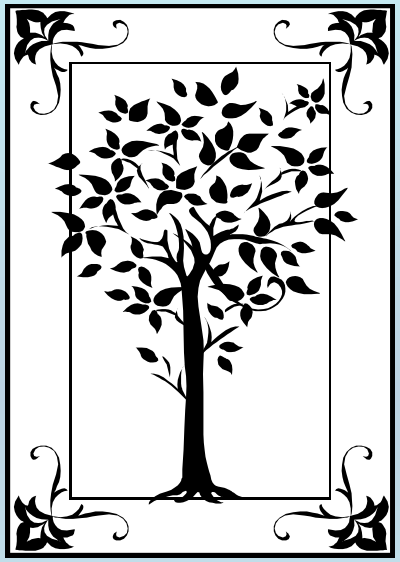
METADATA AND NUMERICAL DATA CAPTURE:
Vapor Pressures
(1 – Component)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for Vapor Pressures of 1 component
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 1997, *42*, 475−487

Thermodynamic Equilibria in Xylene Isomerization. 2. The Thermodynamic Properties of *m*-Xylene†

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Measurements leading to the calculation of the ideal-gas thermodynamic properties for *m*-xylene are reported. Experimental methods included adiabatic heat-capacity calorimetry (5 K to 430 K), vibrating-tube densitometry (323 K to 523 K), comparative ebulliometry (309 K to 453 K), and differential-scanning calorimetry (DSC). The critical temperature was measured by DSC. Saturation heat capacities for the liquid phase between 430 K and 550 K and the critical pressure were derived with the vapor-pressure and DSC results. Results were combined with an enthalpy of combustion reported in the literature to derive standard molar entropies, enthalpies, and Gibbs free energies of formation at selected temperatures between 250 K and 550 K. The standard state is defined as the ideal gas at the pressure $p = p^{\circ} =$ 101.325 kPa. Standard entropies are compared with those calculated statistically on the basis of assigned vibrational spectra for the vapor phase. All results are compared with literature values.

Vapor pressure for 1 component
m-xylene (i.e., 1,3-dimethylbenzene)

Table 2. Summary of Vapor-Pressure Results for *m*-Xylene[a]

standard	*T*/K	*p*/kPa	Δ*p*/kPa	σ/kPa	Δ*T*/K
decane	308.640	1.9992	−0.0003	0.00	
decane	322.290	3.9924	0.0004	0.00	
decane	328.459	5.336	0.000	0.00	
decane	328.459	5.336	0.000	0.00	
decane	337.564	8.001	0.001	0.001	0.010
decane	344.412	10.671	0.000	0.001	0.009
decane	349.946	13.335	0.000	0.002	0.009
decane	355.722	16.679	−0.001	0.002	0.009
decane	360.484	19.931	−0.001	0.002	0.009
decane	366.807	25.036	−0.001	0.003	0.008
water[b]	366.795	25.026	0.000	0.003	0.008
water	373.152	31.185	−0.001	0.003	0.007
water	379.540	38.561	−0.002	0.004	0.008
water	385.969	47.348	−0.002	0.005	0.007
water	392.455	57.780	−0.001	0.006	0.009
water	399.012	70.118	−0.001	0.007	0.011
water	405.601	84.545	−0.001	0.008	0.011
water	412.213	101.299	0.005	0.009	0.014
water	418.893	120.78	0.00	0.01	0.013
water	425.615	143.23	0.01	0.01	0.014
water	432.383	169.01	0.00	0.01	0.014
water	439.202	198.51	0.00	0.02	0.014
water	446.046	231.98	0.00	0.02	0.014
water	452.947	269.98	−0.01	0.02	0.013

