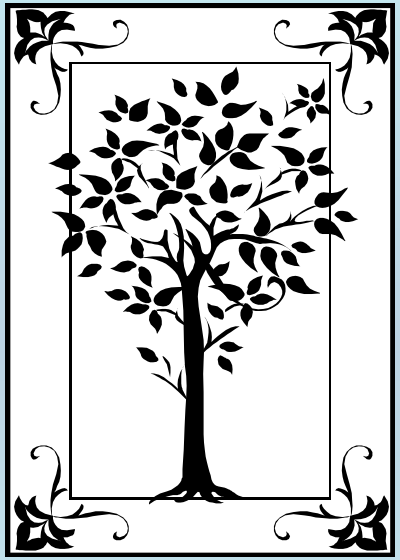
METADATA AND NUMERICAL DATA CAPTURE:
Enthalpy Increments
H(T, p) – H(T', p')

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Enthalpy Increments** ***H(T,p) – H(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:

348 *J. Chem. Eng. Data* 2000, *45,* 348−352

Specific Enthalpy Increments for Pentan-1-ol at Temperatures up to 623.2 K and 10.1 MPa

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Measurements of specific enthalpy increments for pentan-1-ol are reported. A countercurrent water-cooled flow calorimeter was used to measure 102 enthalpy increments over the temperature range 448.2 K to 623.2 K at pressures from 0.1 MPa up to 10.1 MPa. Extrapolation of the gas-phase measurements to zero pressure gave values in excellent agreement with pure component ideal gas enthalpies calculated by extrapolating data on lower alcohols. Values of the specific enthalpy of vaporization derived from the measurements are in agreement with other work and are well fitted by a modification of the Watson equation. A method for the calculation of the two-phase enthalpy−pressure envelope is described.

Enthalpy Increments for **Pentan-1-ol** as a function of ***T*** and ***p***

Table 1. Specific Enthalpy Increments Δh/(kJ·kg^{-1}) for Pentan-1-ol Measured Relative to the Saturation Pressure p_s of the Liquid at the Standard Temperature 298.15 K

T/K	p/MPa	Δh/kJ·kg^{-1}	p/MPa	Δh/kJ·kg^{-1}	p/MPa	Δh/kJ·kg^{-1}	p/MPa	Δh/kJ·kg^{-1}	p/MPa	Δh/kJ·kg^{-1}
448.2	0.25	895	0.77	437	4.32	440	6.50	438	9.32	436
473.2	0.20	947	0.46	927	1.13	517	4.36	518	6.63	51[illegible]
	0.35	937	0.64	527	2.94	519	5.61	517		
498.2	0.17	1005	0.47	995	0.74	970	2.10	600	7.15	6[illegible]4
	0.34	1000	0.57	991	1.20	600	2.78	598	10.1	[illegible]95
523.2	0.15	1072	0.74	1044	1.35	1013	4.07	696	8.18	691
	0.49	1057	1.10	1022	2.33	703	5.38	690	10.1	685
548.2	0.12	1137	0.77	1123	1.88	1070	3.46	798	5.38	786
	0.52	1117	1.29	1103	2.52	800	4.03	790	8.38	785
573.2	0.11	1185	2.72	1112	3.96	905	5.67	885	7.63	872
	0.77	1175	3.50	918	5.12	889	5.98	883	8.31	871
	1.32	1162	3.75	910	5.23	888	6.63	881	9.50	870
586.2	0.11	1221	3.18	1127	4.50	942	5.67	937	8.31	924
	0.78	1210	3.50	1111	5.12	941	5.98	935	9.52	925
	1.33	1197	3.85	970	5.23	940	6.63	93[illegible]		
	2.72	1152	3.96	957	5.48	938	7.63	9[illegible]4		
598.2	0.15	1259	4.13	1106	4.71	1015	5.96	9[illegible]7	10.1	966
	1.09	1232	4.32	1079	5.25	995	6.50	[illegible]81		
	2.59	1200	4.51	1048	5.48	992	8.00	[illegible]68		
	3.84	1135	4.66	1026	5.62	989	9.26	[illegible]68		
623.2	0.40	1307	2.56	1274	5.35	1116	8.96	[illegible]075		
	1.33	1293	4.00	1222	6.63	1086	10.0	[illegible]070		

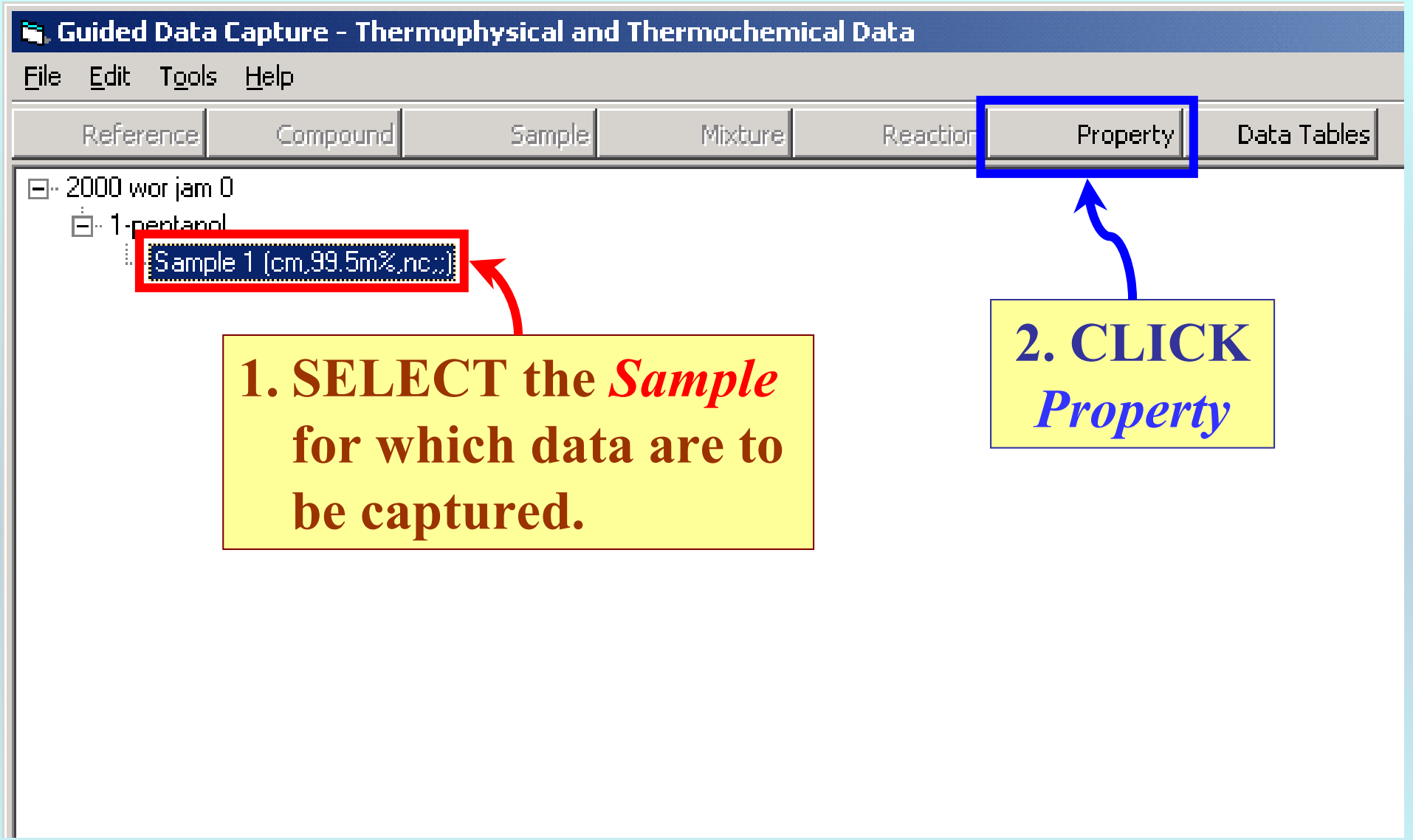
This data set is considered here.

