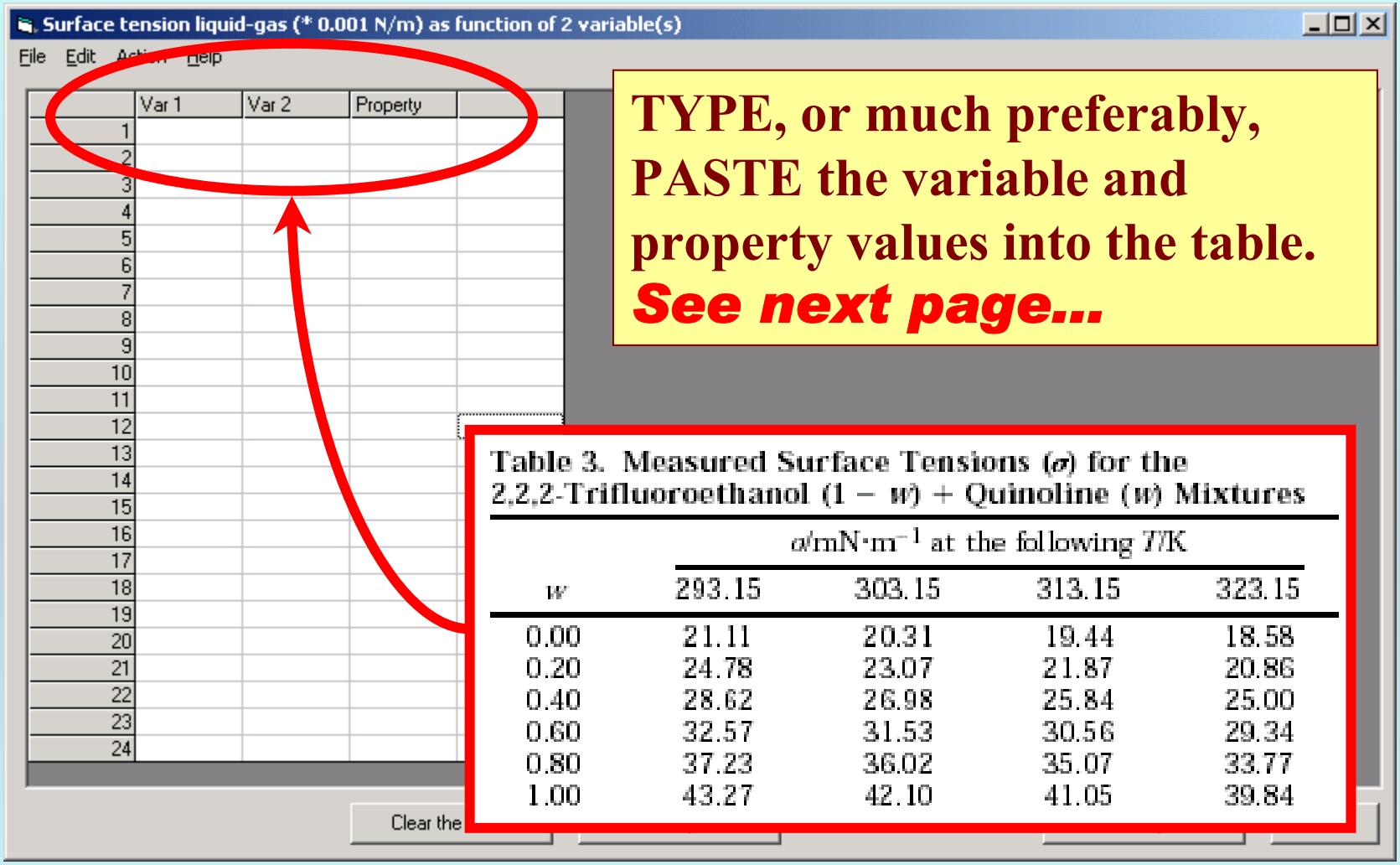


Table 3. Measured Surface Tensions (σ) for the 2,2,2-Trifluoroethanol ($1 - w$) + Quinoline (w) Mixtures

	σ/mN·m^{-1} at the following T/K			
w	293.15	303.15	313.15	323.15
0.00	21.11	20.31	19.44	18.58
0.20	24.78	23.07	21.87	20.86
0.40	28.62	26.98	25.84	25.00
0.60	32.57	31.53	30.56	29.34
0.80	37.23	36.02	35.07	33.77
1.00	43.27	42.10	41.05	39.84

Surface tension liquid-gas (* 0.001 N/m) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	293.15	0.00	21.11
2	293.15	0.20	24.78
3	293.15	0.40	28.62
4	293.15	0.60	32.57
5	293.15	0.80	37.23
6	293.15	1.00	43.27