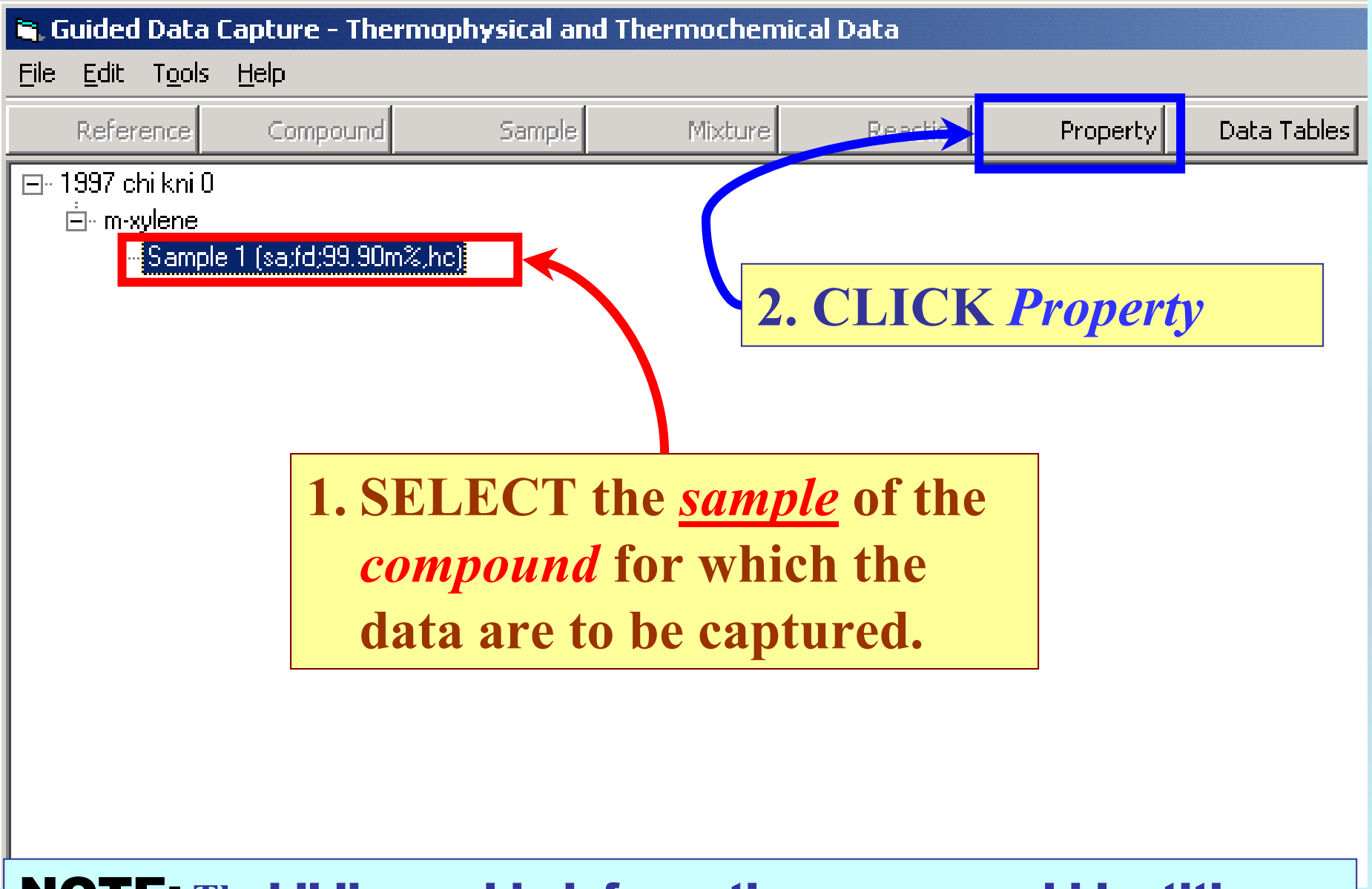
This data set is considered here.

Experimental Method Info :

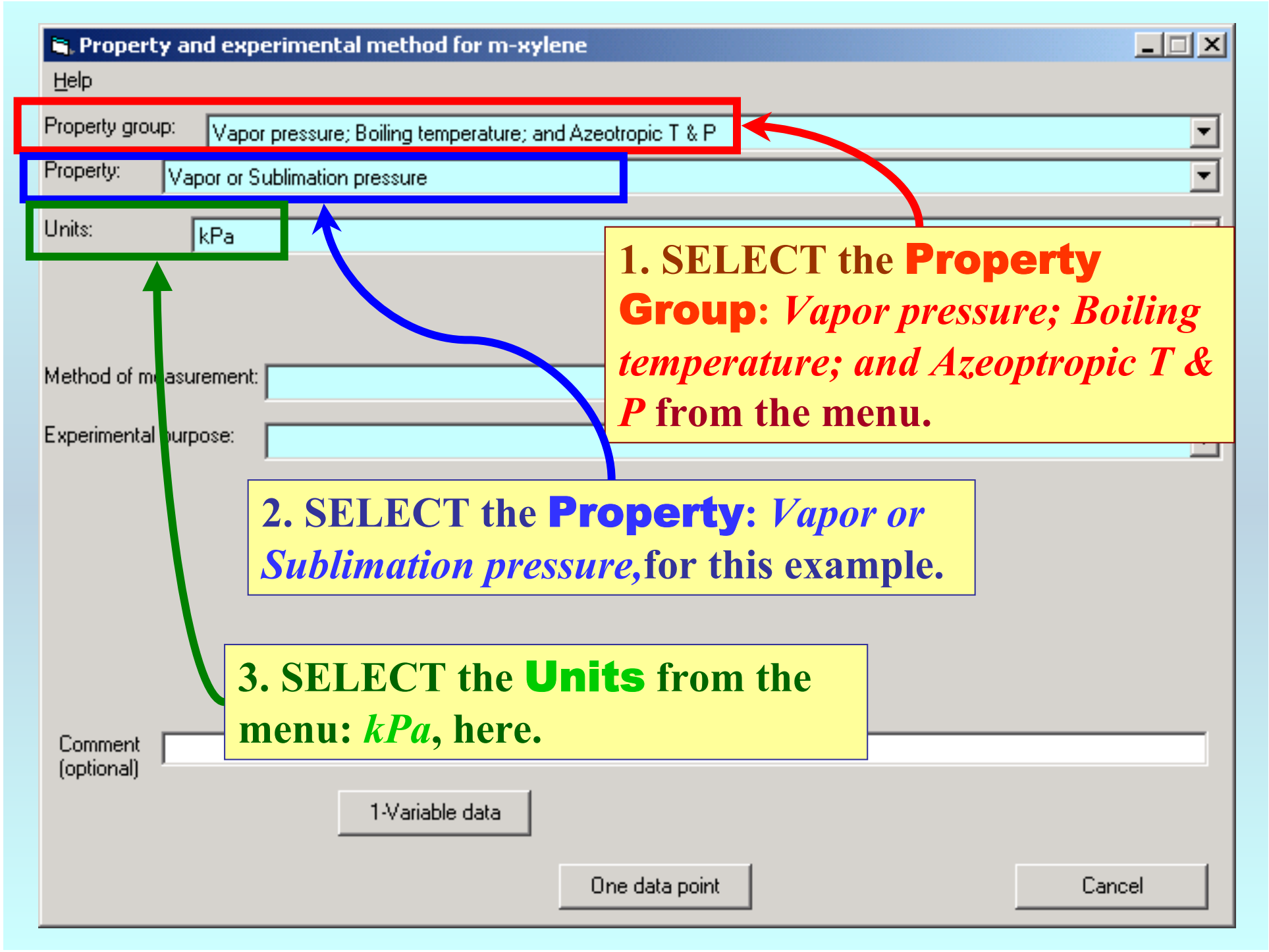
The accuracy and precision of the temperature measurements for the ebulliometric vapor-pressure studies are estimated to be 0.002 K and 0.0005 K, respectively.