NOTE: For $T = 298.15$ K, $p_{sat} = 0.2$ kPa

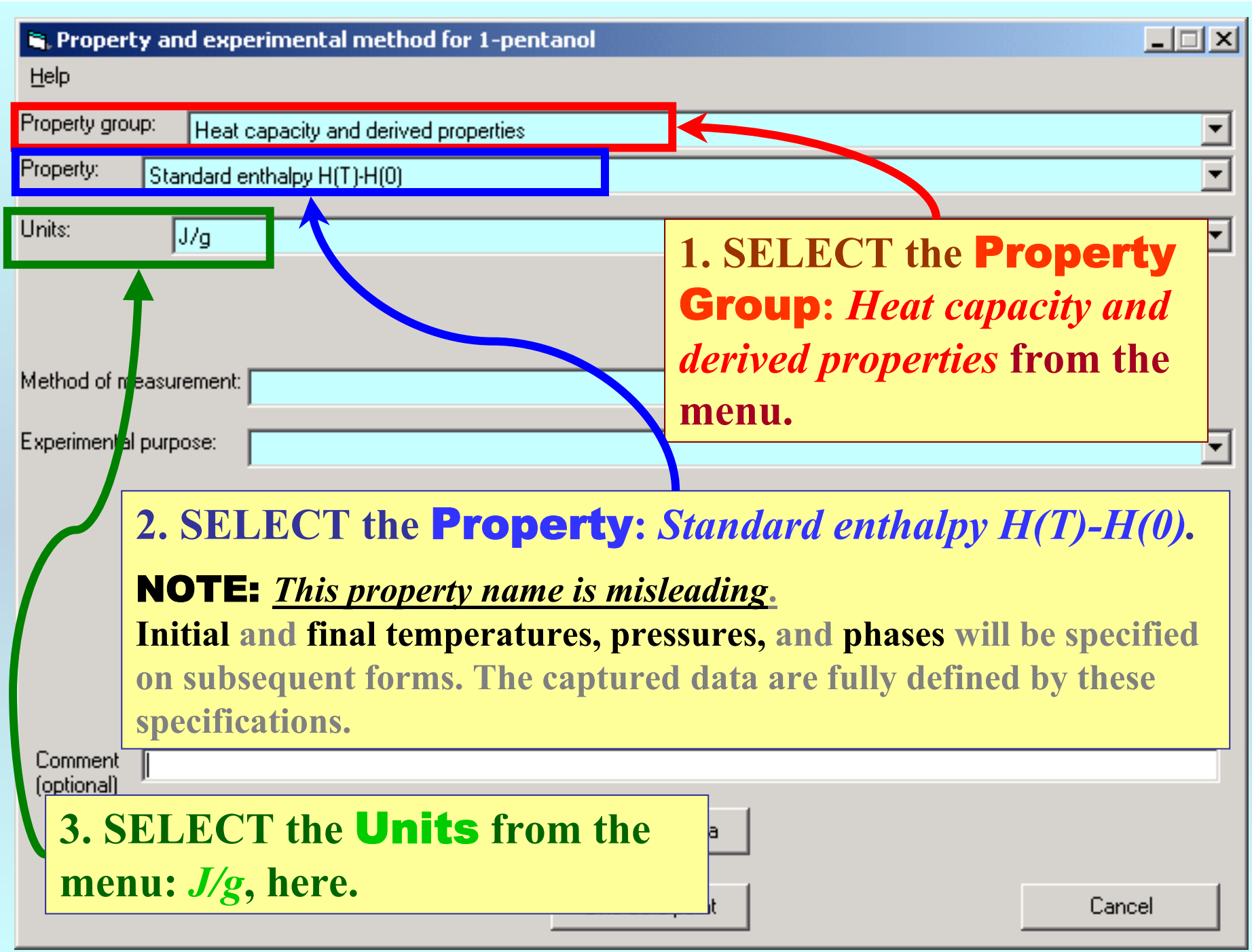
Experimental Method and Uncertainty Information:

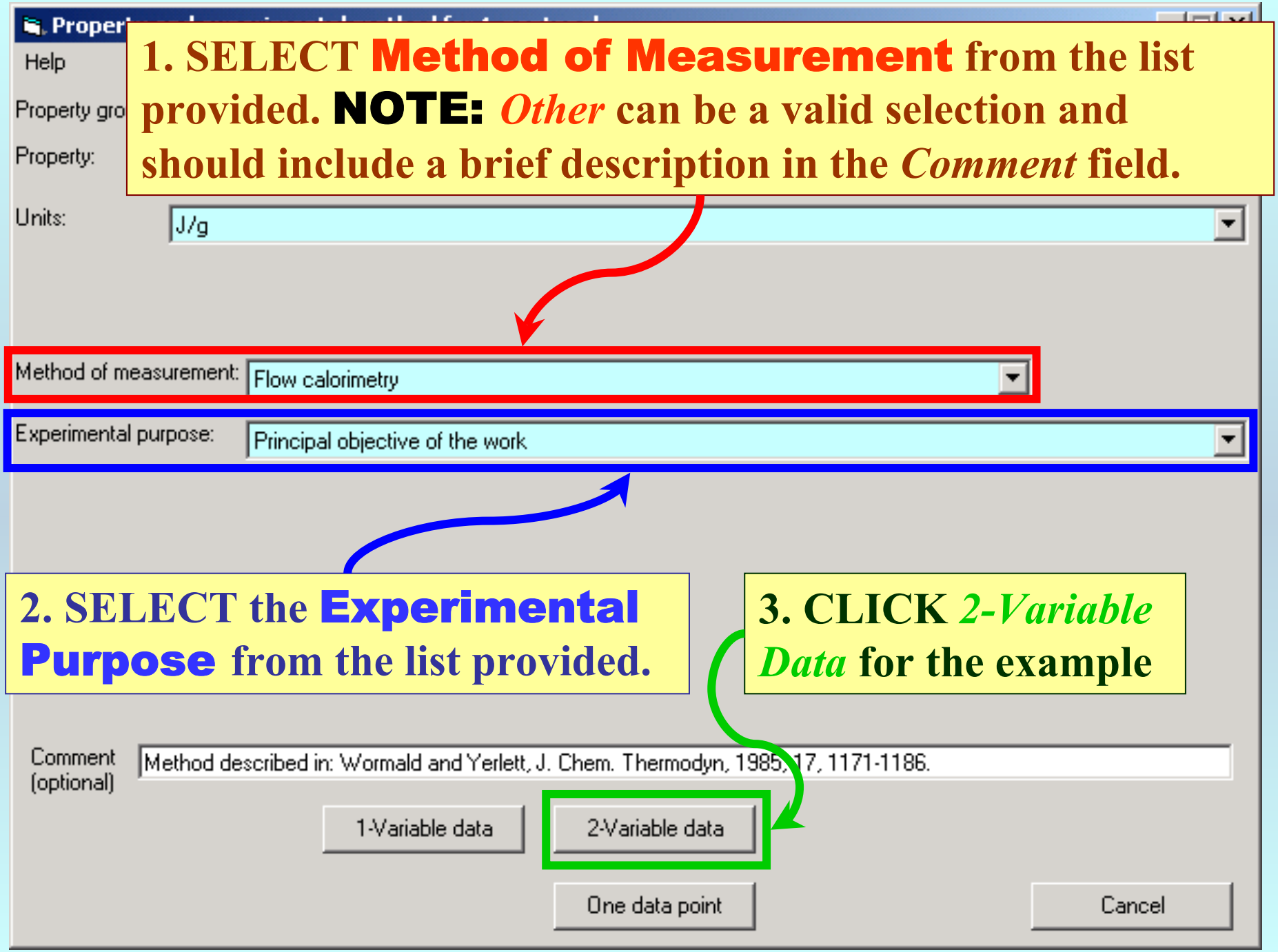
Enthalpy increments were measured with the counter-current heat-exchange calorimetric apparatus described previously (Wormald and Yerlett, 1985).

Systematic errors on the measurements are estimated to be no greater than ± 1 kJ·kg^{-1}. Random errors arose mainly from fluctuations in the operation of the metering pump supplying the alcohol and were estimated to be ± 3 kJ·kg^{-1}.



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 1-pentanol
Help
Property group:
Heat capacity and derived properties
Property:
Standard enthalpy H(T)-H(0)
Units:
J/g
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Heat capacity and derived properties from the menu.
2. SELECT the Property: Standard enthalpy H(T)-H(0).
NOTE: This property name is misleading.
Initial and final temperatures, pressures, and phases will be specified on subsequent forms. The captured data are fully defined by these specifications.
Comment (optional)
3. SELECT the Units from the menu: J/g, here.
Cancel

