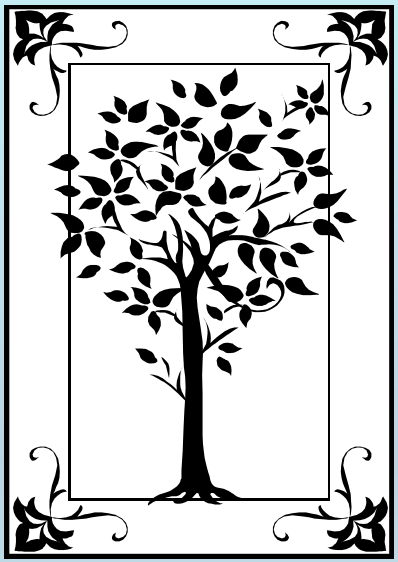
METADATA AND NUMERICAL DATA CAPTURE:
Excess Enthalpy: $H^E_{m,123}$
(3 Individual Components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **3 individual components:**
(i.e., NOT 1 component added to a binary)
EXCESS ENTHALPY: $H^E_{m,123}$
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:

124 *J. Chem. Eng. Data* 2000, *45,* 124−130

Excess Enthalpies and Volumes of Ternary Mixtures Containing 1-Propanol or 1-Butanol, an Ether (Diisopropyl Ether or Dibutyl Ether), and Heptane

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Experimental data are reported at 298.15 K of excess molar volumes V^E and of excess molar enthalpies H^E for binary and ternary mixtures of an alkanol (1-propanol or 1-butanol), an ether (diisopropyl ether or dibutyl ether), and an alkane (heptane). A vibrating-tube densitometer was used to determine V^E. H^E was measured using a quasi-isothermal flow calorimeter. The experimental results are used to test the applicability of the modified UNIFAC model for correlating H^E and of the ERAS model for describing both V^E and H^E of binary mixtures as well as for predicting the excess properties of ternary mixtures containing an alkanol, an ether, and an alkane. For all investigated binary systems, a better description of the experimental data was achieved with the ERAS model in comparison with the modified UNIFAC model.

Excess Enthalpy (H^E) for the ternary system
1-propanol + diisopropyl ether + heptane
at p = 101.3 kPa and T = 298.15 K

Table 3. Experimental Excess Molar Enthalpies H^E at 298.15 K for the Ternary Mixture $x_A = (1 - x_B - x_C)$ 1-Propanol + x_B DIPE + x_C Heptane

x_A	x_B	x_C	H^E/J·mol^{-1}	x_A	x_B	x_C	H^E/J·mol^{-1}
x_B/x_C = 0.20/0.80				x_B/x_C = 0.40/0.60			
0.1040	0.1844	0.7116	572.6	0.1040	0.3718	0.5242	557.6
0.2070	0.1632	0.6298	670.6	0.2070	0.3290	0.4640	664.7
0.3090	0.1422	0.5488	678.6	0.3090	0.2867	0.4043	676.3
0.4090	0.1216	0.4694	645.4	0.4090	0.2452	0.3458	610.6
0.5090	0.1010	0.3900	583.3	0.5090	0.2037	0.2873	567.7
0.6100	0.0802	0.3098	489.3	0.6100	0.1618	0.2282	463.5
0.7080	0.0601	0.2319	390.6	0.7080	0.1212	0.1708	379.9
0.8060	0.0399	0.1541	265.6	0.8060	0.0805	0.1135	259.3
0.9040	0.0205	0.0755	141.1	0.9040	0.0398	0.0562	126.1
x_B/x_C = 0.60/0.40				x_B/x_C = 0.80/0.20			
0.1020	0.5442	0.3538	562.6	0.1020	0.7301	0.1679	420.5
0.2040	0.4824	0.3136	663.6	0.2040	0.6472	0.1488	525.1
0.3050	0.3606	0.2738	673.5	0.3050	0.5650	0.1300	542.6
0.4050	0.3606	0.2344	626.6	0.4050	0.4837	0.1113	512.0
0.5050	0.3000	0.1950	554.5	0.5050	0.4024	0.0926	450.9
0.6050	0.2394	0.1556	456.5	0.6050	0.3211	0.0739	366.3
0.7040	0.1794	0.1166	341.9	0.7040	0.2407	0.0553	267.9
0.8030	0.1194	0.0776	223.5	0.8030	0.1602	0.0368	167.0
0.9020	0.0594	0.0386	108.9	0.9020	0.0797	0.0183	71.2

