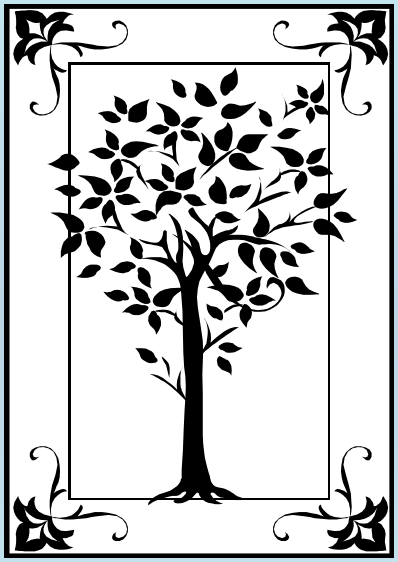
METADATA AND NUMERICAL DATA CAPTURE:
Derived *Thermodynamic Functions*
From adiabatic calorimetry
(for 1 – Component)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Derived Thermodynamic Functions**
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.

Derived Thermodynamic Functions: $C_{sat,m}(T)$, {H(T)-H(0)}, S(T)-S(0)
m-xylene

Table 9. Molar Thermodynamic Functions at Vapor-Saturation Pressure for *m*-Xylene[a] ($R = 8.314\ 51$ J·K^{-1}·mol^{-1})

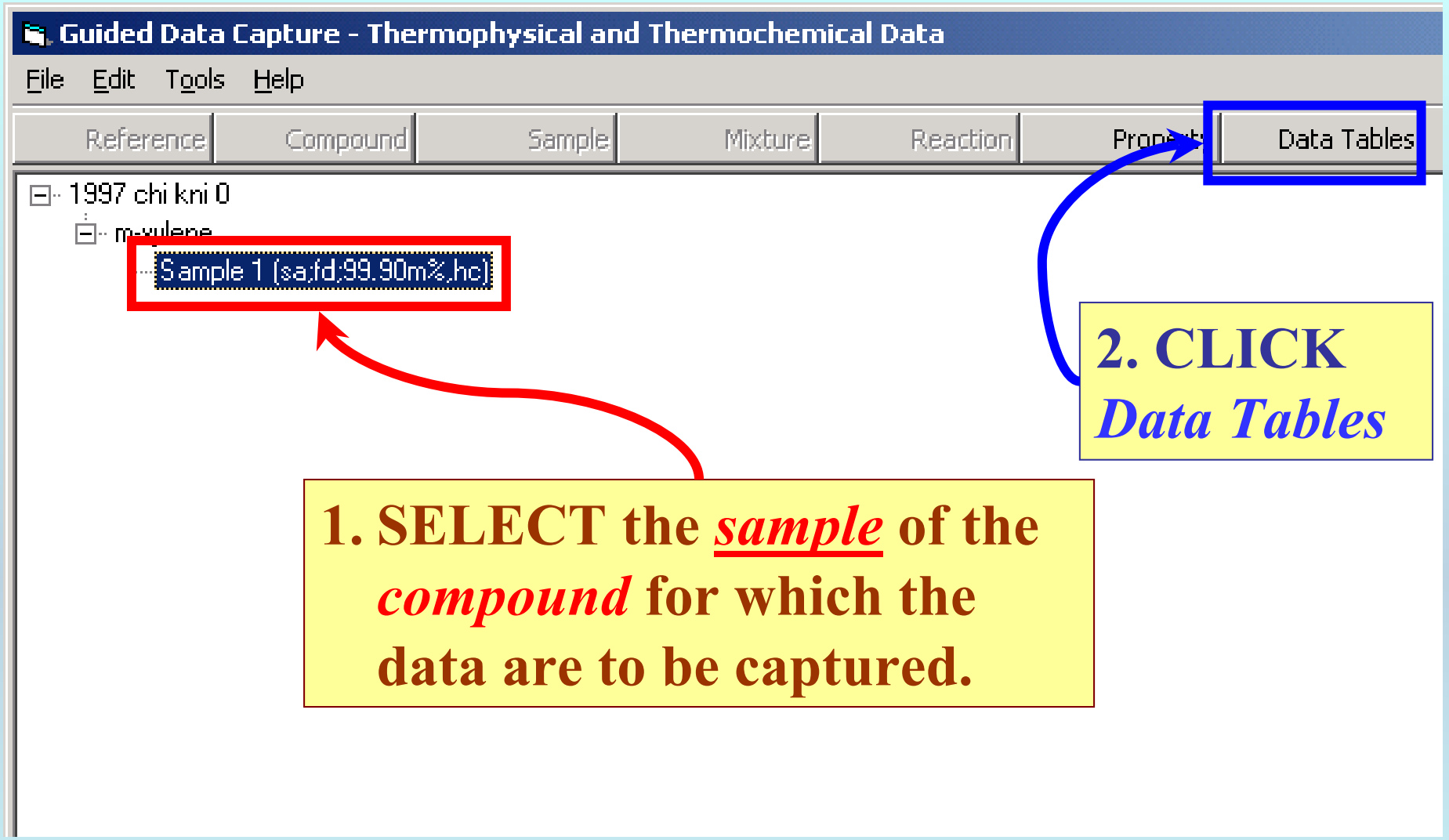
T/K	$C_{sat,m}/R$	$\Delta_0^T S_m/R$	$\Delta_0^T H_m/RT$	T/K	$C_{sat,m}/R$	$\Delta_0^T S_m/R$	$\Delta_0^T H_m/RT$
			Crystals				
5.00	0.028	0.009	0.007	90.00	8.292	8.281	4.699
10.00	0.265	0.082	0.062	100.00	8.745	9.178	5.081
15.00	0.844	0.287	0.217	120.00	9.654	10.853	5.767
20.00	1.651	0.637	0.472	140.00	10.577	12.410	6.388
30.00	3.431	1.645	1.163	160.00	11.535	13.885	6.971
40.00	4.937	2.849	1.928	180.00	12.521	15.300	7.533
50.00	6.002	4.073	2.643	200.00	13.527	16.671	8.082
60.00	6.749	5.237	3.268	220.00	14.582	18.009	8.624
70.00	7.322	6.322	3.808	225.30	14.880	18.359	8.768
80.00	7.821	7.333	4.279				
			Liquid				
225.30	19.362	24.575	14.984	400.00	26.444	37.351	18.308
240.00	19.772	25.812	15.264	420.00	27.419	38.665	18.719
260.00	20.410	27.419	15.635				
280.00	21.133	28.958	16.001				
298.15	21.848	30.307	16.335				
300.00	21.923	30.442	16.369				
320.00	22.765	31.884	16.743				
340.00	23.642	33.290	17.122				
360.00	24.554	34.667	17.510				
380.00	25.490	36.020	17.905				

Data sets considered here.

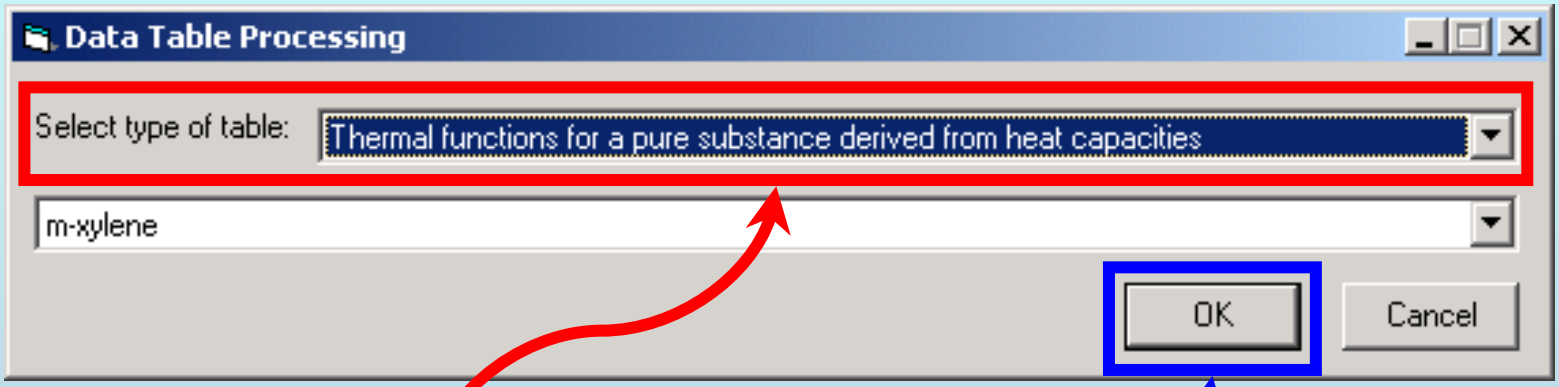
NOTE: **Each phase will be considered separately**

Experimental Method Info :

Adiabatic Calorimetry



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.)



1. SELECT the type of table: *Thermal functions for a pure substance derived from heat capacities.*

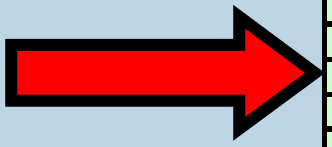
2. CLICK *OK*.

Transform the multi-column data into single columns.

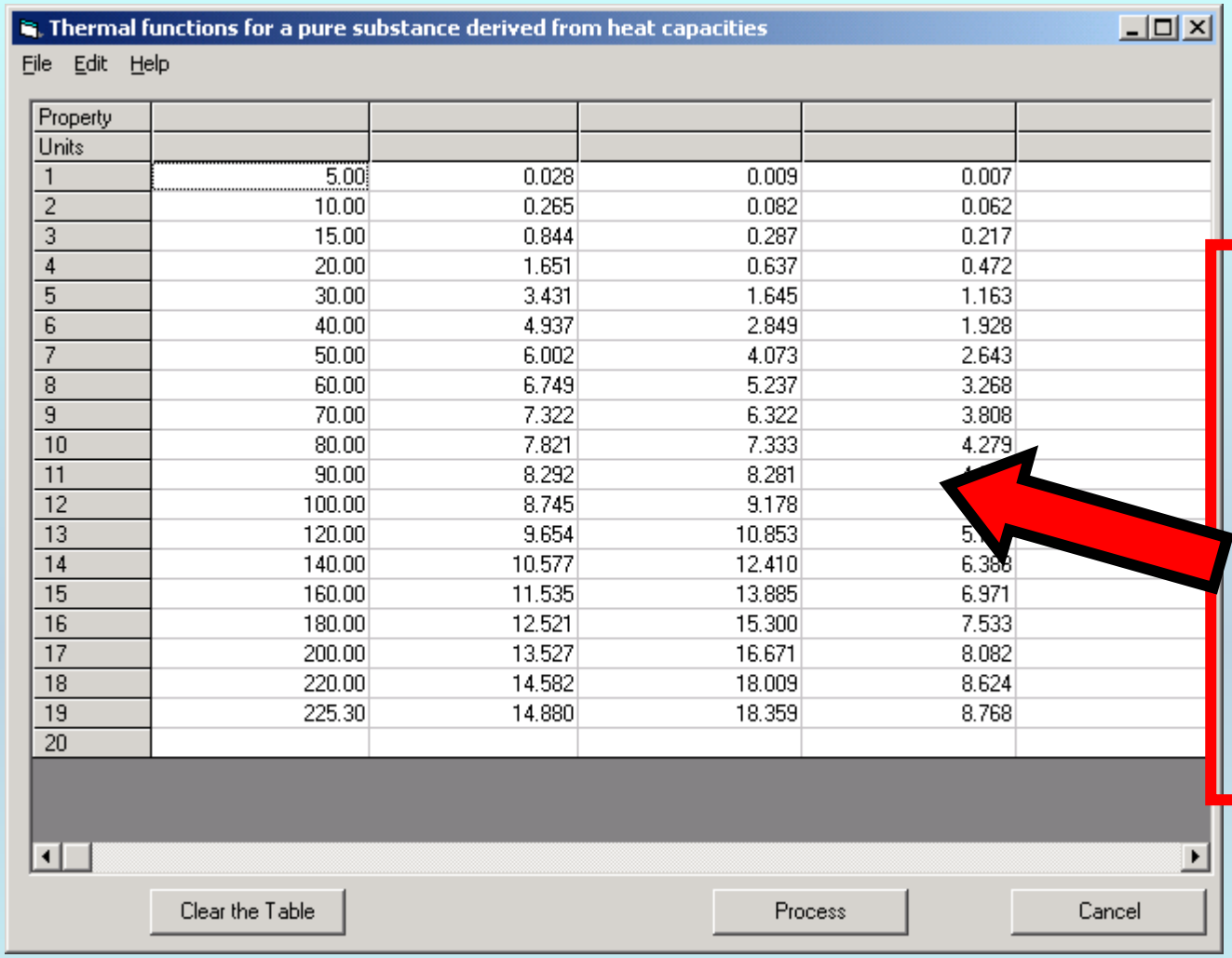
NOTE: **This can be done in any spreadsheet software (e.g., EXCEL)**