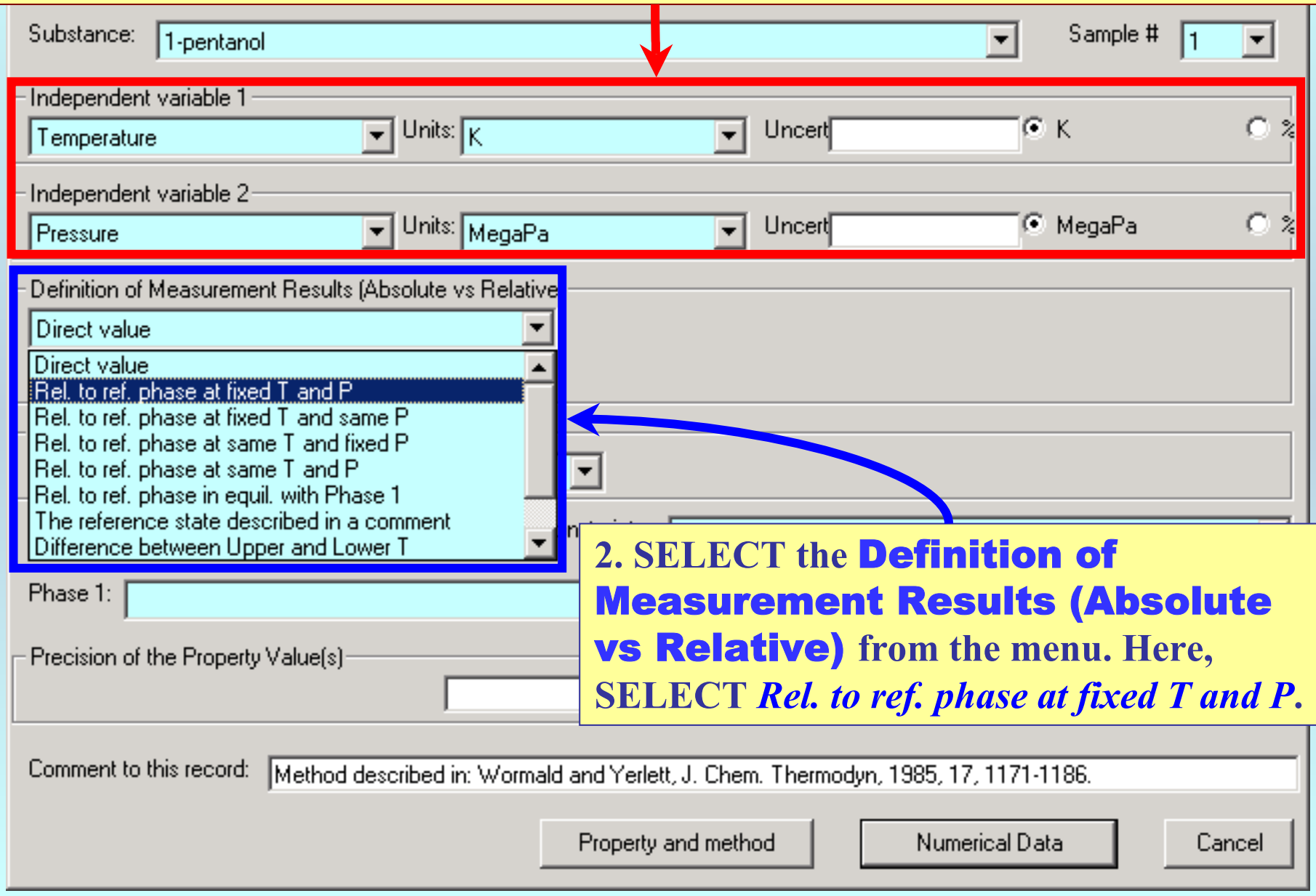


1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the *Comment* field.

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

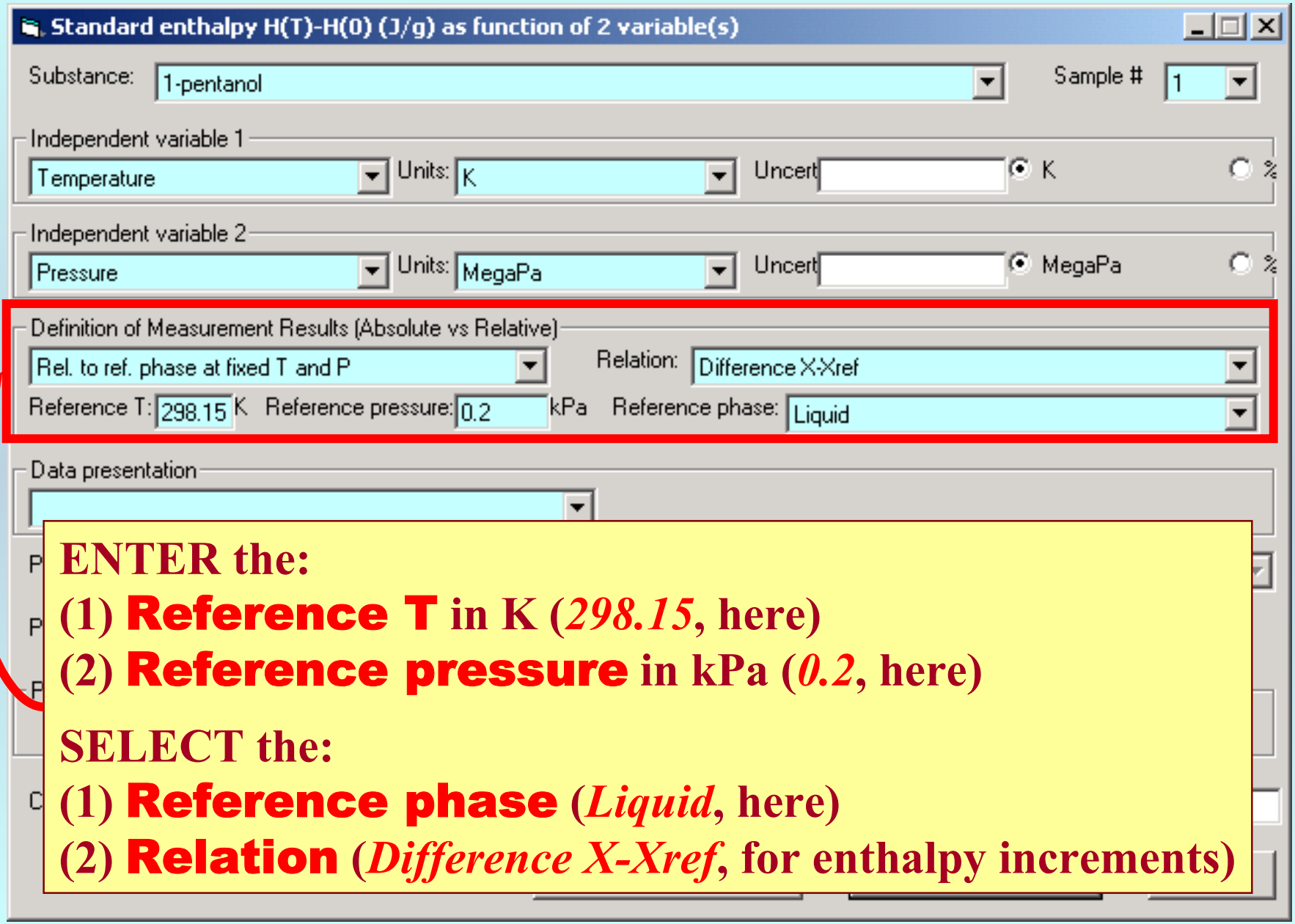
3. CLICK *2-Variable Data* for the example

1. SELECT the Independent variable(s) with Units; *Temperature* (*K*) and *Pressure* (*MegaPa*), here. Include Uncertainties, if known.



2. SELECT the Definition of Measurement Results (Absolute vs Relative) from the menu. Here, SELECT *Rel. to ref. phase at fixed T and P*.