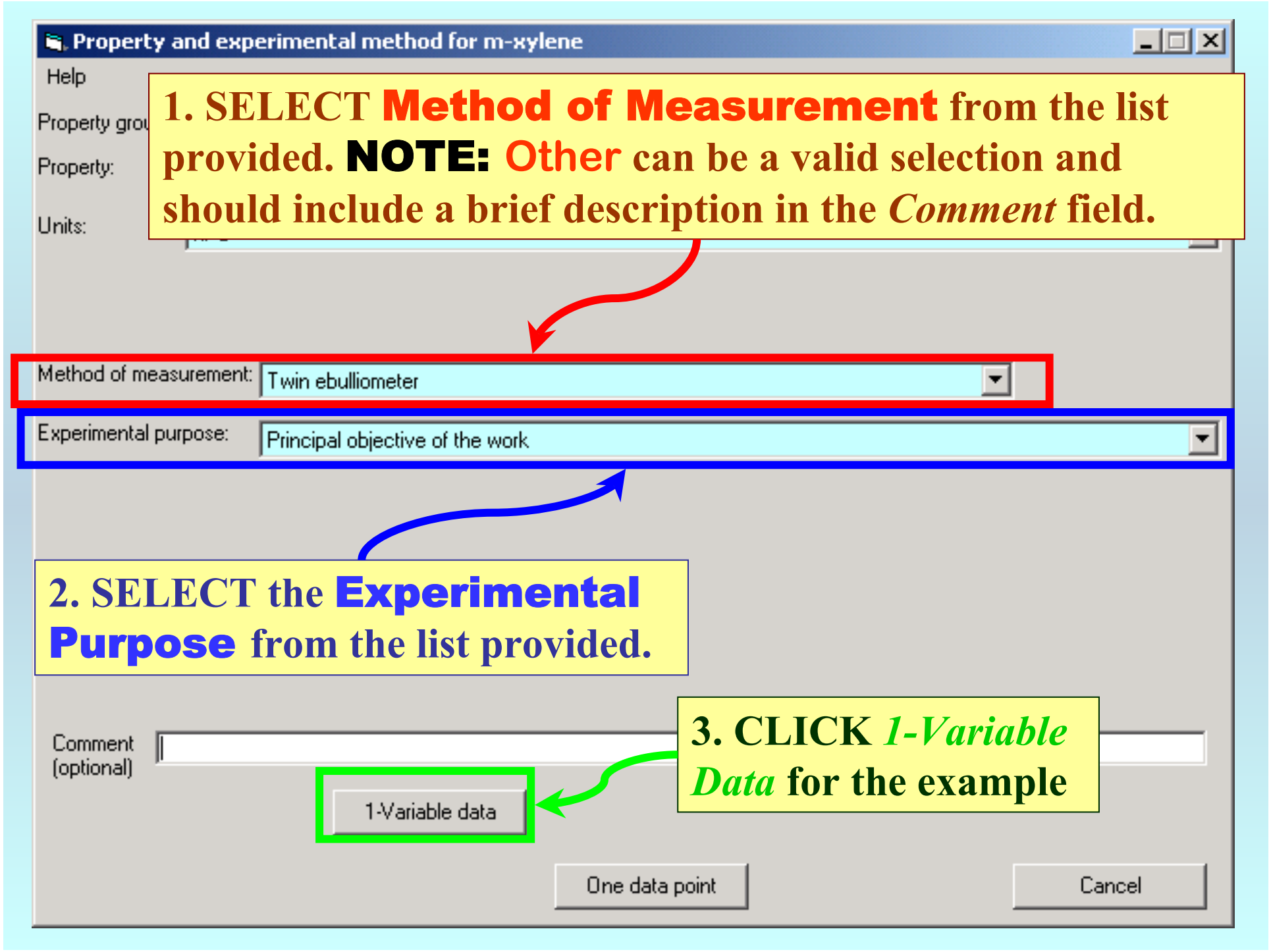
Uncertainty estimates:

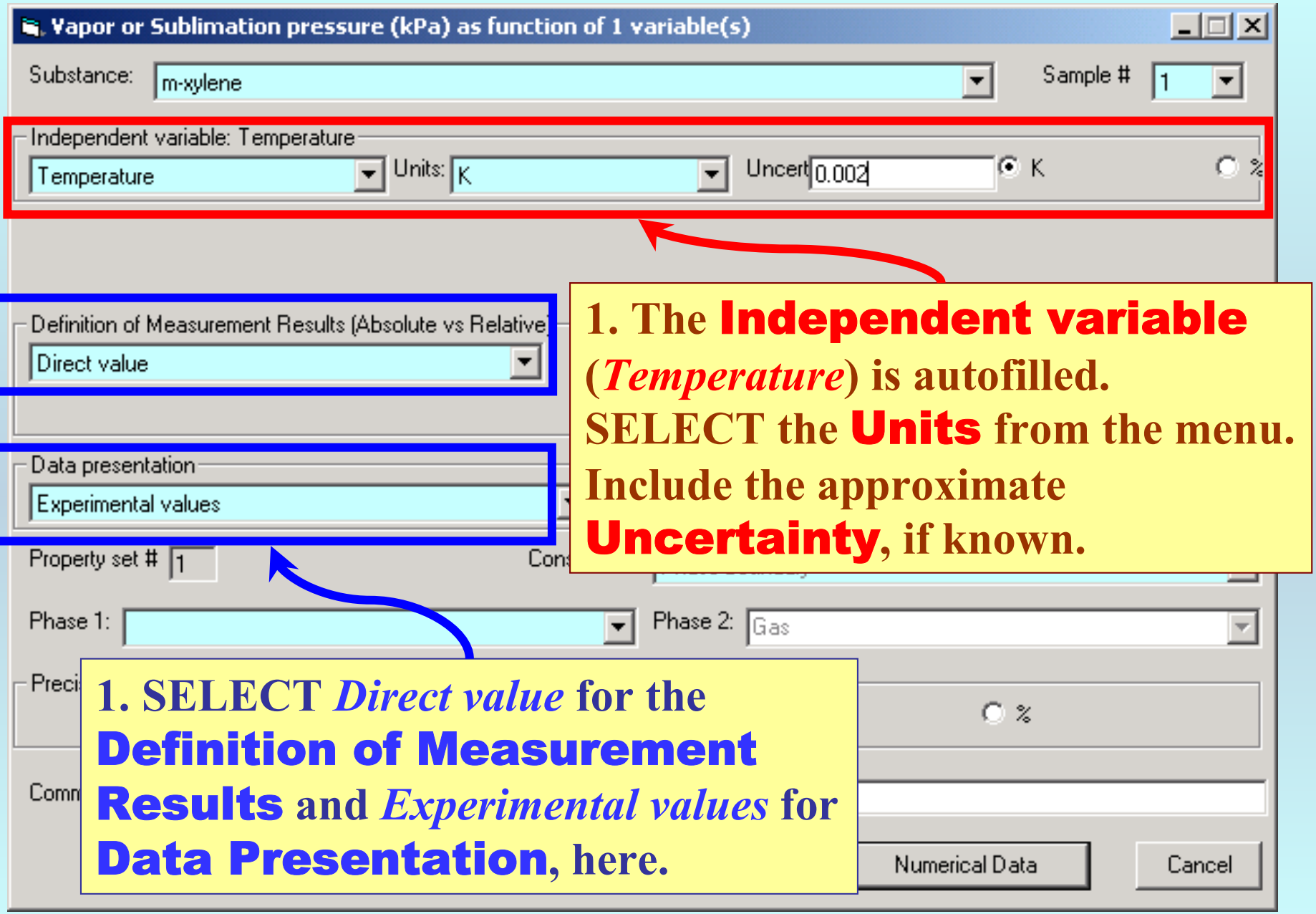
Given in the data table.