Table 9. Molar Thermodynamic Functions at Vapor-Saturation Pressure for *m*-Xylene[a] ($R = 8.314\ 51$ J·K^{-1}·mol^{-1})

T/K	$C_{sat,m}/R$	$\Delta_0^T S_m/R$	$\Delta_0^T H_m/RT$	T/K	$C_{sat,m}/R$	$\Delta_0^T S_m/R$	$\Delta_0^T H_m/RT$
			Crystals				
5.00	0.028	0.009	0.007	90.00	8.292	8.281	4.699
10.00	0.265	0.082	0.062	100.00	8.745	9.178	5.081
15.00	0.844	0.287	0.217	120.00	9.654	10.853	5.767
20.00	1.651	0.637	0.472	140.00	10.577	12.410	6.388
30.00	3.431	1.645	1.163	160.00	11.535	13.885	6.971
40.00	4.937	2.849	1.928	180.00	12.521	15.300	7.533
50.00	6.002	4.073	2.643	200.00	13.527	16.671	8.082
60.00	6.749	5.237	3.268	220.00	14.582	18.009	8.624
70.00	7.322	6.322	3.808	225.30	14.880	18.359	8.768
80.00	7.821	7.333	4.279				
			Liquid				
225.30	19.362	24.575	14.984	400.00	26.444	37.351	18.308
240.00	19.772	25.812	15.264	420.00	27.419	38.665	18.719
260.00	20.410	27.419	15.635	440.00[b]	28.41	39.96	19.14
280.00	21.133	28.958	16.001	460.00[b]	29.44	41.25	19.56
298.15	21.848	30.307	16.335	480.00[b]	30.51	42.52	20.00
300.00	21.923	30.442	16.369	500.00[b]	31.65	43.79	20.44
320.00	22.765	31.884	16.743	520.00[b]	32.89	45.06	20.89
340.00	23.642	33.290	17.122	540.00[b]	34.30	46.33	21.36
360.00	24.554	34.667	17.510	550.00[b]	35.10	46.96	21.61
380.00	25.490	36.020	17.905				



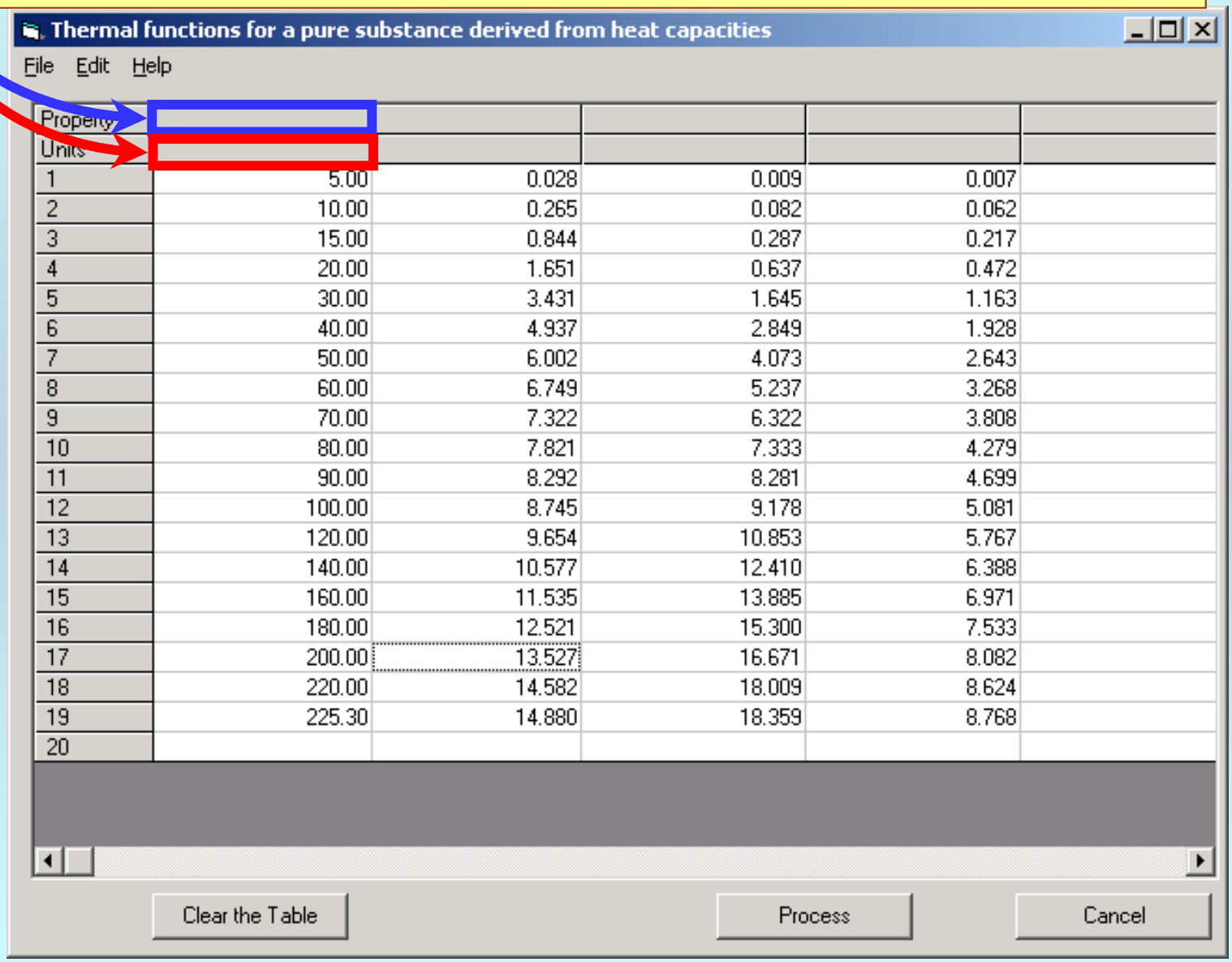
T/K	Csat/R	S/R	(H-H0)/RT
crystals			
5.00	0.028	0.009	0.007
10.00	0.265	0.082	0.062
15.00	0.844	0.287	0.217
20.00	1.651	0.637	0.472
30.00	3.431	1.645	1.163
40.00	4.937	2.849	1.928
50.00	6.002	4.073	2.643
60.00	6.749	5.237	3.268
70.00	7.322	6.322	3.808
80.00	7.821	7.333	4.279
90.00	8.292	8.281	4.699
100.00	8.745	9.178	5.081
120.00	9.654	10.853	5.767
140.00	10.577	12.410	6.388
160.00	11.535	13.885	6.971
180.00	12.521	15.300	7.533
200.00	13.527	16.671	8.082
220.00	14.582	18.009	8.624
225.30	14.880	18.359	8.768
liquid			
225.30	19.362	24.575	14.984
240.00	19.772	25.812	15.264
260.00	20.410	27.419	15.635
280.00	21.133	28.958	16.001
298.15	21.848	30.307	16.335
300.00	21.923	30.442	16.369
320.00	22.765	31.884	16.743
340.00	23.642	33.290	17.122
360.00	24.554	34.667	17.510
380.00	25.490	36.020	17.905
400.00	26.444	37.351	18.308
420.00	27.419	38.665	18.719



T/K	Csat/R	S/R	(H-H0)/RT
	crystals		
5.00	0.028	0.009	0.007
10.00	0.265	0.082	0.062
15.00	0.844	0.287	0.217
20.00	1.651	0.637	0.472
30.00	3.431	1.645	1.163
40.00	4.937	2.849	1.928
50.00	6.002	4.073	2.643
60.00	6.749	5.237	3.268
70.00	7.322	6.322	3.808
80.00	7.821	7.333	4.279
90.00	8.292	8.281	4.699
100.00	8.745	9.178	5.081
120.00	9.654	10.853	5.767
140.00	10.577	12.410	6.388
160.00	11.535	13.885	6.971
180.00	12.521	15.300	7.533
200.00	13.527	16.671	8.082
220.00	14.582	18.009	8.624
225.30	14.880	18.359	8.768
	liquid		
225.30	19.362	24.575	14.984
240.00	19.772	25.812	15.264
260.00	20.410	27.419	15.635
280.00	21.133	28.958	16.001
298.15	21.848	30.307	16.335
300.00	21.923	30.442	16.369
320.00	22.765	31.884	16.743
340.00	23.642	33.290	17.122
360.00	24.554	34.667	17.510
380.00	25.490	36.020	17.905
400.00	26.444	37.351	18.308
420.00	27.419	38.665	18.719