NOTE: Additional fields appear



ENTER the:

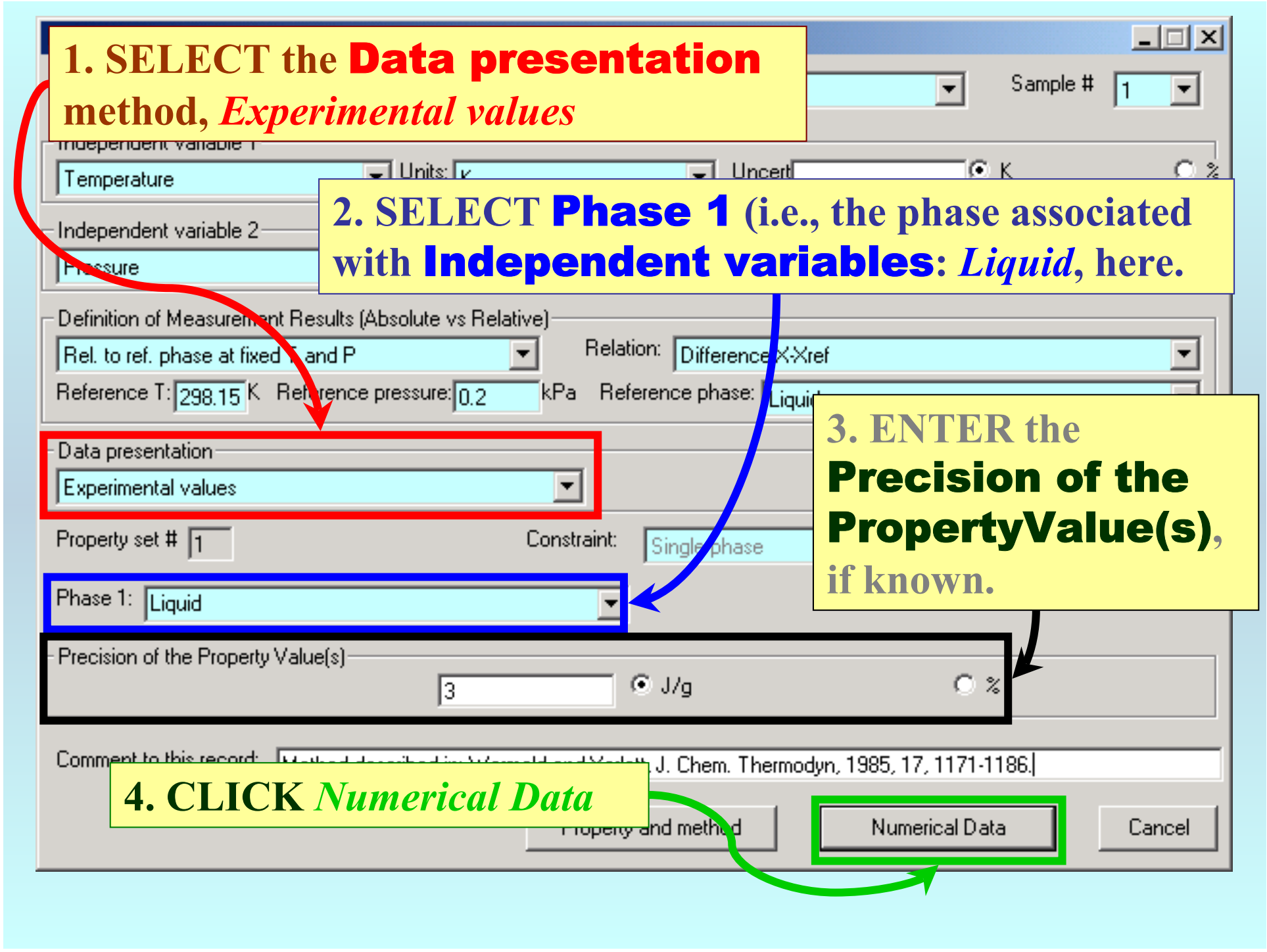
(1) **Reference T** in K (*298.15*, here)

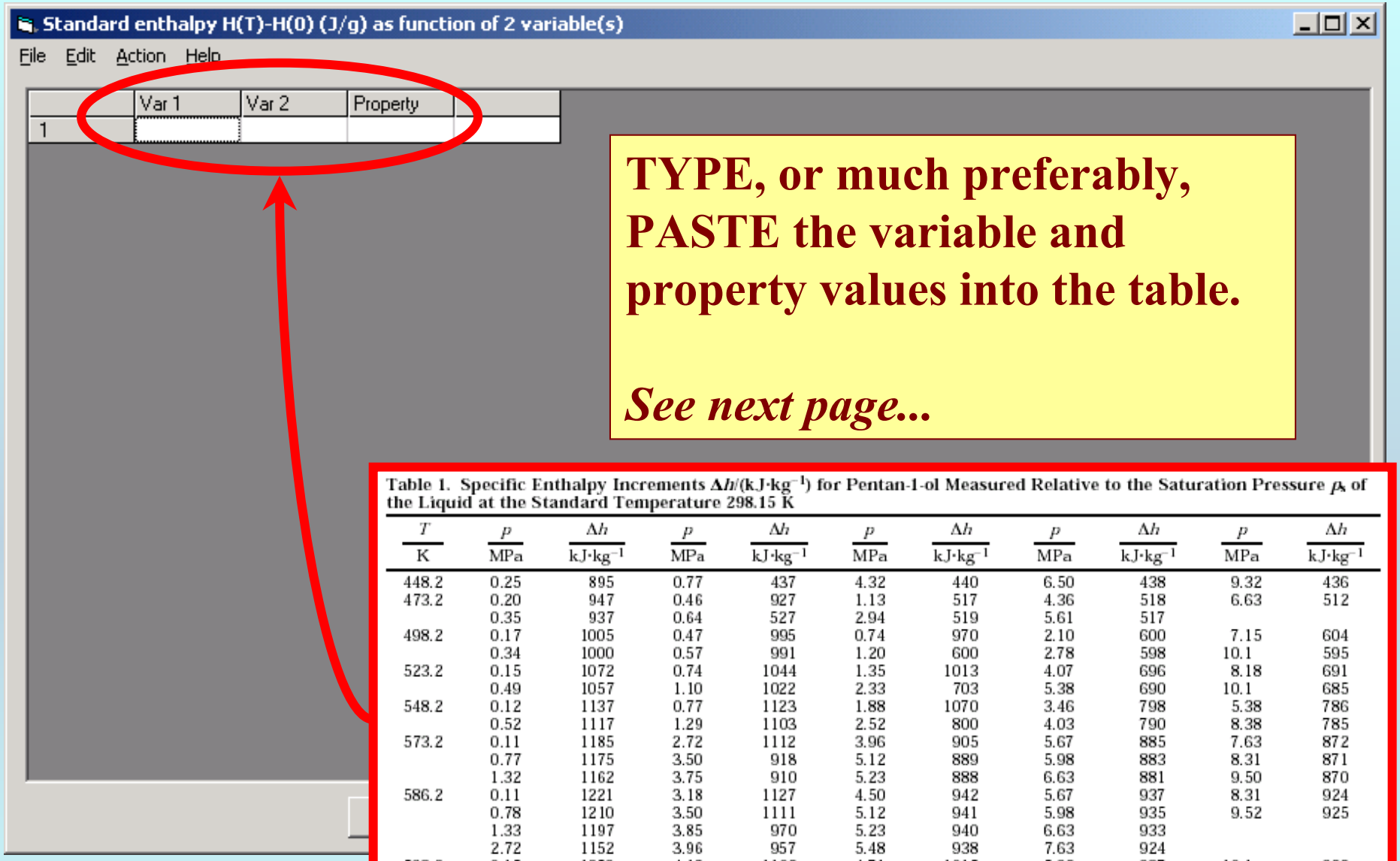
(2) **Reference pressure** in kPa (*0.2*, here)