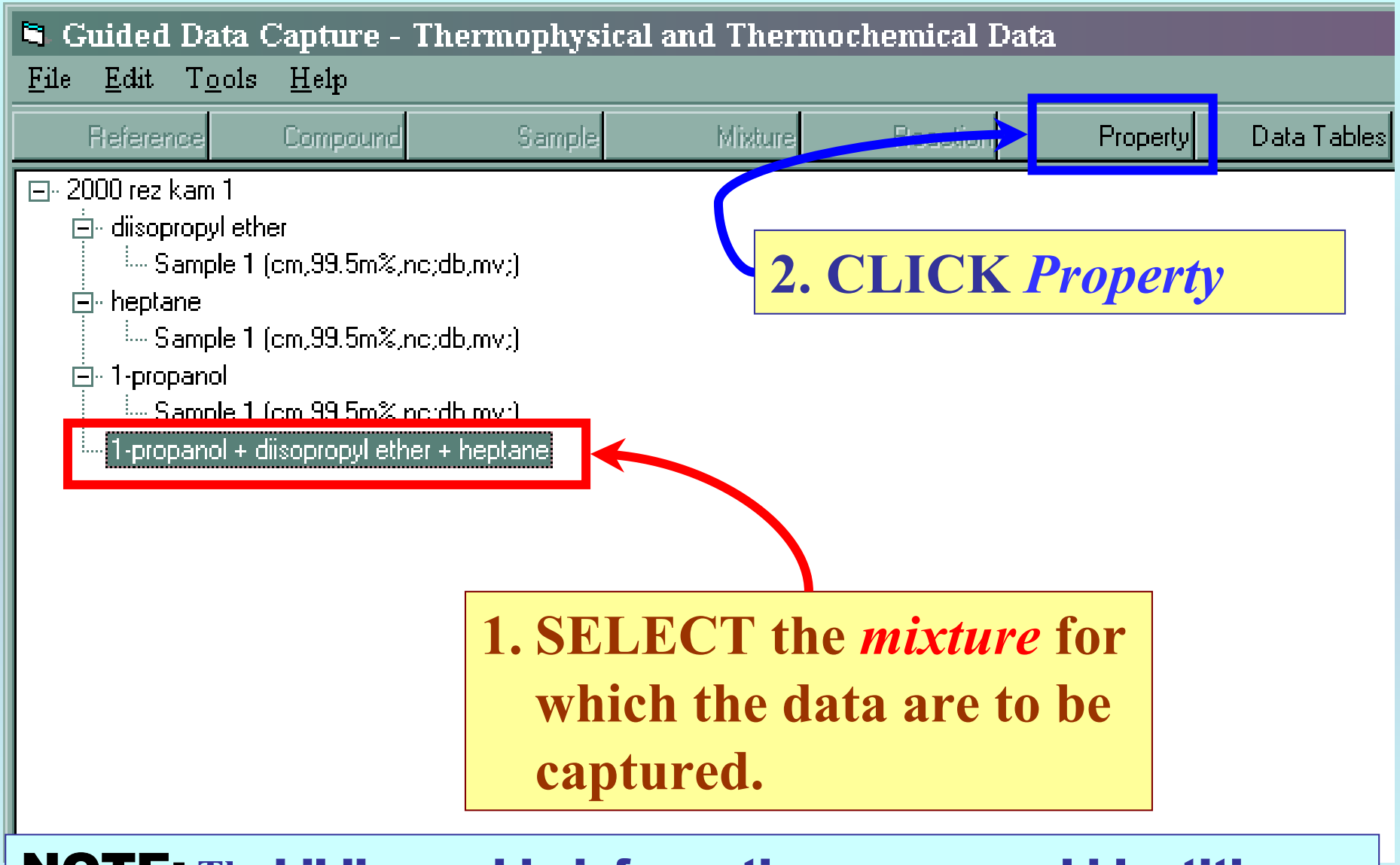
This data set is considered here.