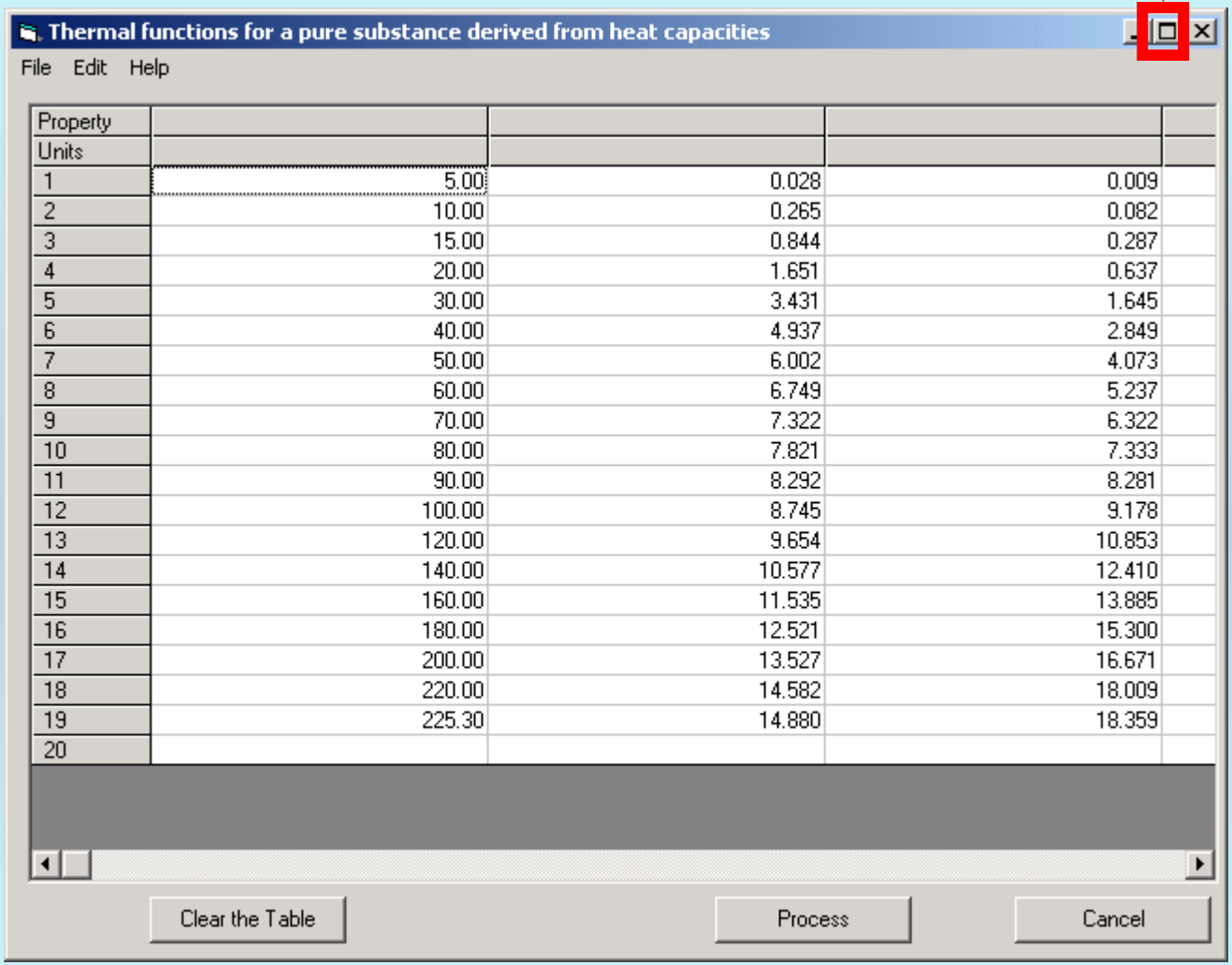
PASTE the data for the first phase (*crystals*, here) into the table.

DOUBLE CLICK in each box above the columns to select the Property and Units for each column from the menus, which appear after double clicking.

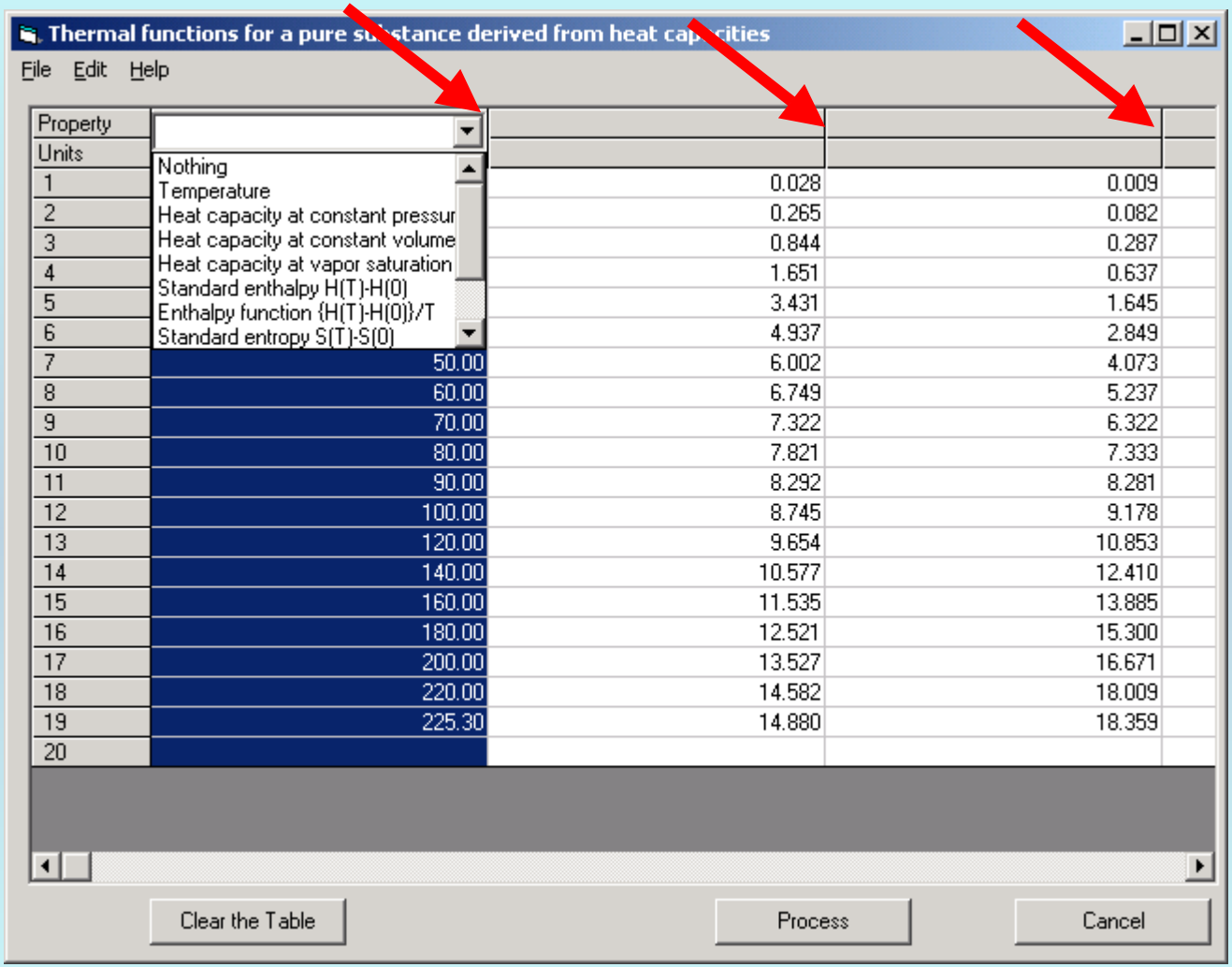


Property					
Units					
1	5.00	0.028	0.009	0.007	
2	10.00	0.265	0.082	0.062	
3	15.00	0.844	0.287	0.217	
4	20.00	1.651	0.637	0.472	
5	30.00	3.431	1.645	1.163	
6	40.00	4.937	2.849	1.928	
7	50.00	6.002	4.073	2.643	
8	60.00	6.749	5.237	3.268	
9	70.00	7.322	6.322	3.808	
10	80.00	7.821	7.333	4.279	
11	90.00	8.292	8.281	4.699	
12	100.00	8.745	9.178	5.081	
13	120.00	9.654	10.853	5.767	
14	140.00	10.577	12.410	6.388	
15	160.00	11.535	13.885	6.971	
16	180.00	12.521	15.300	7.533	
17	200.00	13.527	16.671	8.082	
18	220.00	14.582	18.009	8.624	
19	225.30	14.880	18.359	8.768	
20					

CLICK here to fill the screen with the table.

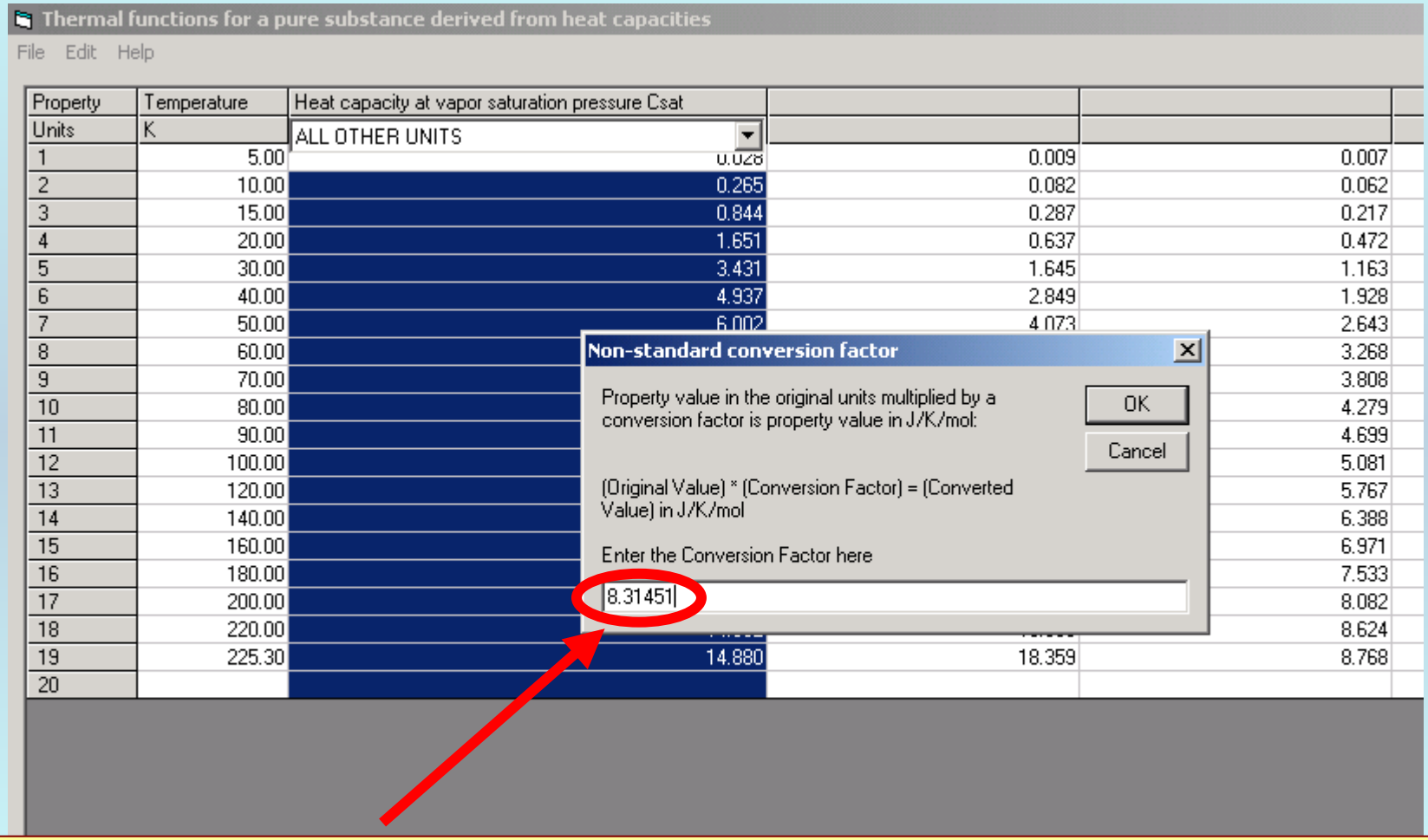


Some menu items are wide. Column widths can be adjusted by moving the dividers. This will allow the full text to be seen.