7	303.15	0.00	20.31
8	303.15	0.20	23.07
9	303.15	0.40	26.98
10	303.15	0.60	31.53
11	303.15	0.80	36.02
12	303.15	1.00	42.10
13	313.15	0.00	19.44
14	313.15	0.20	21.87
15	313.15	0.40	25.84
16	313.15	0.60	30.56
17	313.15	0.80	35.07
18	313.15	1.00	41.05
19	323.15	0.00	18.58
20	323.15	0.20	20.86
21	323.15	0.40	25.00
22	323.15	0.60	29.34
23	323.15	0.80	33.77
24	323.15	1.00	39.84

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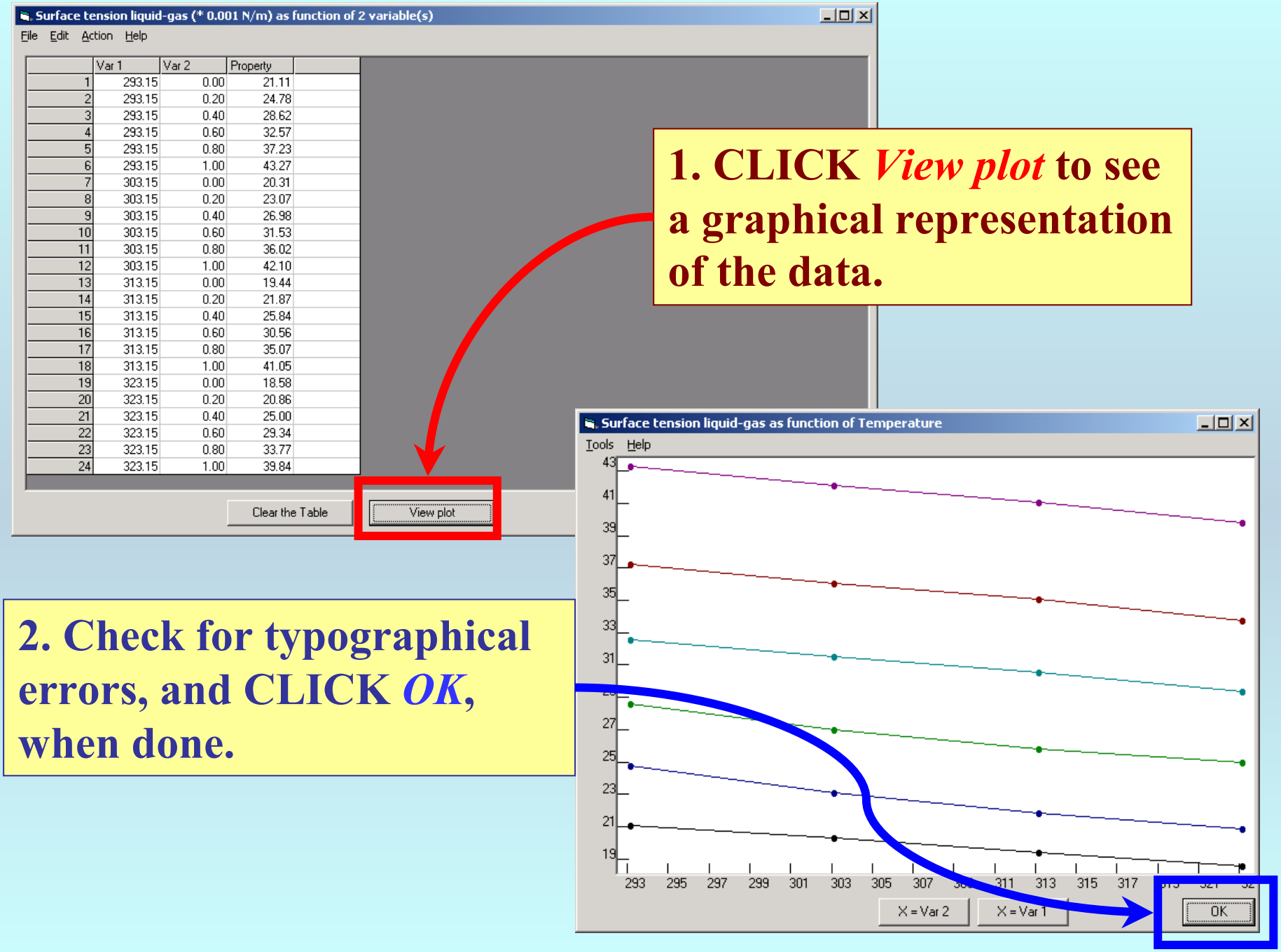
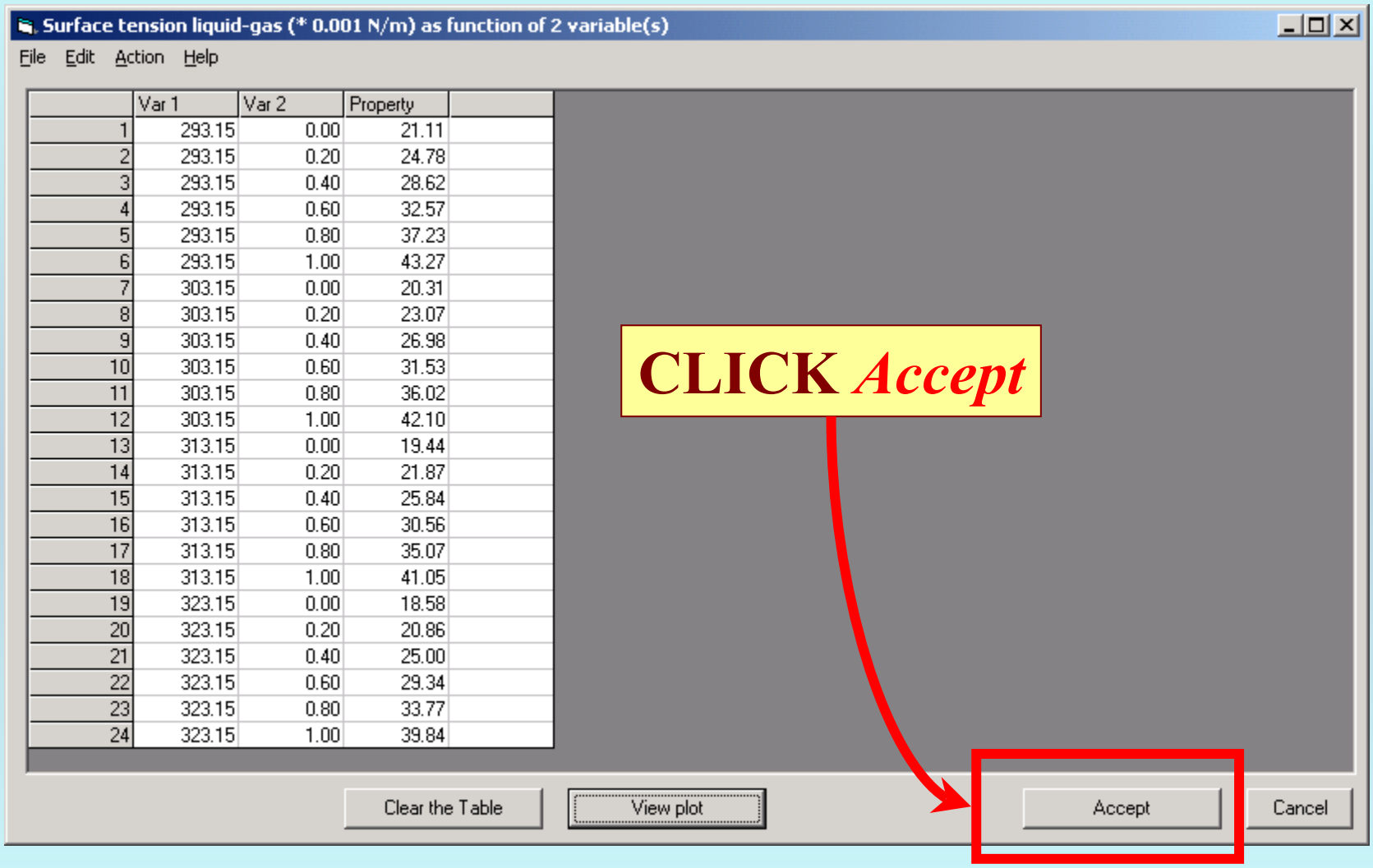
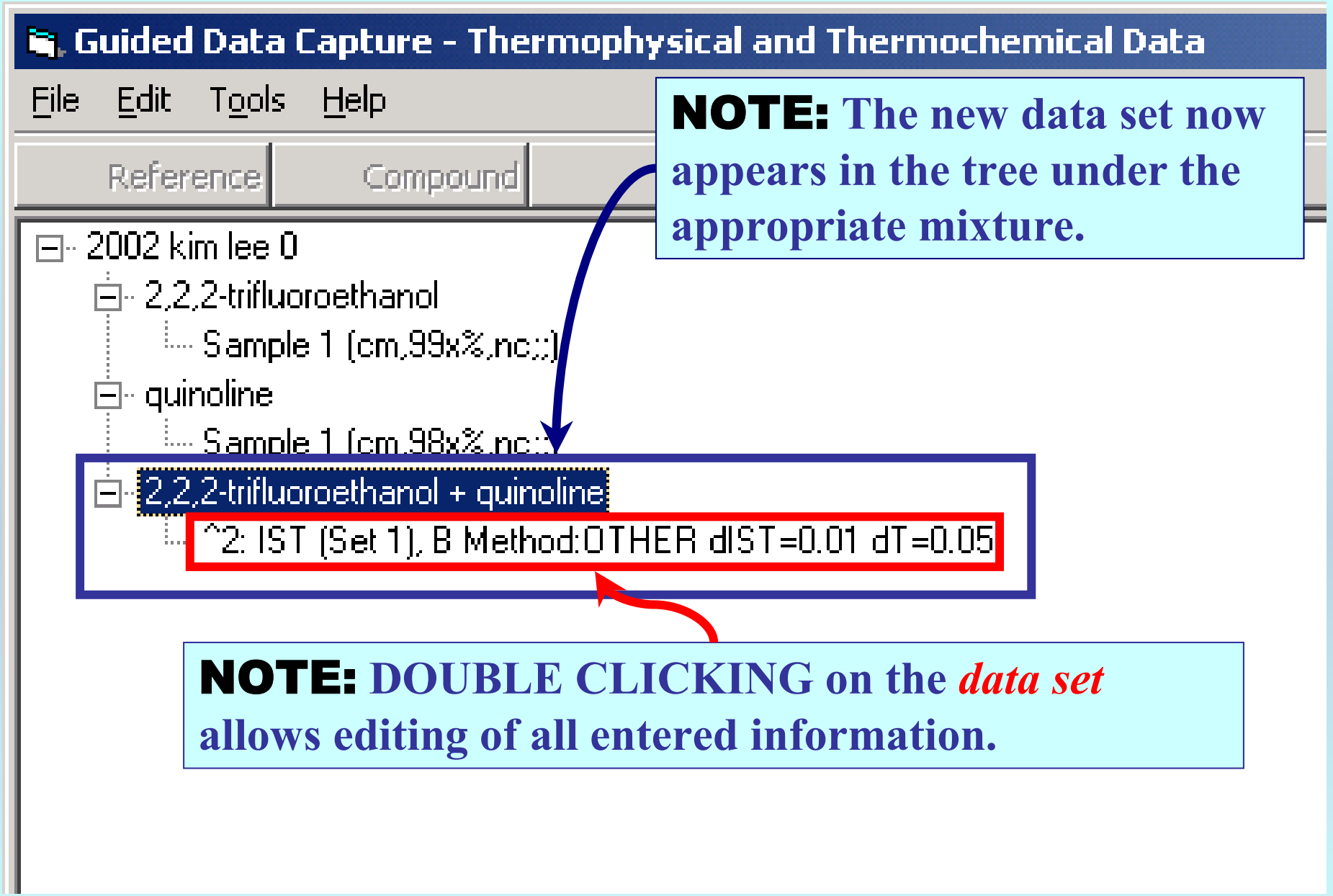
0.80	37.23	36.02	35.07	33.77
1.00	43.27	42.10	41.05	39.84