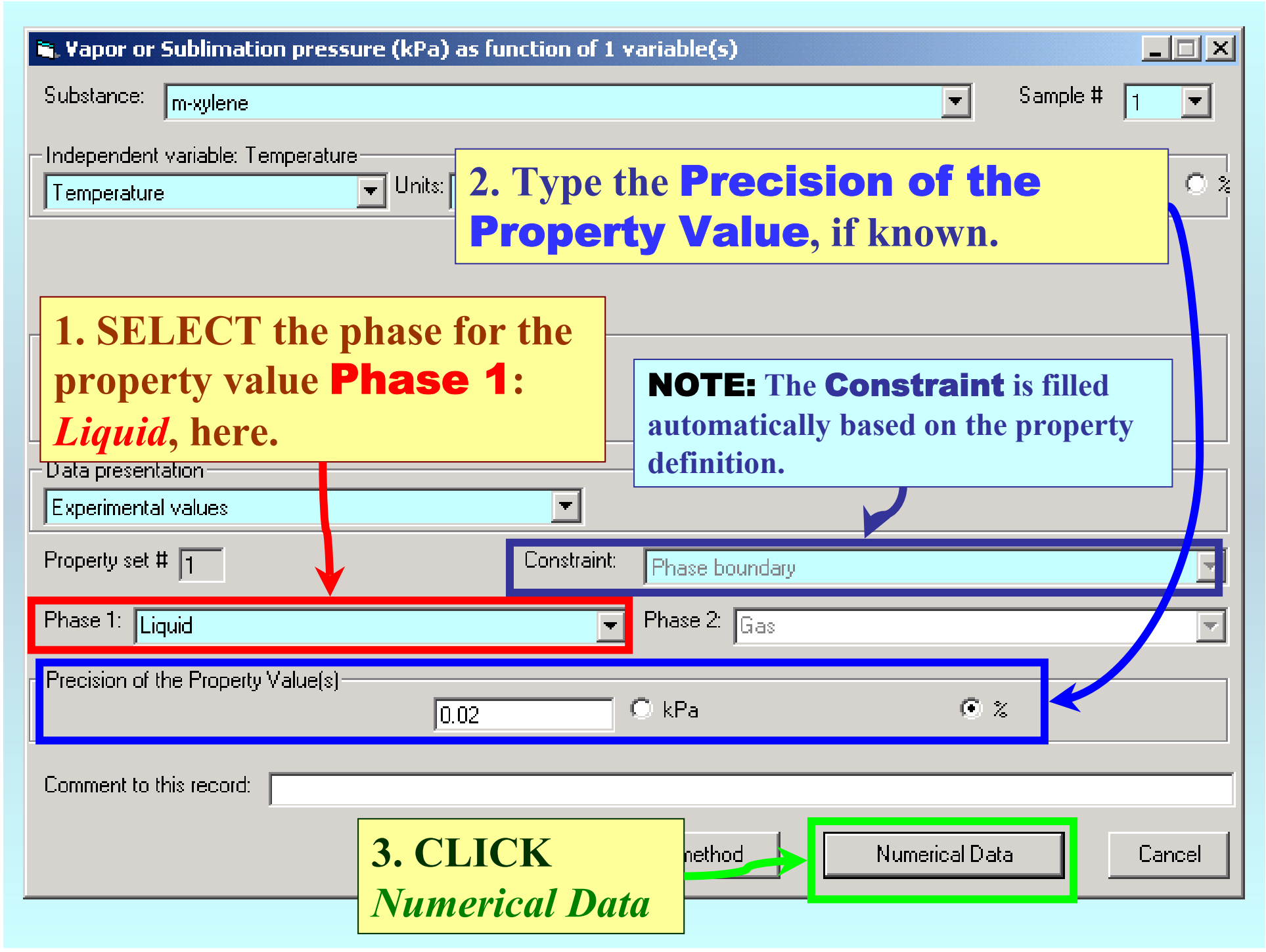


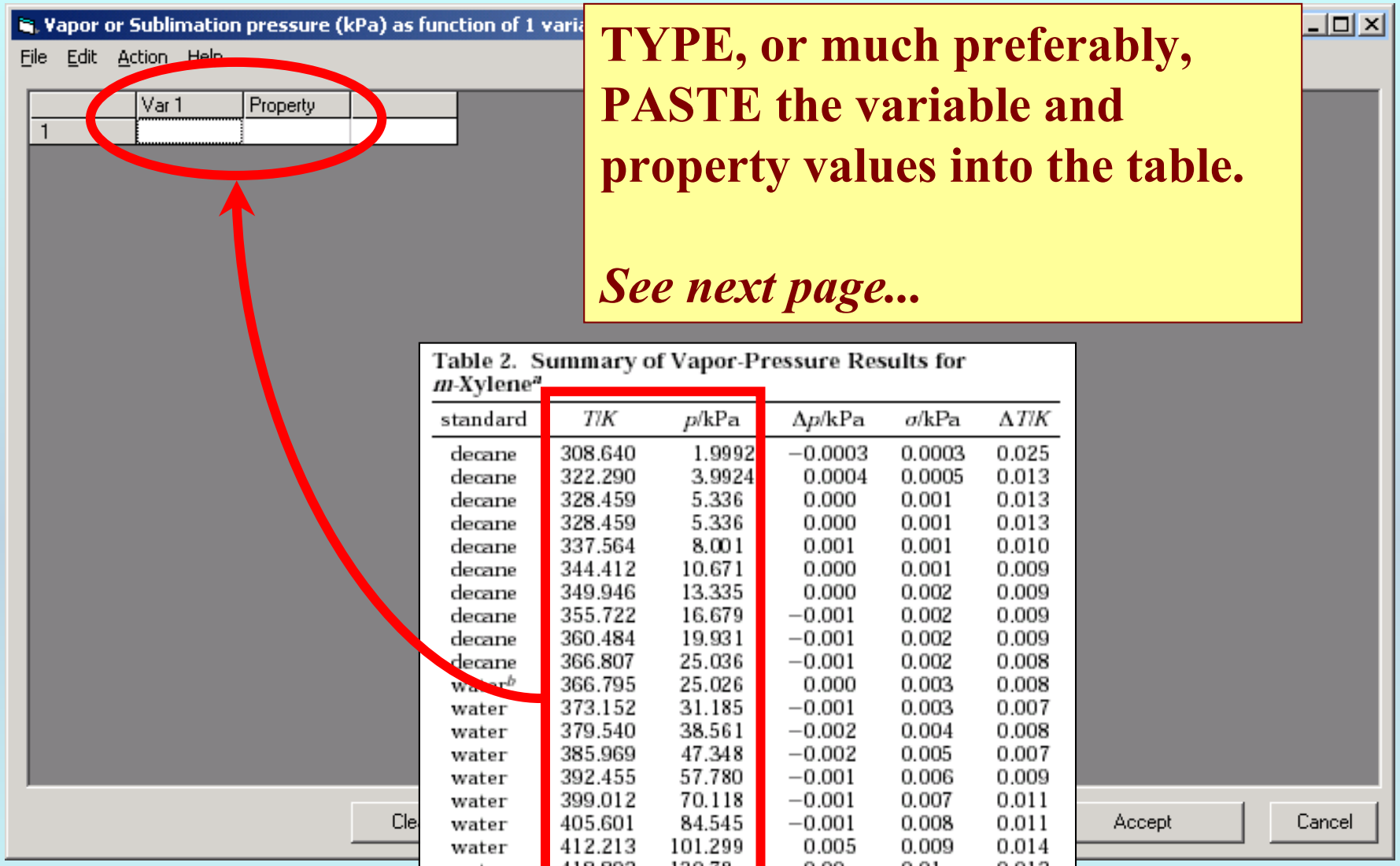
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for m-xylene
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Vapor or Sublimation pressure
Units:
kPa
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Vapor pressure; Boiling temperature; and Azeoptropic T & P from the menu.
2. SELECT the Property: Vapor or Sublimation pressure, for this example.
3. SELECT the Units from the menu: kPa, here.
Comment (optional)
1-Variable data
One data point
Cancel


Property and experimental method for m-xylene
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:
Twin ebulliometer
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK 1-Variable Data for the example
1-Variable data
One data point
Cancel


Vapor or Sublimation pressure (kPa) as function of 1 variable(s)
Substance:
m-xylene
Sample #
1
Independent variable: Temperature
Temperature
Units:
K
Uncert
0.002
K
%
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Property set #
1
Phase 1:
Phase 2:
Gas
%
Numerical Data
Cancel
1. The Independent variable (Temperature) is autofilled.
SELECT the Units from the menu.
Include the approximate Uncertainty, if known.
1. SELECT Direct value for the Definition of Measurement Results and Experimental values for Data Presentation, here.