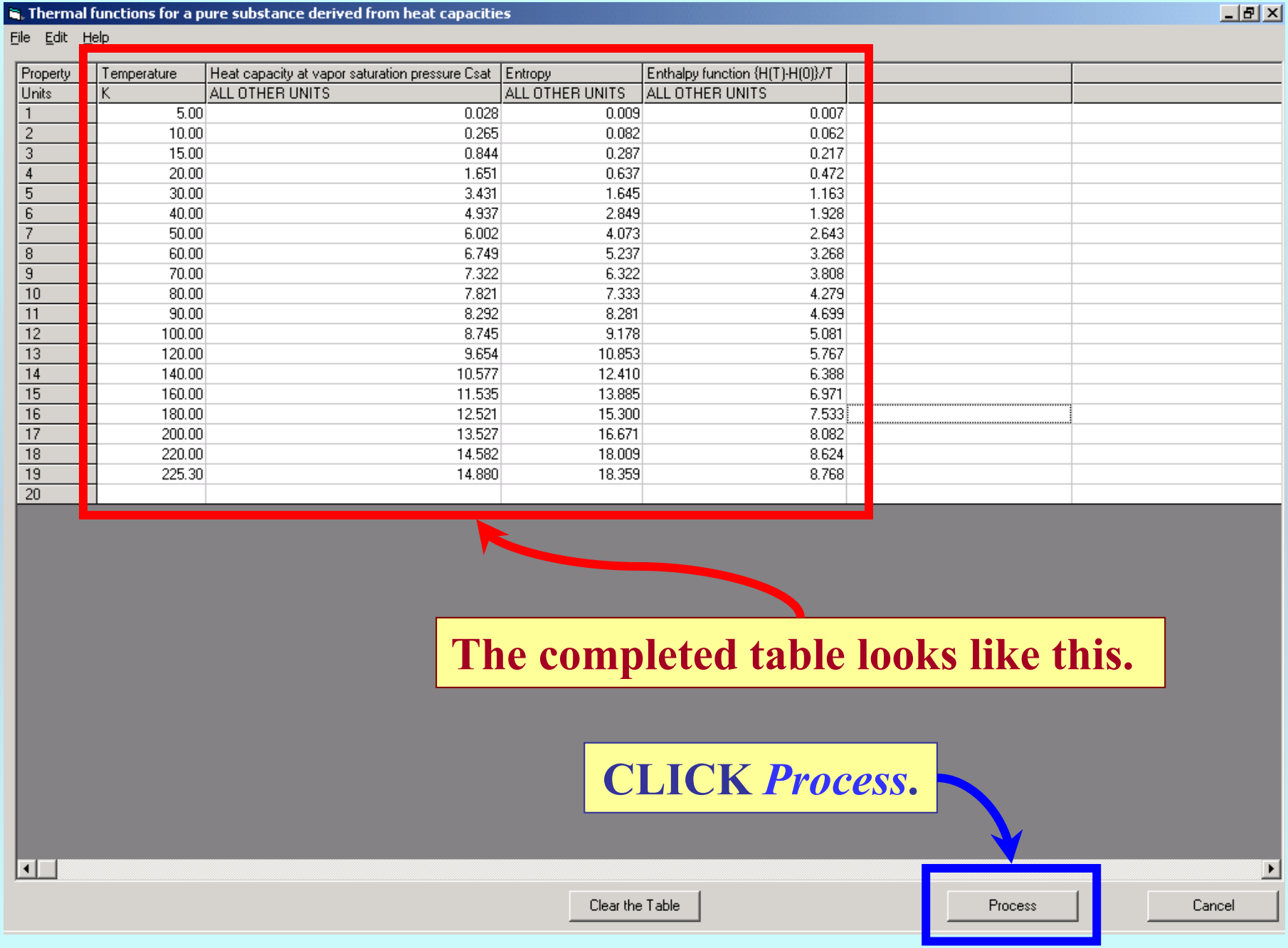


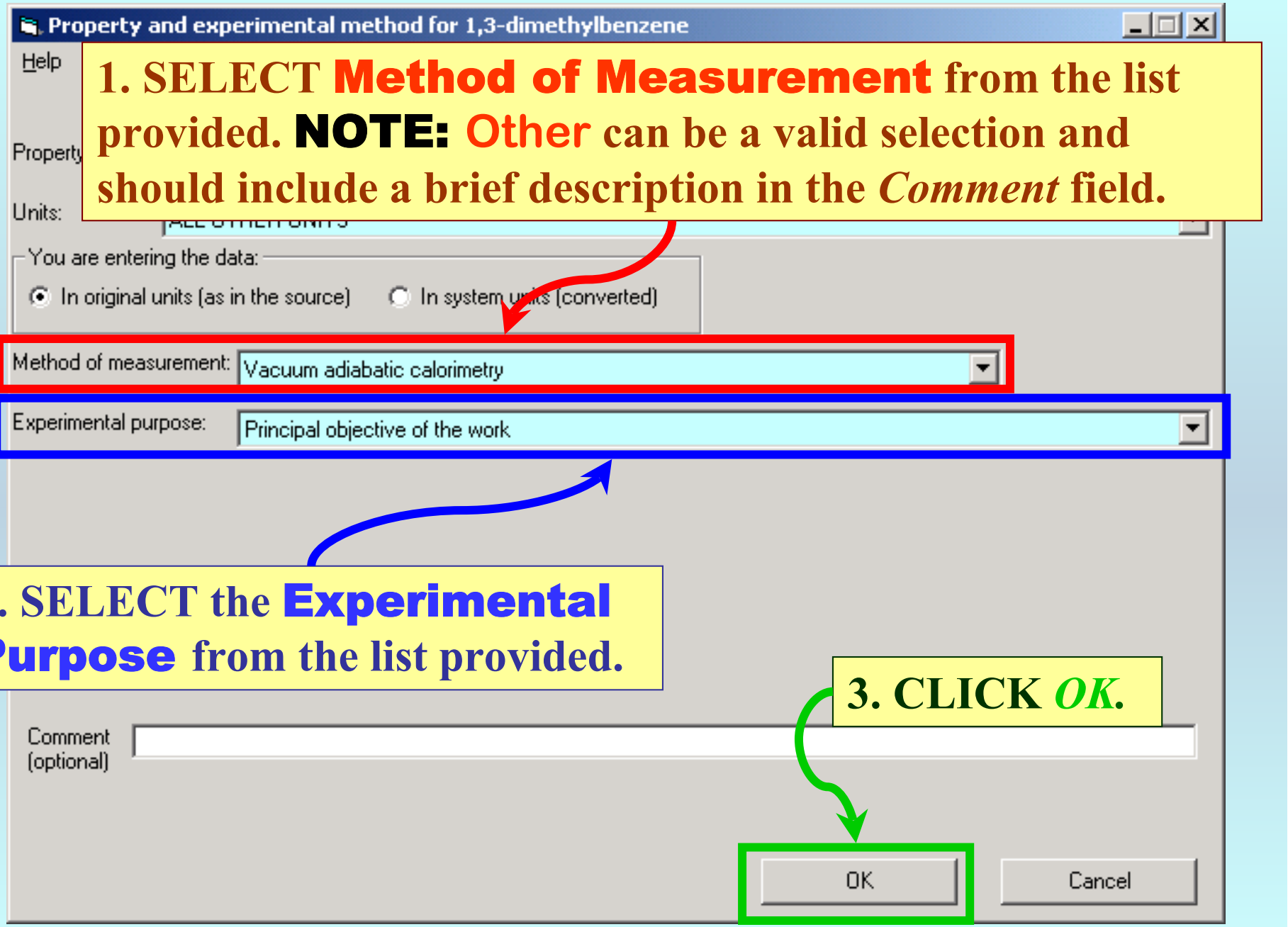
Property				
Units				
1		0.028	0.009	
2		0.265	0.082	
3		0.844	0.287	
4		1.651	0.637	
5		3.431	1.645	
6		4.937	2.849	
7	50.00	6.002	4.073	
8	60.00	6.749	5.237	
9	70.00	7.322	6.322	
10	80.00	7.821	7.333	
11	90.00	8.292	8.281	
12	100.00	8.745	9.178	
13	120.00	9.654	10.853	
14	140.00	10.577	12.410	
15	160.00	11.535	13.885	
16	180.00	12.521	15.300	
17	200.00	13.527	16.671	
18	220.00	14.582	18.009	
19	225.30	14.880	18.359	
20				

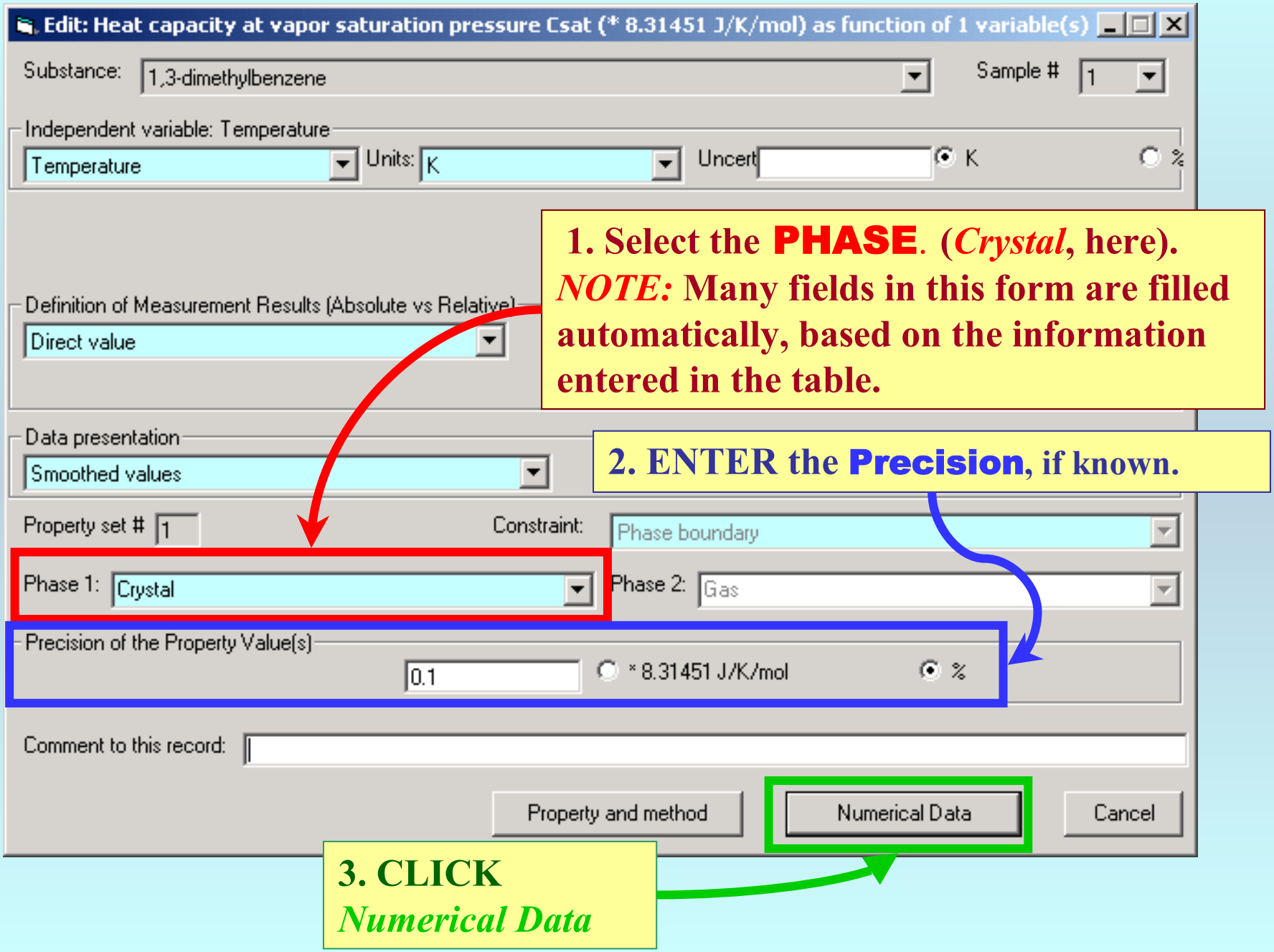
Non-standard units **can be used by selecting *ALL OTHER UNITS* from the menu and entering an appropriate conversion factor to the indicated unit.**