Experimental Method & Uncertainty Estimates:

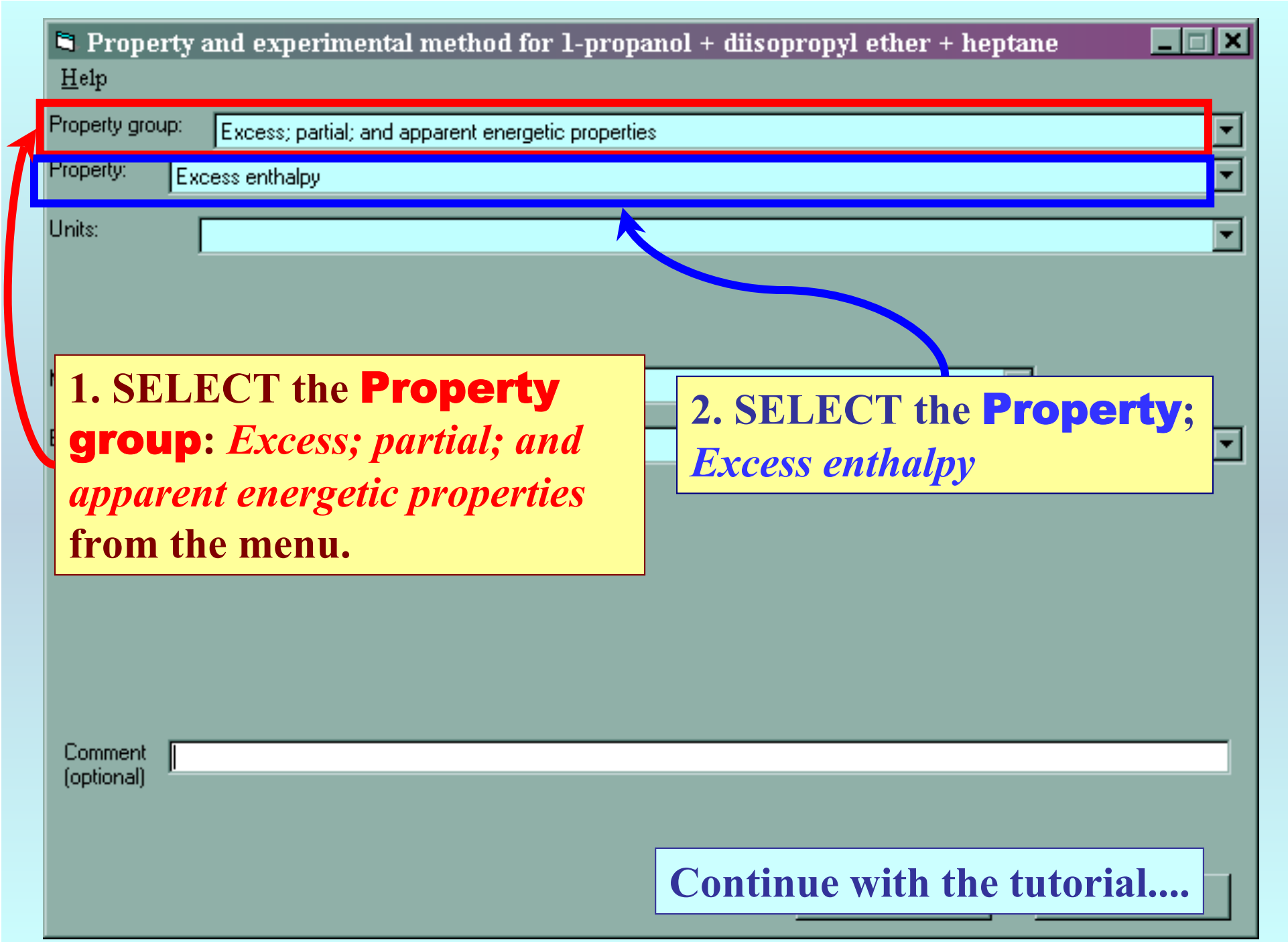
Excess molar enthalpies were measured using a modified TRONAC 1250 calorimeter. This quasi-isothermal flow calorimeter and the operating procedure have been described in detail by Heintz and Lichtenthaler (1979). The mole fraction x is accurate to the third decimal place.