Vapor or Sublimation pressure (kPa) as function of 1 variable(s)
Substance:
m-xylene
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)
0.02
kPa
%
Comment to this record:
3. CLICK Numerical Data
Numerical Data
Cancel



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

See next page...

Table 2. Summary of Vapor-Pressure Results for *m*-Xylene[a]

standard	*T*/K	*p*/kPa	Δ*p*/kPa	*σ*/kPa	Δ*T*/K
decane	308.640	1.9992	−0.0003	0.0003	0.025
decane	322.290	3.9924	0.0004	0.0005	0.013
decane	328.459	5.336	0.000	0.001	0.013
decane	328.459	5.336	0.000	0.001	0.013
decane	337.564	8.001	0.001	0.001	0.010
decane	344.412	10.671	0.000	0.001	0.009
decane	349.946	13.335	0.000	0.002	0.009
decane	355.722	16.679	−0.001	0.002	0.009
decane	360.484	19.931	−0.001	0.002	0.009
decane	366.807	25.036	−0.001	0.002	0.008
[illegible][b]	366.795	25.026	0.000	0.003	0.008
water	373.152	31.185	−0.001	0.003	0.007
water	379.540	38.561	−0.002	0.004	0.008
water	385.969	47.348	−0.002	0.005	0.007
water	392.455	57.780	−0.001	0.006	0.009
water	399.012	70.118	−0.001	0.007	0.011
water	405.601	84.545	−0.001	0.008	0.011
water	412.213	101.299	0.005	0.009	0.014
water	418.893	120.78	0.00	0.01	0.013
water	425.615	143.23	0.01	0.01	0.014
water	432.383	169.01	0.00	0.01	0.014
water	439.202	198.51	0.00	0.02	0.014
water	446.046	231.98	0.00	0.02	0.014
water	452.947	269.98	−0.01	0.02	0.013

Vapor or Sublimation pressure (kPa) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	308.640	1.9992
2	322.290	3.9924
3	328.459	5.336
4	328.459	5.336
5	337.564	8.001
6	344.412	10.671
7	349.946	13.335
8	355.722	16.679
9	360.484	19.931
10	366.807	25.036
11	366.795	25.026
12	373.152	31.185
13	379.540	38.561
14	385.969	47.348
15	392.455	57.780
16	399.012	70.118
17	405.601	84.545
18	412.213	101.299
19	418.893	120.78
20	425.615	143.23
21	432.383	169.01
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Table 2. Summary of Vapor-Pressure Results for *m*-Xylene[a]

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decane	308.640	1.9992	−0.0003	0.0003	0.025
decane	322.290	3.9924	0.0004	0.0005	0.013
decane	328.459	5.336	0.000	0.001	0.013
decane	328.459	5.336	0.000	0.001	0.013
decane	337.564	8.001	0.001	0.001	0.010
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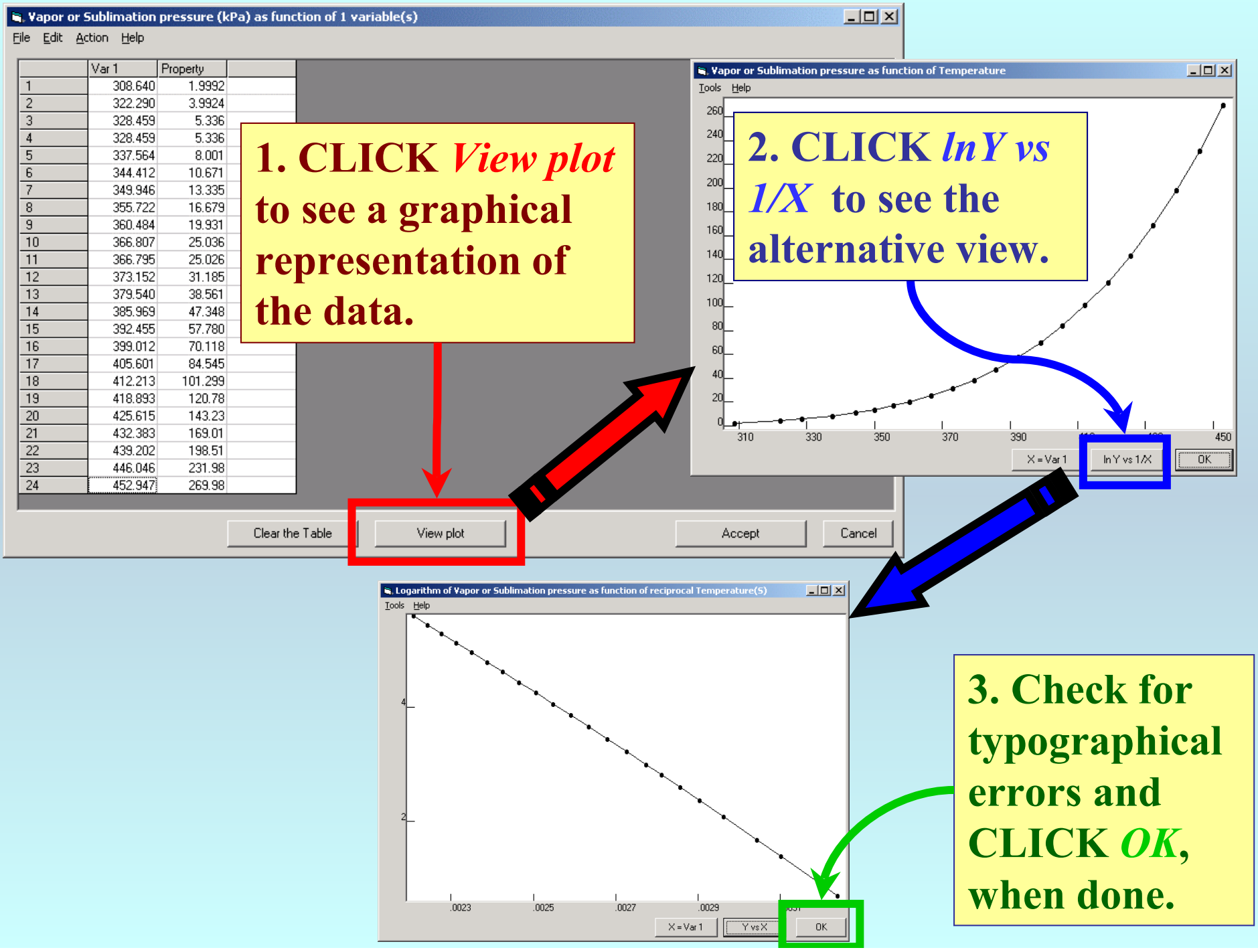
water	446.046	231.98	0.00	0.02	0.014
water	452.947	269.98	−0.01	0.02	0.013