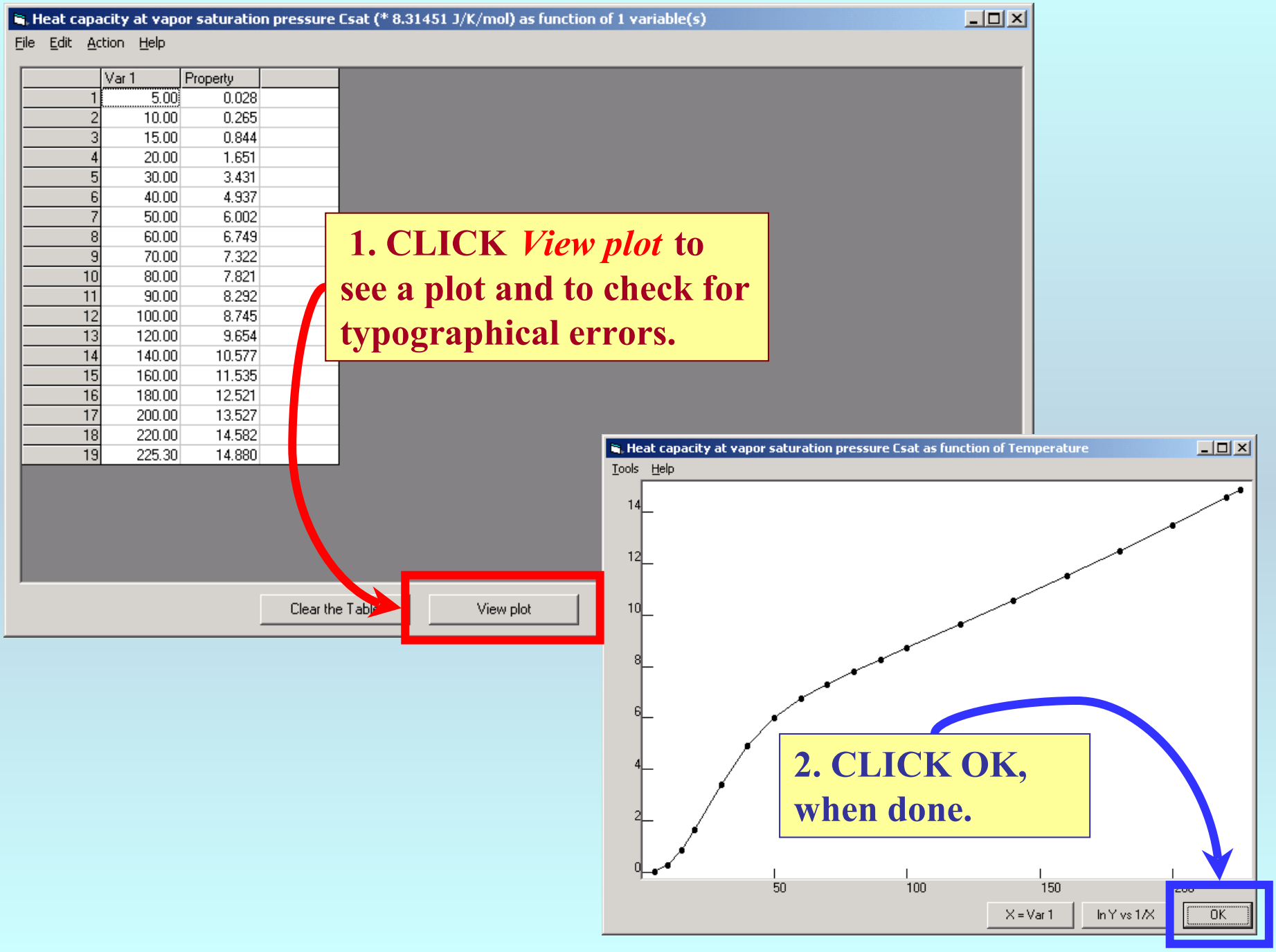


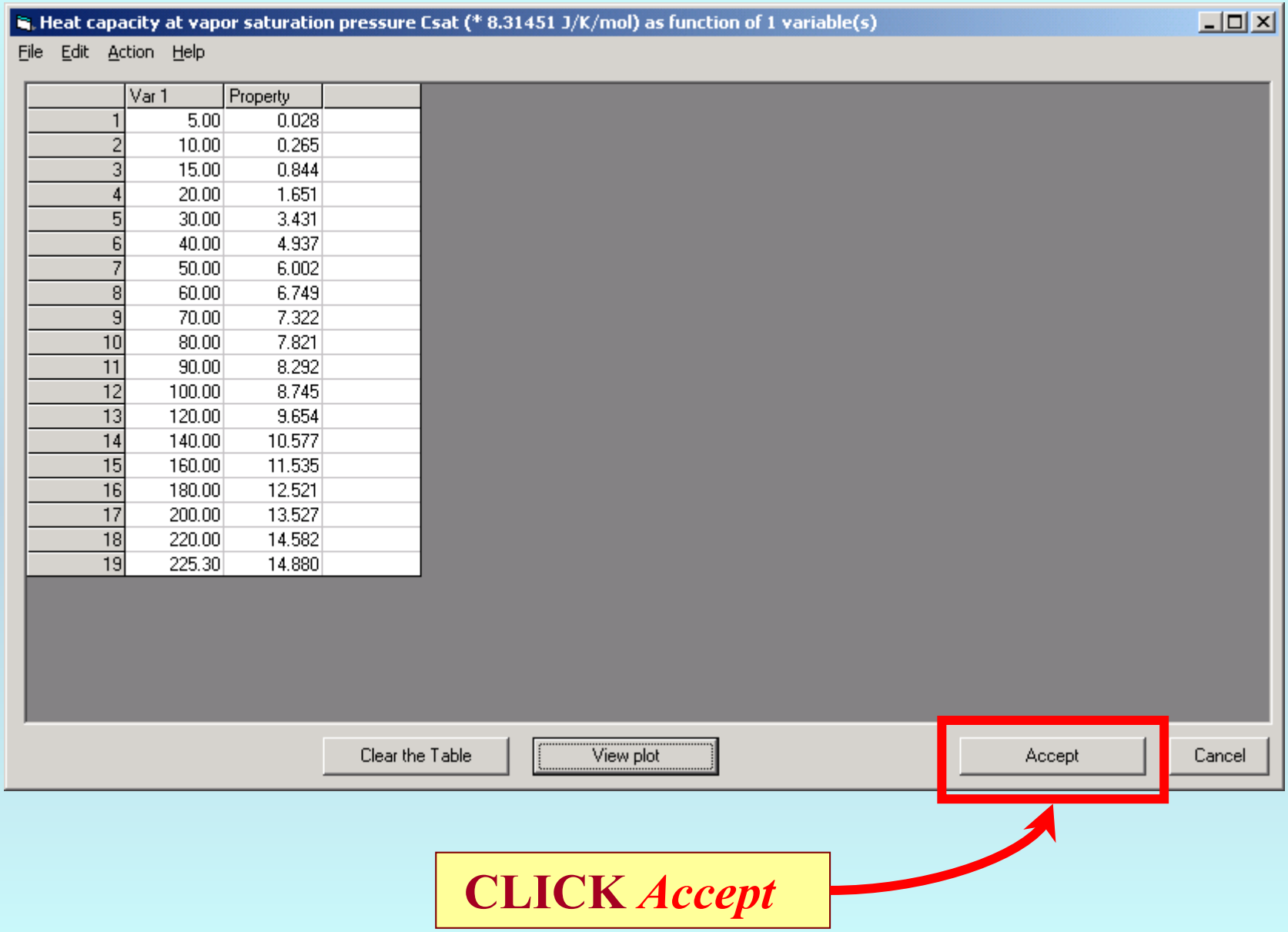
In the example, $C_{sat,m}/R$ values are converted to J/K/mol with the conversion factor 8.31451 given by the authors.


Thermal functions for a pure substance derived from heat capacities
File Edit Help
Property | Temperature | Heat capacity at vapor saturation pressure Csat | Entropy | Enthalpy function {H(T)-H(0)}/T
Units | K | ALL OTHER UNITS | ALL OTHER UNITS | ALL OTHER UNITS
1 5.00 0.028 0.009 0.007
2 10.00 0.265 0.082 0.062
3 15.00 0.844 0.287 0.217
4 20.00 1.651 0.637 0.472
5 30.00 3.431 1.645 1.163
6 40.00 4.937 2.849 1.928
7 50.00 6.002 4.073 2.643
8 60.00 6.749 5.237 3.268
9 70.00 7.322 6.322 3.808
10 80.00 7.821 7.333 4.279
11 90.00 8.292 8.281 4.699
12 100.00 8.745 9.178 5.081
13 120.00 9.654 10.853 5.767
14 140.00 10.577 12.410 6.388
15 160.00 11.535 13.885 6.971
16 180.00 12.521 15.300 7.533
17 200.00 13.527 16.671 8.082
18 220.00 14.582 18.009 8.624
19 225.30 14.880 18.359 8.768
20
The completed table looks like this.
CLICK Process.
Clear the Table
Process
Cancel