SELECT the:

(1) **Reference phase** (*Liquid*, here)

(2) **Relation** (*Difference X-Xref*, for enthalpy increments)


1. SELECT the Data presentation method, Experimental values
2. SELECT Phase 1 (i.e., the phase associated with Independent variables: Liquid, here.
3. ENTER the Precision of the PropertyValue(s), if known.
4. CLICK Numerical Data
Sample #
1
Temperature
Units:
Uncert
K
%
Independent variable 2
Definition of Measurement Results (Absolute vs Relative)
Rel. to ref. phase at fixed T and P
Relation:
Difference X-Xref
Reference T:
298.15
K
Reference pressure:
0.2
kPa
Reference phase:
Data presentation
Experimental values
Property set #
1
Constraint:
Single phase
Phase 1:
Liquid
Precision of the Property Value(s)
3
J/g
%
Comment to this record:
J. Chem. Thermodyn, 1985, 17, 1171-1186.
Property and method
Numerical Data
Cancel



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

See next page...

Table 1. Specific Enthalpy Increments Δh/(kJ·kg^{-1}) for Pentan-1-ol Measured Relative to the Saturation Pressure p_s of the Liquid at the Standard Temperature 298.15 K

T/K	p/MPa	Δh/kJ·kg^{-1}	p/MPa	Δh/kJ·kg^{-1}	p/MPa	Δh/kJ·kg^{-1}	p/MPa	Δh/kJ·kg^{-1}	p/MPa	Δh/kJ·kg^{-1}
448.2	0.25	895	0.77	437	4.32	440	6.50	438	9.32	436
473.2	0.20	947	0.46	927	1.13	517	4.36	518	6.63	512
	0.35	937	0.64	527	2.94	519	5.61	517		
498.2	0.17	1005	0.47	995	0.74	970	2.10	600	7.15	604
	0.34	1000	0.57	991	1.20	600	2.78	598	10.1	595
523.2	0.15	1072	0.74	1044	1.35	1013	4.07	696	8.18	691
	0.49	1057	1.10	1022	2.33	703	5.38	690	10.1	685
548.2	0.12	1137	0.77	1123	1.88	1070	3.46	798	5.38	786
	0.52	1117	1.29	1103	2.52	800	4.03	790	8.38	785
573.2	0.11	1185	2.72	1112	3.96	905	5.67	885	7.63	872
	0.77	1175	3.50	918	5.12	889	5.98	883	8.31	871
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	1.33	1197	3.85	970	5.23	940	6.63	933		
	2.72	1152	3.96	957	5.48	938	7.63	924		
598.2	0.15	1259	4.13	1106	4.71	1015	5.96	987	10.1	966
	1.09	1232	4.32	1079	5.25	995	6.50	981		
	2.59	1200	4.51	1048	5.48	992	8.00	968		
	3.84	1135	4.66	1026	5.62	989	9.26	968		
623.2	0.40	1307	2.56	1274	5.35	1116	8.96	1075		
	1.33	1293	4.00	1222	6.63	1086	10.0	1070		

Standard enthalpy H(T)-H(0) (J/g) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	448.2	0.25	895
2	448.2	0.77	437
3	448.2	4.32	440
4	448.2	6.50	438
5	448.2	9.32	436
6	473.2	0.20	947
7	473.2	0.35	937
8	473.2	0.46	927
9	473.2	0.64	527
10	473.2	1.13	517
11	473.2	2.94	519
12	473.2	4.36	518
13	473.2	5.61	517
14	473.2	6.63	512
15	498.2	0.17	1005
16	498.2	0.34	1000
17	498.2	0.47	995
18	498.2	0.57	991
19	498.2	0.74	970
20	498.2	1.20	600
21	498.2	2.10	600
22	498.2	2.78	598
23	498.2	7.15	604
24	498.2	10.10	595
25	523.2	0.15	1072

Clear the

Table 1. Specific Enthalpy Increments Δh/(kJ·kg^{-1}) for Pentan-1-ol Measured Relative to the Saturation Pressure p_s of the Liquid at the Standard Temperature 298.15 K