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.)


Surface tension liquid-gas (* 0.001 N/m) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 293.15 0.00 21.11
2 293.15 0.20 24.78
3 293.15 0.40 28.62
4 293.15 0.60 32.57
5 293.15 0.80 37.23
6 293.15 1.00 43.27
7 303.15 0.00 20.31
8 303.15 0.20 23.07
9 303.15 0.40 26.98
10 303.15 0.60 31.53
11 303.15 0.80 36.02
12 303.15 1.00 42.10
13 313.15 0.00 19.44
14 313.15 0.20 21.87
15 313.15 0.40 25.84
16 313.15 0.60 30.56
17 313.15 0.80 35.07
18 313.15 1.00 41.05
19 323.15 0.00 18.58
20 323.15 0.20 20.86
21 323.15 0.40 25.00
22 323.15 0.60 29.34
23 323.15 0.80 33.77
24 323.15 1.00 39.84
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
Surface tension liquid-gas as function of Temperature
Tools Help
43
41
39
37
35
33
31
27
25
23
21
19
293 295 297 299 301 303 305 307 311 313 315 317
X = Var 2
X = Var 1
OK
2. Check for typographical errors, and CLICK OK, when done.


Surface tension liquid-gas (* 0.001 N/m) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 293.15 0.00 21.11
2 293.15 0.20 24.78
3 293.15 0.40 28.62
4 293.15 0.60 32.57
5 293.15 0.80 37.23
6 293.15 1.00 43.27
7 303.15 0.00 20.31
8 303.15 0.20 23.07
9 303.15 0.40 26.98
10 303.15 0.60 31.53
11 303.15 0.80 36.02
12 303.15 1.00 42.10
13 313.15 0.00 19.44
14 313.15 0.20 21.87
15 313.15 0.40 25.84
16 313.15 0.60 30.56
17 313.15 0.80 35.07
18 313.15 1.00 41.05
19 323.15 0.00 18.58
20 323.15 0.20 20.86
21 323.15 0.40 25.00
22 323.15 0.60 29.34
23 323.15 0.80 33.77
24 323.15 1.00 39.84
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
2002 kim lee 0
2,2,2-trifluoroethanol
Sample 1 (cm,99x%,nc::)
quinoline
Sample 1 (cm,98x%,nc::)
2,2,2-trifluoroethanol + quinoline
^2: IST (Set 1), B Method:OTHER dIST=0.01 dT=0.05
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.**