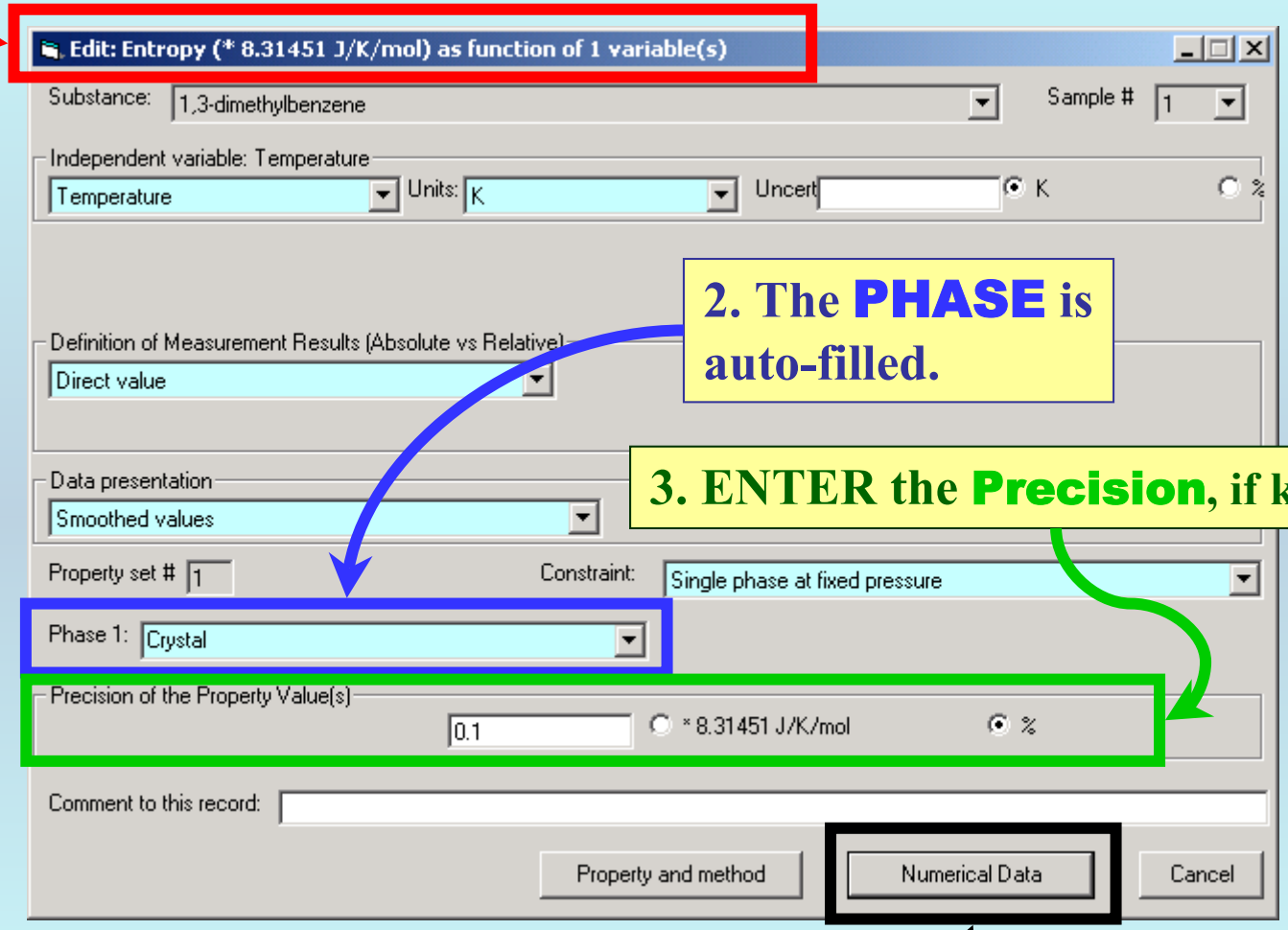

Property and experimental method for 1,3-dimethylbenzene
Help
Property
Units:
You are entering the data:
In original units (as in the source)
In system units (converted)
Method of measurement:
Vacuum adiabatic calorimetry
Experimental purpose:
Principal objective of the work
Comment (optional)
OK
Cancel
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.


Edit: Heat capacity at vapor saturation pressure Csat (* 8.31451 J/K/mol) as function of 1 variable(s)
Substance: 1,3-dimethylbenzene
Sample # 1
Independent variable: Temperature
Temperature
Units: K
Uncert
K
%
1. Select the PHASE. (Crystal, here).
NOTE: Many fields in this form are filled automatically, based on the information entered in the table.
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Smoothed values
2. ENTER the Precision, if known.
Property set # 1
Constraint:
Phase boundary
Phase 1: Crystal
Phase 2: Gas
Precision of the Property Value(s)
0.1
* 8.31451 J/K/mol
%
Comment to this record:
Property and method
Numerical Data
Cancel
3. CLICK
Numerical Data


Heat capacity at vapor saturation pressure Csat (* 8.31451 J/K/mol) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 5.00 0.028
2 10.00 0.265
3 15.00 0.844
4 20.00 1.651
5 30.00 3.431
6 40.00 4.937
7 50.00 6.002
8 60.00 6.749
9 70.00 7.322
10 80.00 7.821
11 90.00 8.292
12 100.00 8.745
13 120.00 9.654
14 140.00 10.577
15 160.00 11.535
16 180.00 12.521
17 200.00 13.527
18 220.00 14.582
19 225.30 14.880
1. CLICK View plot to see a plot and to check for typographical errors.
Clear the Table
View plot
Heat capacity at vapor saturation pressure Csat as function of Temperature
Tools Help
14
12
10
8
6
4
2
0
50
100
150
2. CLICK OK, when done.
X = Var 1
ln Y vs 1/X
OK


Heat capacity at vapor saturation pressure Csat (* 8.31451 J/K/mol) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 5.00 0.028
2 10.00 0.265
3 15.00 0.844
4 20.00 1.651
5 30.00 3.431
6 40.00 4.937
7 50.00 6.002
8 60.00 6.749
9 70.00 7.322
10 80.00 7.821
11 90.00 8.292
12 100.00 8.745
13 120.00 9.654
14 140.00 10.577
15 160.00 11.535
16 180.00 12.521
17 200.00 13.527
18 220.00 14.582
19 225.30 14.880
Clear the Table
View plot
Accept
Cancel
CLICK Accept

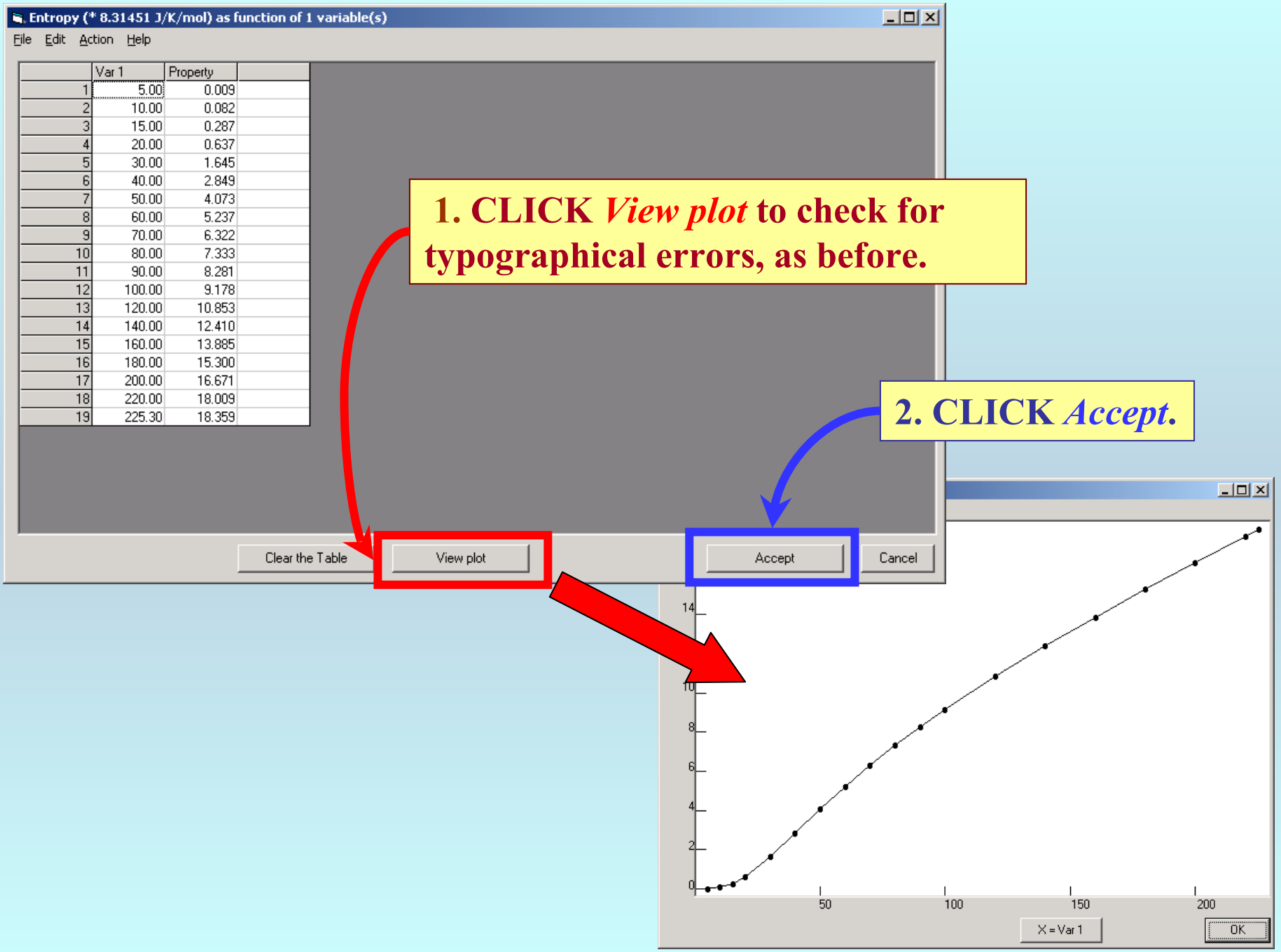
1. The form for the next column (*entropy*, here) will appear.



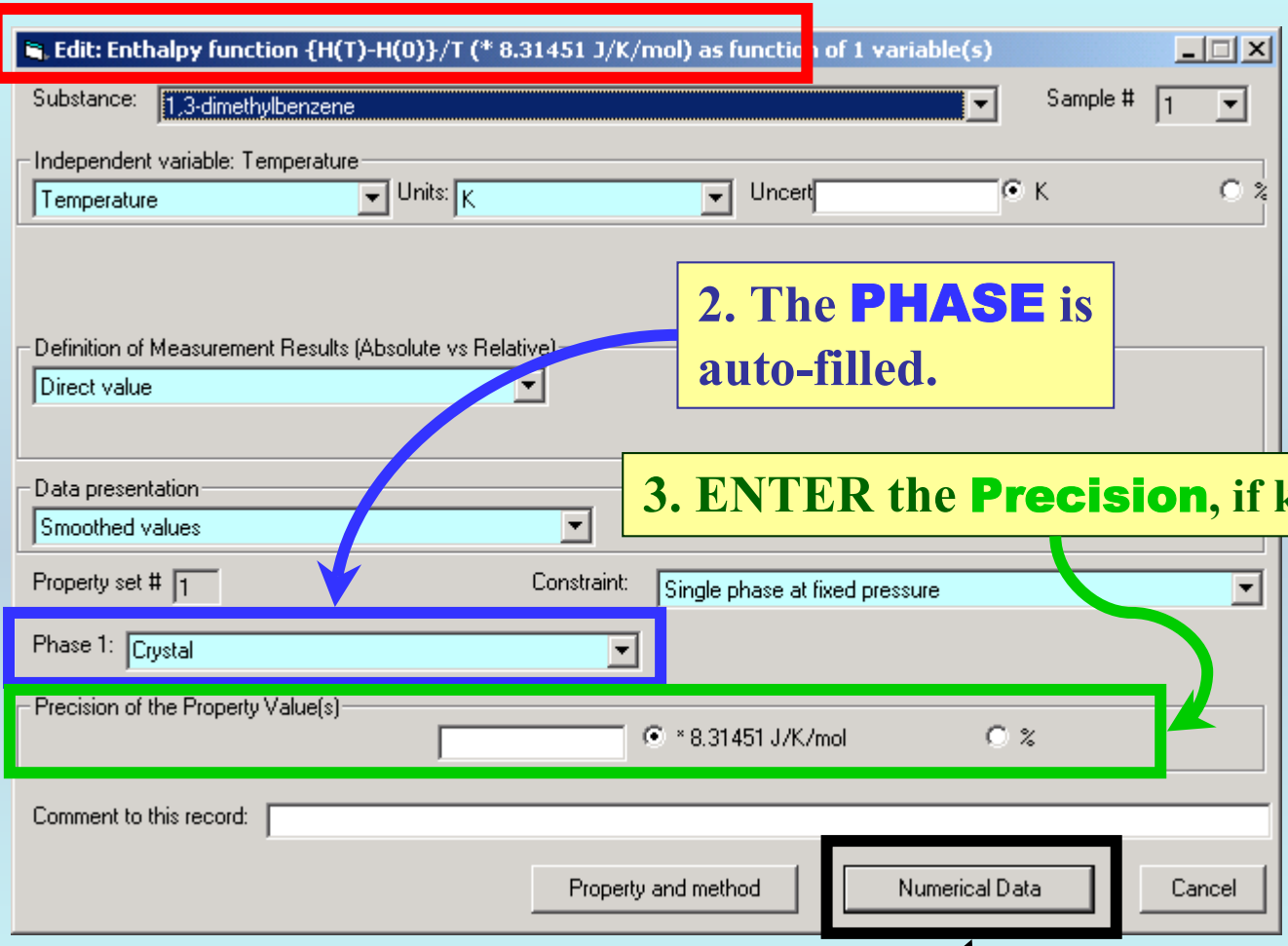
2. The **PHASE** is auto-filled.