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	1.33	1197	3.85	970	5.23	940	6.63	933		
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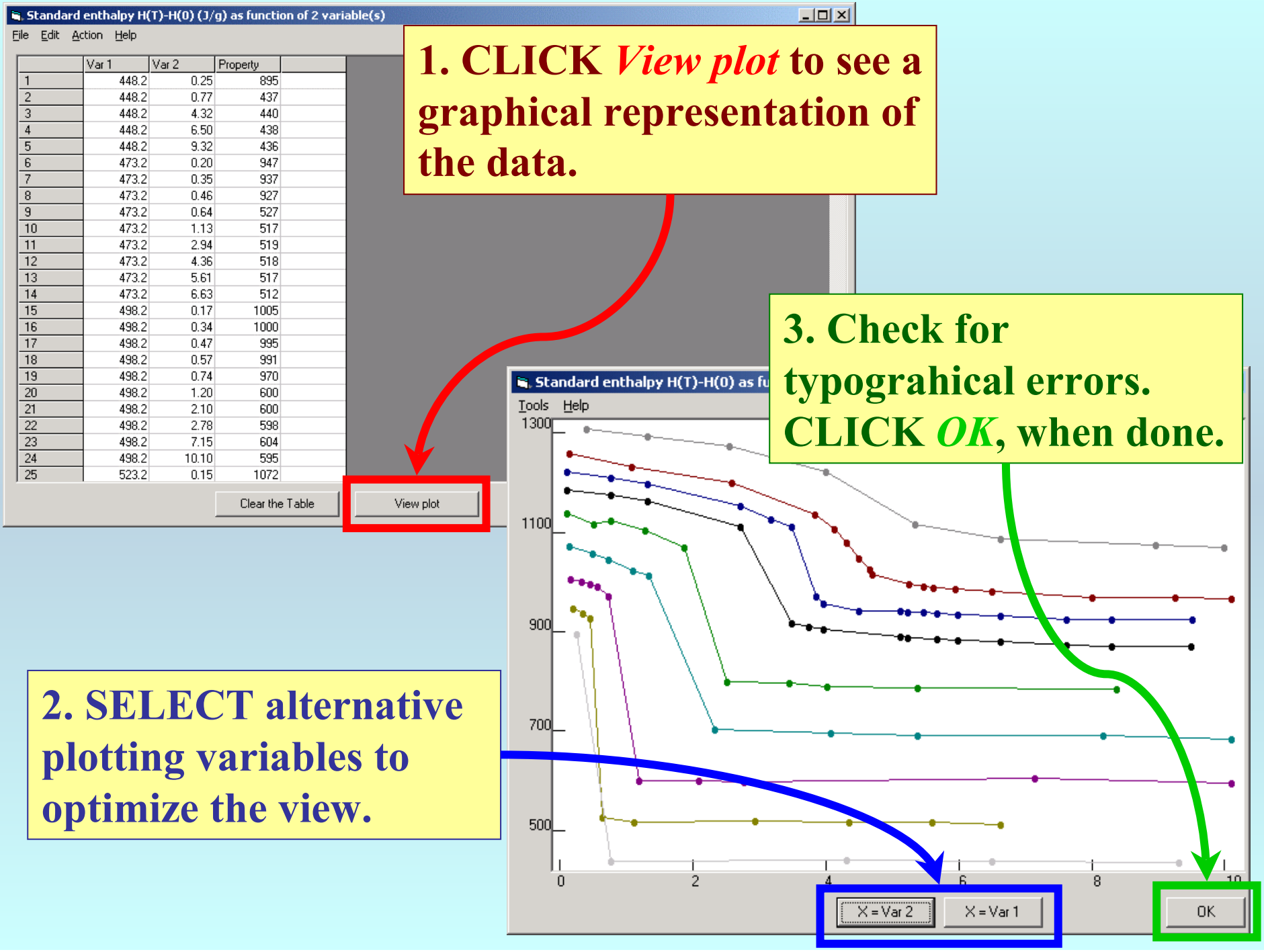
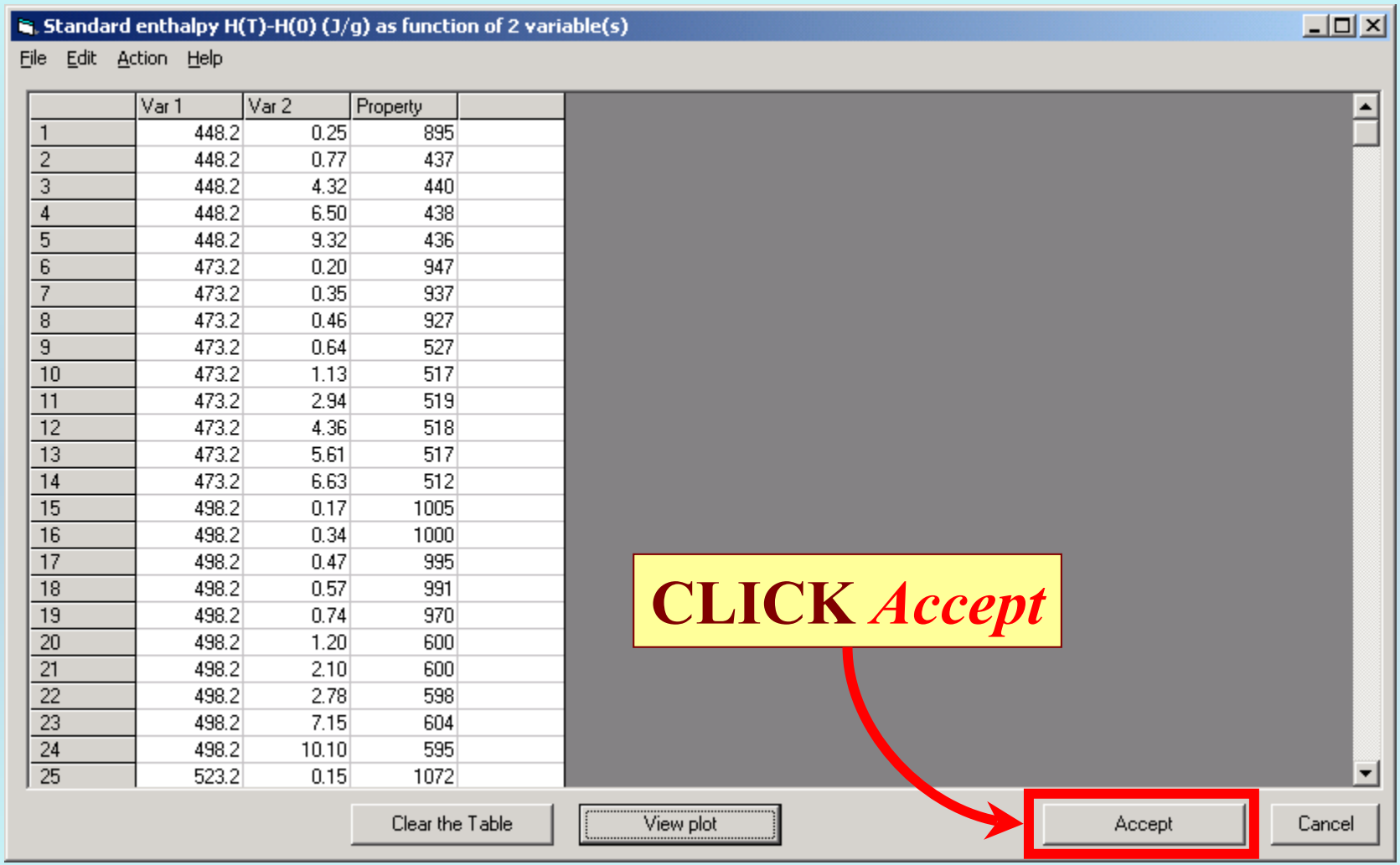
	1.09	1232	4.32	1079	5.25	995	6.50	981		
	2.59	1200	4.51	1048	5.48	992	8.00	968		
	3.84	1135	4.66	1026	5.62	989	9.26	968		
623.2	0.40	1307	2.56	1274	5.35	1116	8.96	1075		
	1.33	1293	4.00	1222	6.63	1086	10.0	1070		

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.)