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.)


Vapor or Sublimation pressure (kPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 308.640 1.9992
2 322.290 3.9924
3 328.459 5.336
4 328.459 5.336
5 337.564 8.001
6 344.412 10.671
7 349.946 13.335
8 355.722 16.679
9 360.484 19.931
10 366.807 25.036
11 366.795 25.026
12 373.152 31.185
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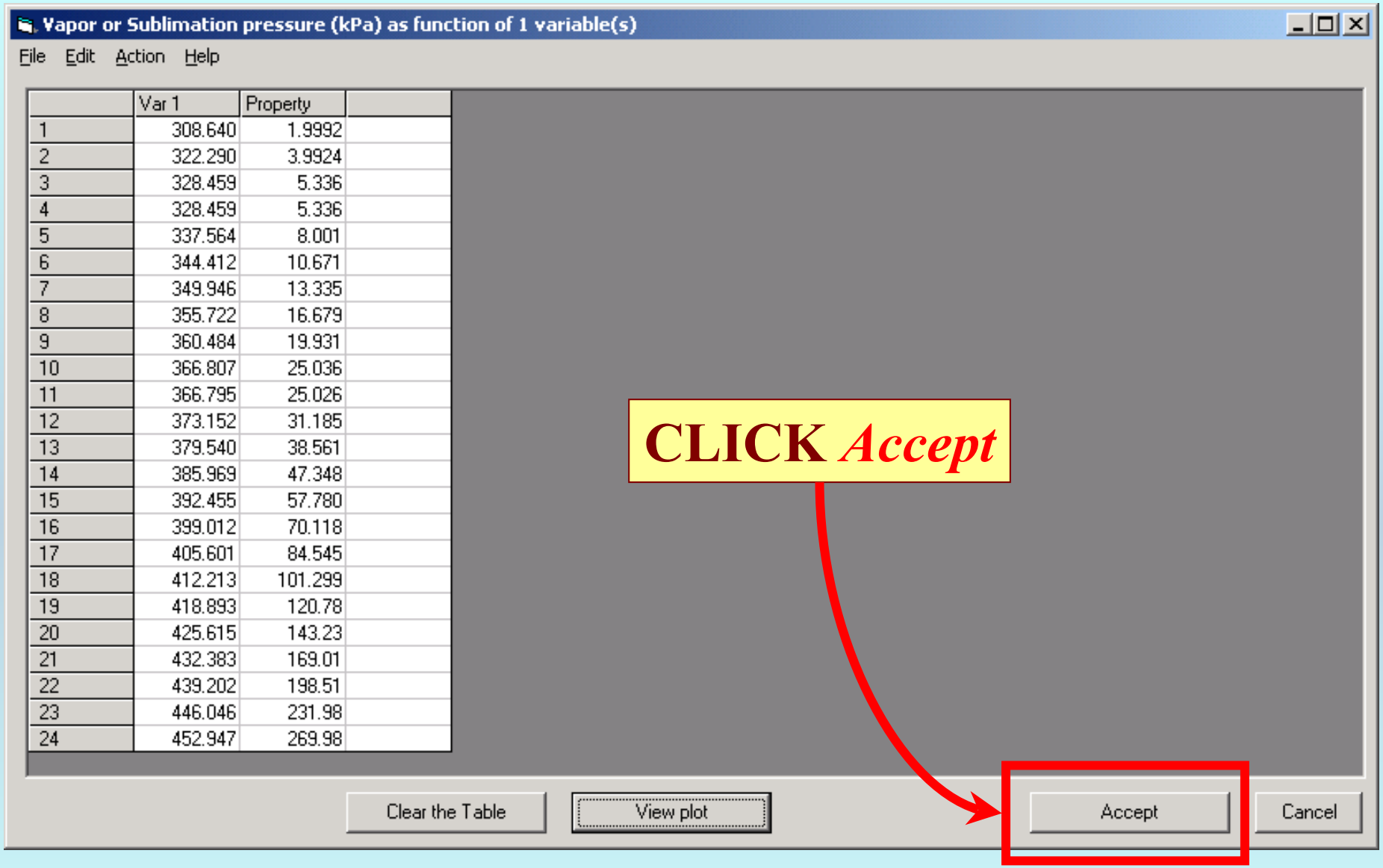
15 392.455 57.780
16 399.012 70.118
17 405.601 84.545
18 412.213 101.299
19 418.893 120.78
20 425.615 143.23
21 432.383 169.01
22 439.202 198.51
23 446.046 231.98
24 452.947 269.98
Clear the Table
View plot
Accept
Cancel
1. CLICK View plot to see a graphical representation of the data.
Vapor or Sublimation pressure as function of Temperature
Tools Help
260
240
220
200
180
160
140
120
100
80
60
40
20
0
310
330
350
370
390
450
X = Var 1
ln Y vs 1/X
OK
2. CLICK lnY vs 1/X to see the alternative view.
Logarithm of Vapor or Sublimation pressure as function of reciprocal Temperature(S)
Tools Help
4
2
.0023
.0025
.0027
.0029
X = Var 1
Y vs X
OK
3. Check for typographical errors and CLICK OK, when done.