3. ENTER the **Precision**, if known.

4. CLICK *Numerical Data*


Entropy (* 8.31451 J/K/mol) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 5.00 0.009
2 10.00 0.082
3 15.00 0.287
4 20.00 0.637
5 30.00 1.645
6 40.00 2.849
7 50.00 4.073
8 60.00 5.237
9 70.00 6.322
10 80.00 7.333
11 90.00 8.281
12 100.00 9.178
13 120.00 10.853
14 140.00 12.410
15 160.00 13.885
16 180.00 15.300
17 200.00 16.671
18 220.00 18.009
19 225.30 18.359
1. CLICK View plot to check for typographical errors, as before.
2. CLICK Accept.
Clear the Table
View plot
Accept
Cancel
14
10
8
6
4
2
0
50
100
150
200
X = Var 1
OK

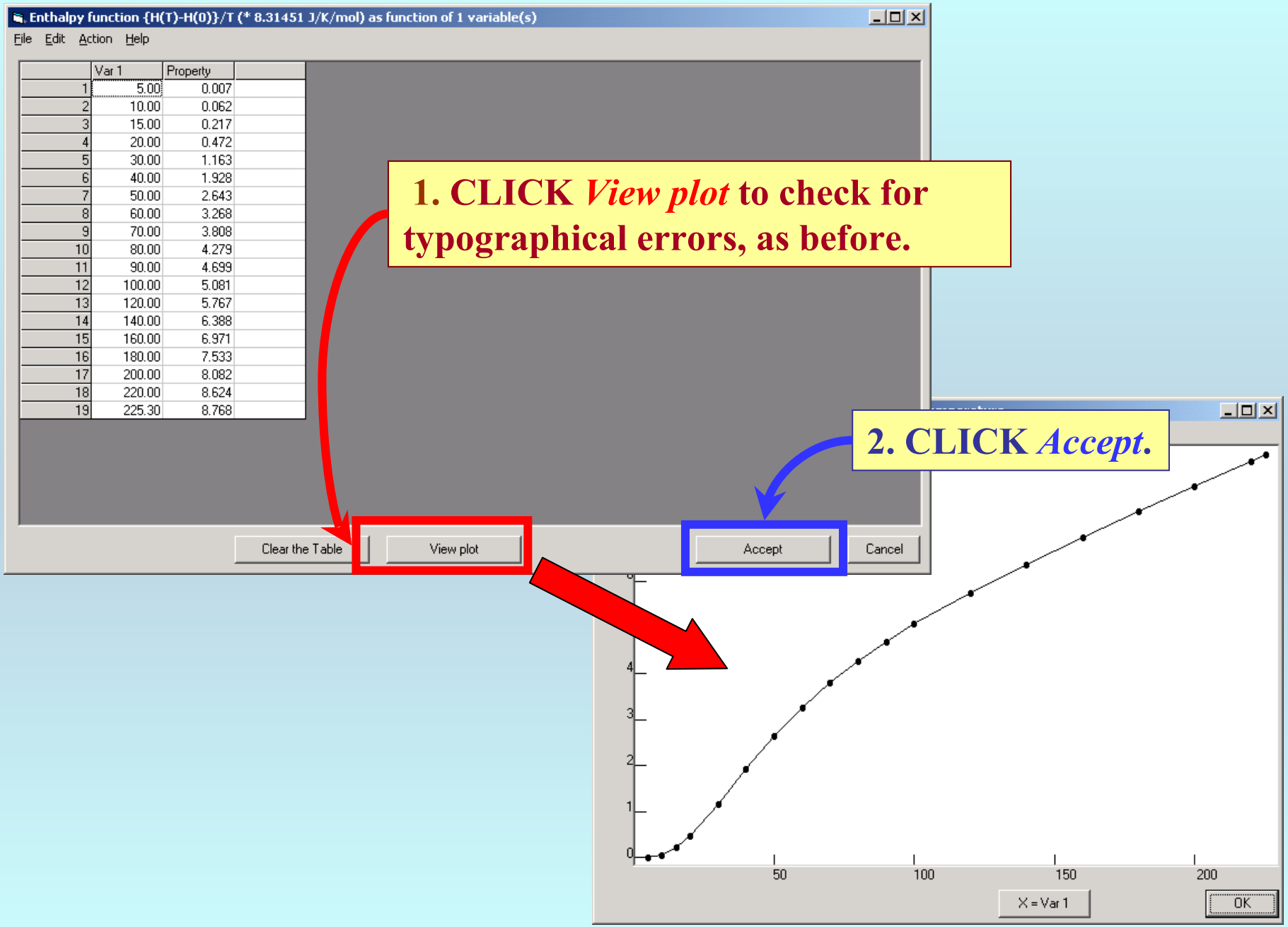
1. The form for the *final* column (*enthalpy function*, here) will appear.

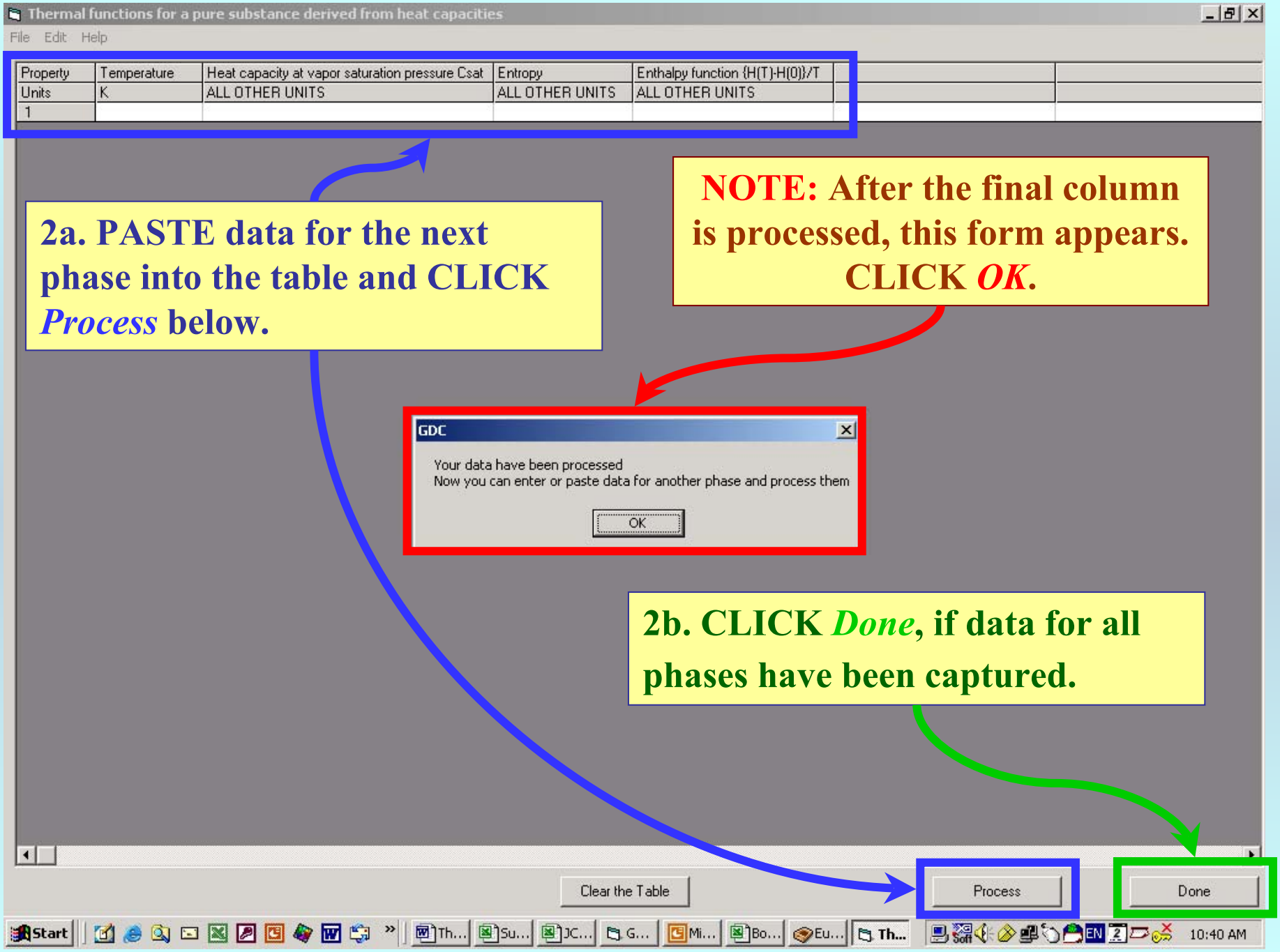


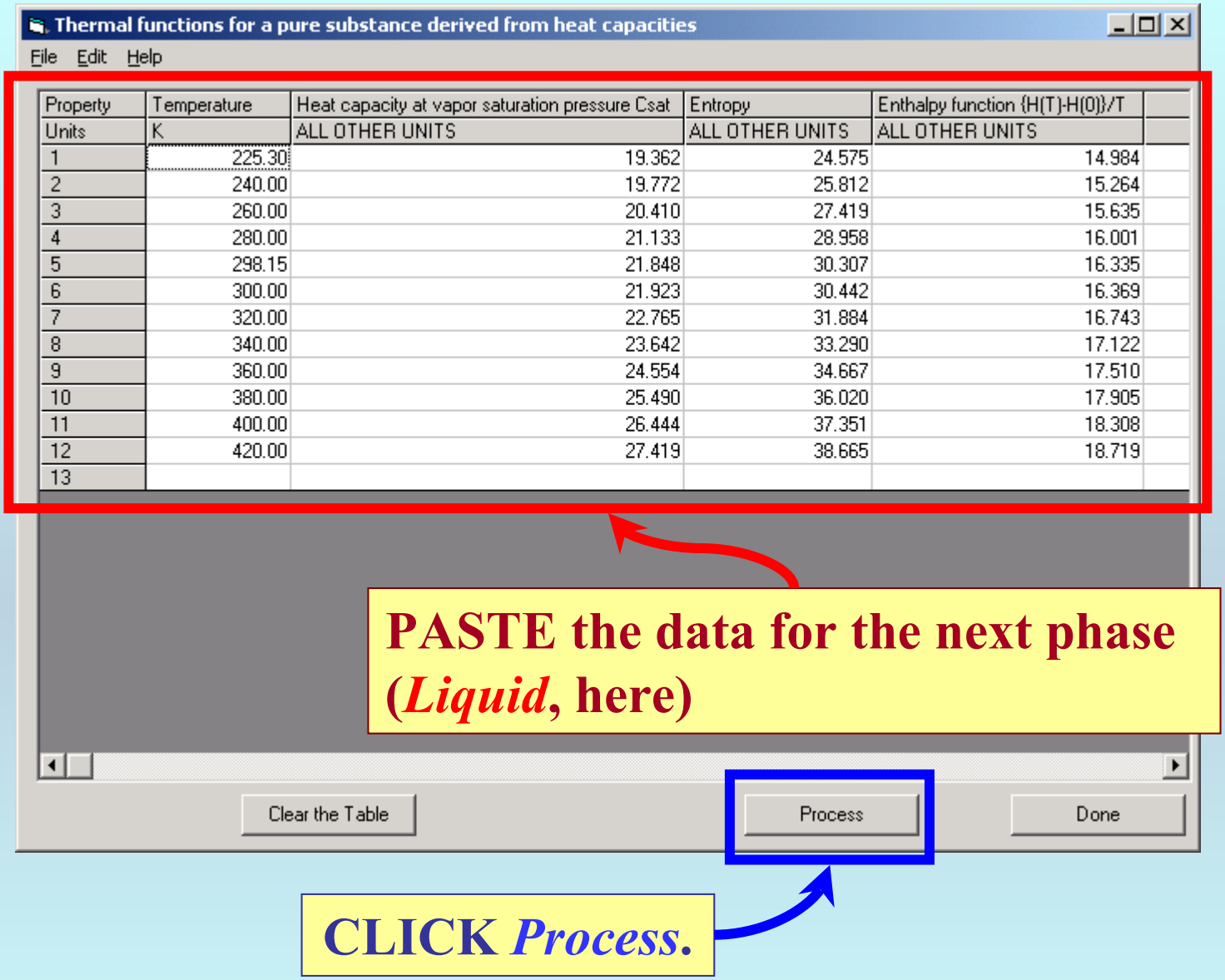
2. The **PHASE** is auto-filled.