Standard enthalpy H(T)-H(0) (J/g) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 448.2 0.25 895
2 448.2 0.77 437
3 448.2 4.32 440
4 448.2 6.50 438
5 448.2 9.32 436
6 473.2 0.20 947
7 473.2 0.35 937
8 473.2 0.46 927
9 473.2 0.64 527
10 473.2 1.13 517
11 473.2 2.94 519
12 473.2 4.36 518
13 473.2 5.61 517
14 473.2 6.63 512
15 498.2 0.17 1005
16 498.2 0.34 1000
17 498.2 0.47 995
18 498.2 0.57 991
19 498.2 0.74 970
20 498.2 1.20 600
21 498.2 2.10 600
22 498.2 2.78 598
23 498.2 7.15 604
24 498.2 10.10 595
25 523.2 0.15 1072
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
Standard enthalpy H(T)-H(0) as fu
Tools Help
1300
1100
900
700
500
0
2
4
6
8
10
X = Var 2
X = Var 1
OK
3. Check for typograhical errors. CLICK OK, when done.
2. SELECT alternative plotting variables to optimize the view.


Standard enthalpy H(T)-H(0) (J/g) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 448.2 0.25 895
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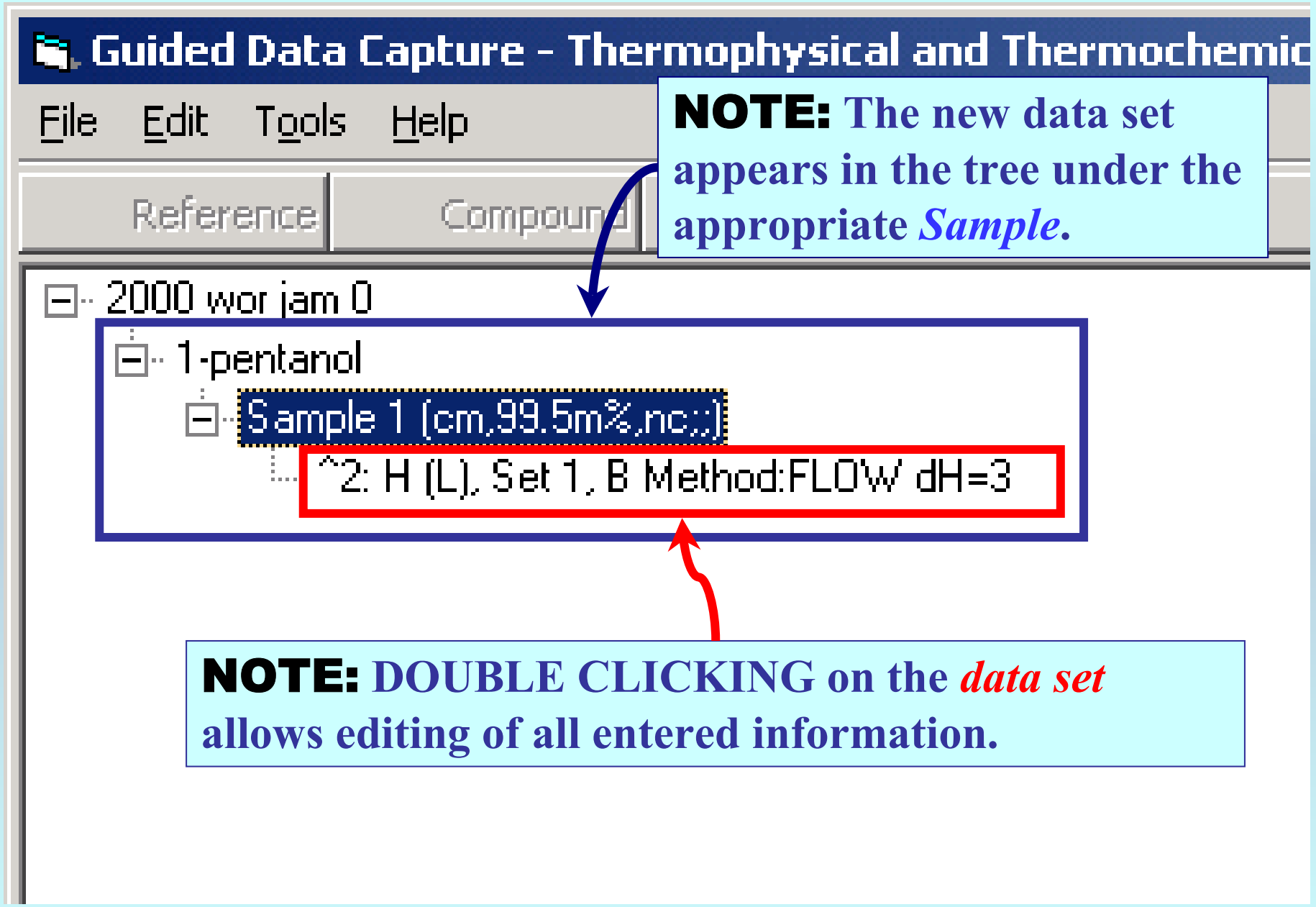
20 498.2 1.20 600
21 498.2 2.10 600
22 498.2 2.78 598
23 498.2 7.15 604
24 498.2 10.10 595
25 523.2 0.15 1072
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemic
File Edit Tools Help
Reference
Compound
NOTE: The new data set appears in the tree under the appropriate Sample.
2000 wor jam 0
1-pentanol
Sample 1 (cm,99.5m%,nc;;)
^2: H (L), Set 1, B Method:FLOW dH=3
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.**