Vapor or Sublimation pressure (kPa) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 308.640 1.9992
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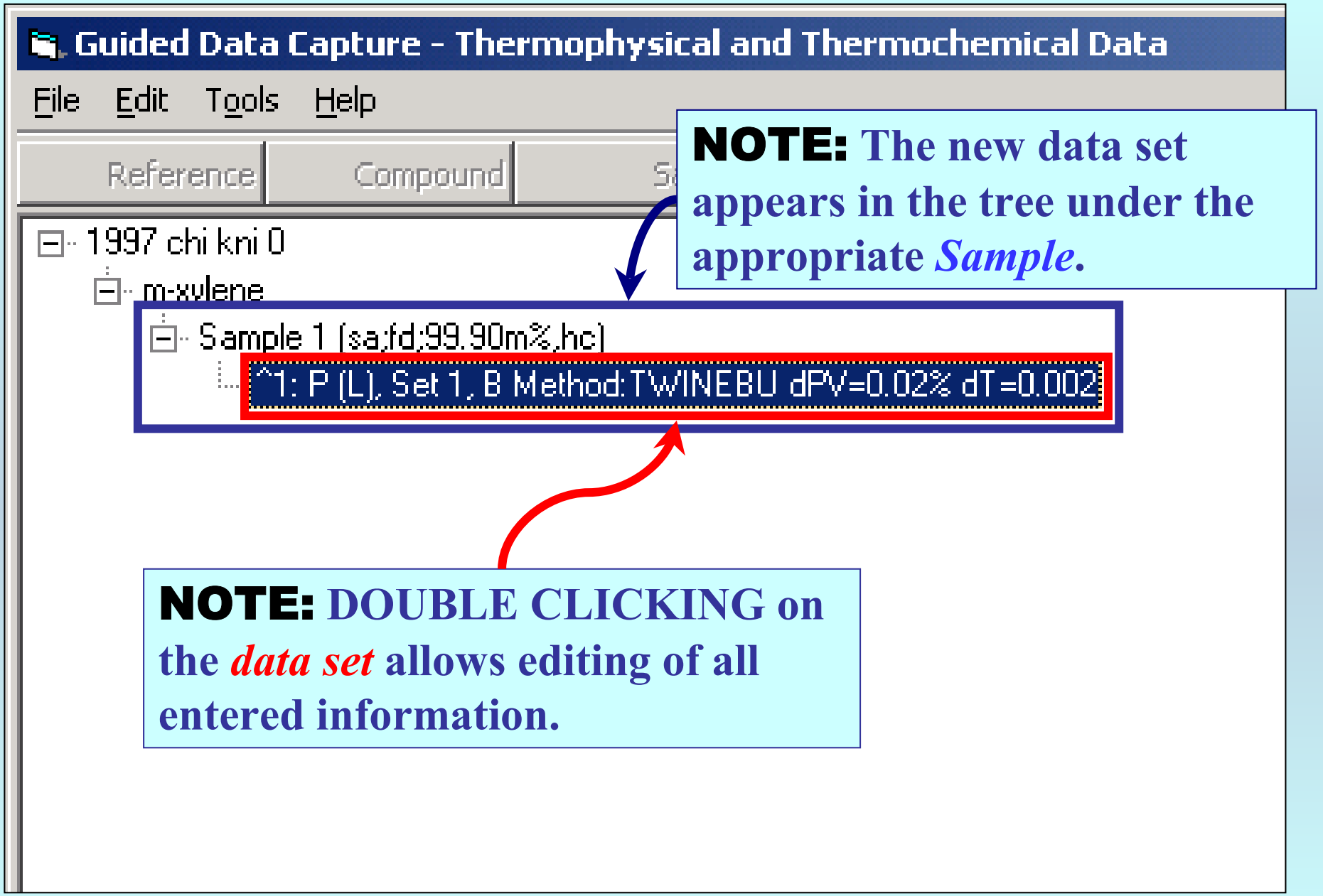
21 432.383 169.01
22 439.202 198.51
23 446.046 231.98
24 452.947 269.98
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
1997 chi kni 0
m-xylene
Sample 1 [sa;fd;99.90m%,hc]
^1: P (L), Set 1, B Method:TWINEBU dPV=0.02% dT=0.002
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.**