3. ENTER the **Precision**, if known.

4. CLICK
Numerical Data

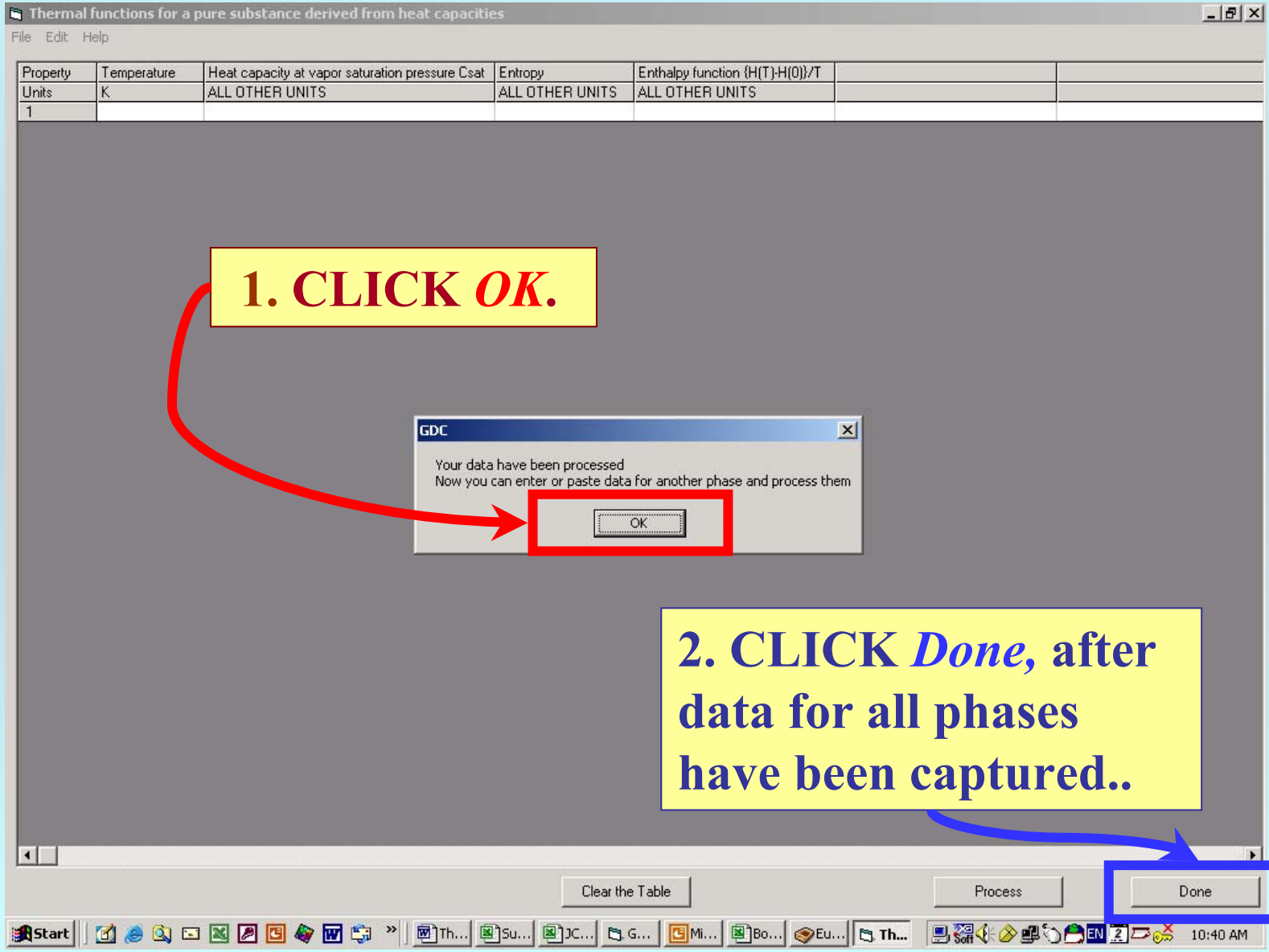

Enthalpy function {H(T)-H(0)}/T (* 8.31451 J/K/mol) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 5.00 0.007
2 10.00 0.062
3 15.00 0.217
4 20.00 0.472
5 30.00 1.163
6 40.00 1.928
7 50.00 2.643
8 60.00 3.268
9 70.00 3.808
10 80.00 4.279
11 90.00 4.699
12 100.00 5.081
13 120.00 5.767
14 140.00 6.388
15 160.00 6.971
16 180.00 7.533
17 200.00 8.082
18 220.00 8.624
19 225.30 8.768
1. CLICK View plot to check for typographical errors, as before.
2. CLICK Accept.
Clear the Table
View plot
Accept
Cancel
0
1
2
3
4
50
100
150
200
X = Var 1
OK

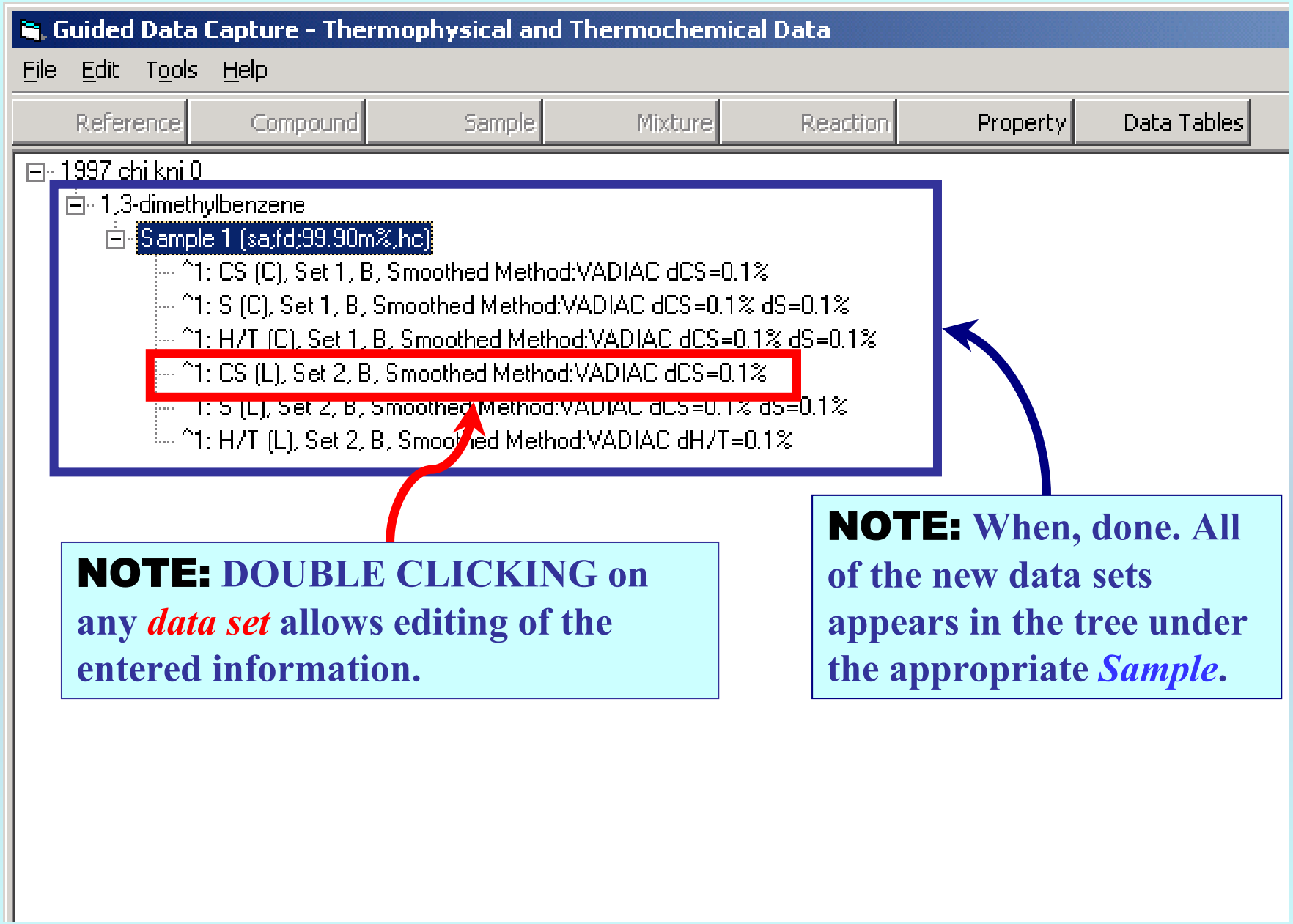

Thermal functions for a pure substance derived from heat capacities
File Edit Help
Property | Temperature | Heat capacity at vapor saturation pressure Csat | Entropy | Enthalpy function {H(T)-H(0)}/T
Units | K | ALL OTHER UNITS | ALL OTHER UNITS | ALL OTHER UNITS
1
2a. PASTE data for the next phase into the table and CLICK Process below.
NOTE: After the final column is processed, this form appears. CLICK OK.
GDC
Your data have been processed
Now you can enter or paste data for another phase and process them
OK
2b. CLICK Done, if data for all phases have been captured.
Clear the Table
Process
Done
Start
10:40 AM



Data capture continues for the next phase exactly as shown in pages 13 through 22 of this PDF example.

When data capture for the phase is complete, this screen will reappear. Continue with any additional PHASES or CLICK OK and Done, as indicated below.




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property Data Tables
1997 chi kni 0
1,3-dimethylbenzene
Sample 1 (sa;fd;99.90m%;hc)
^1: CS (C), Set 1, B, Smoothed Method:VADIAC dCS=0.1%
^1: S (C), Set 1, B, Smoothed Method:VADIAC dCS=0.1% dS=0.1%
^1: H/T (C), Set 1, B, Smoothed Method:VADIAC dCS=0.1% dS=0.1%
^1: CS (L), Set 2, B, Smoothed Method:VADIAC dCS=0.1%
^1: S (L), Set 2, B, Smoothed Method:VADIAC dCS=0.1% dS=0.1%
^1: H/T (L), Set 2, B, Smoothed Method:VADIAC dH/T=0.1%
NOTE: DOUBLE CLICKING on any data set allows editing of the entered information.
NOTE: When, done. All of the new data sets appears in the tree under the appropriate Sample.

END

Continue with other compounds, samples, properties, reactions, etc...

***or* save your file and exit the program.**