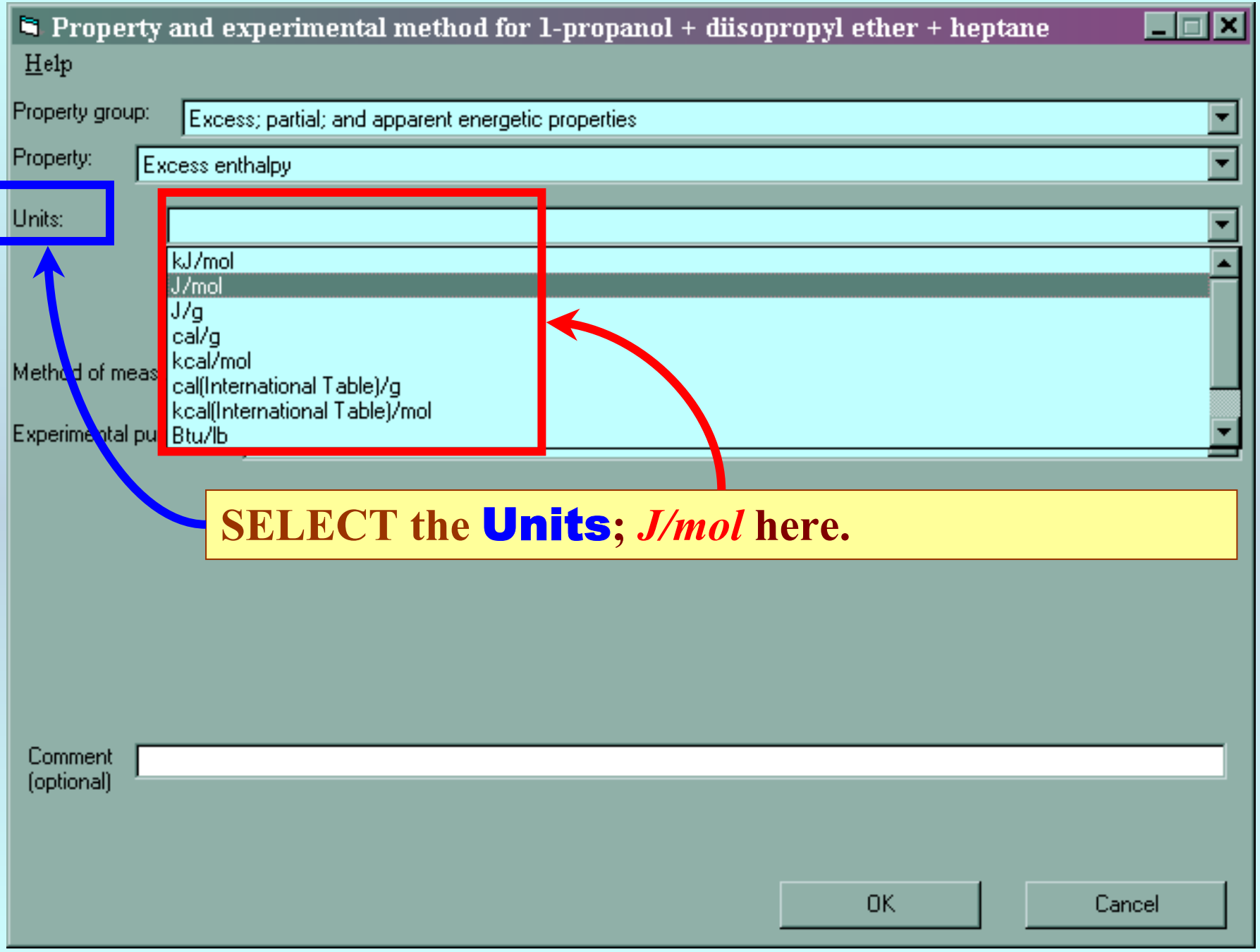
Uncertainty estimates:

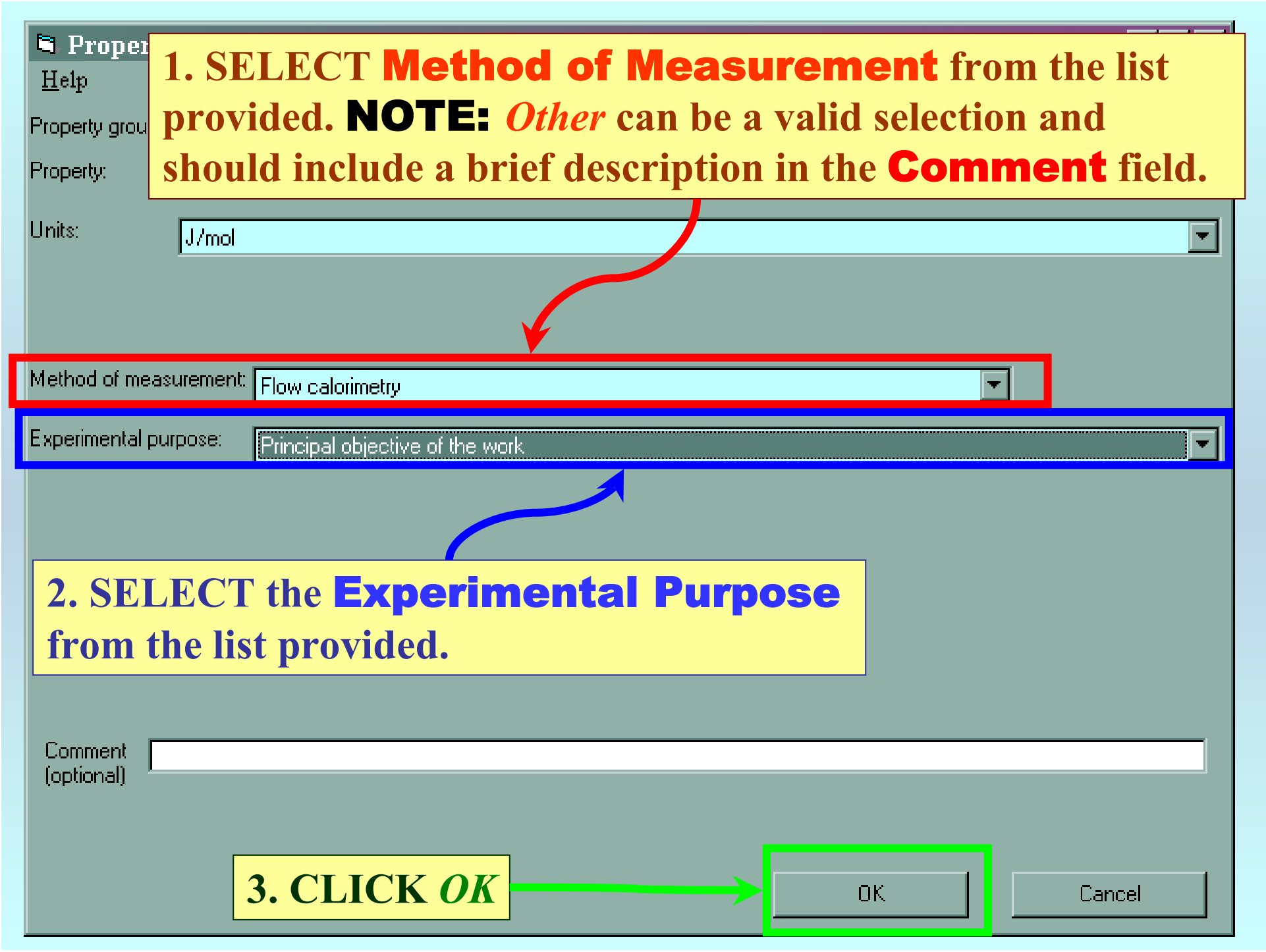
The error of the H^E data obtained is estimated to be $<\pm 0.01$ H^E (at least ± 1 J·mol^{-1}).



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-propanol + diisopropyl ether + heptane
Help
Property group:
Excess; partial; and apparent energetic properties
Property:
Excess enthalpy
Units:
1. SELECT the Property group: Excess; partial; and apparent energetic properties from the menu.
2. SELECT the Property; Excess enthalpy
Comment (optional)
Continue with the tutorial....


Property and experimental method for 1-propanol + diisopropyl ether + heptane
Help
Property group:
Excess; partial; and apparent energetic properties
Property:
Excess enthalpy
Units:
kJ/mol
J/mol
J/g
cal/g
kcal/mol
cal(International Table)/g
kcal(International Table)/mol
Btu/lb
Method of meas
Experimental pu
SELECT the Units; J/mol here.
Comment (optional)
OK
Cancel

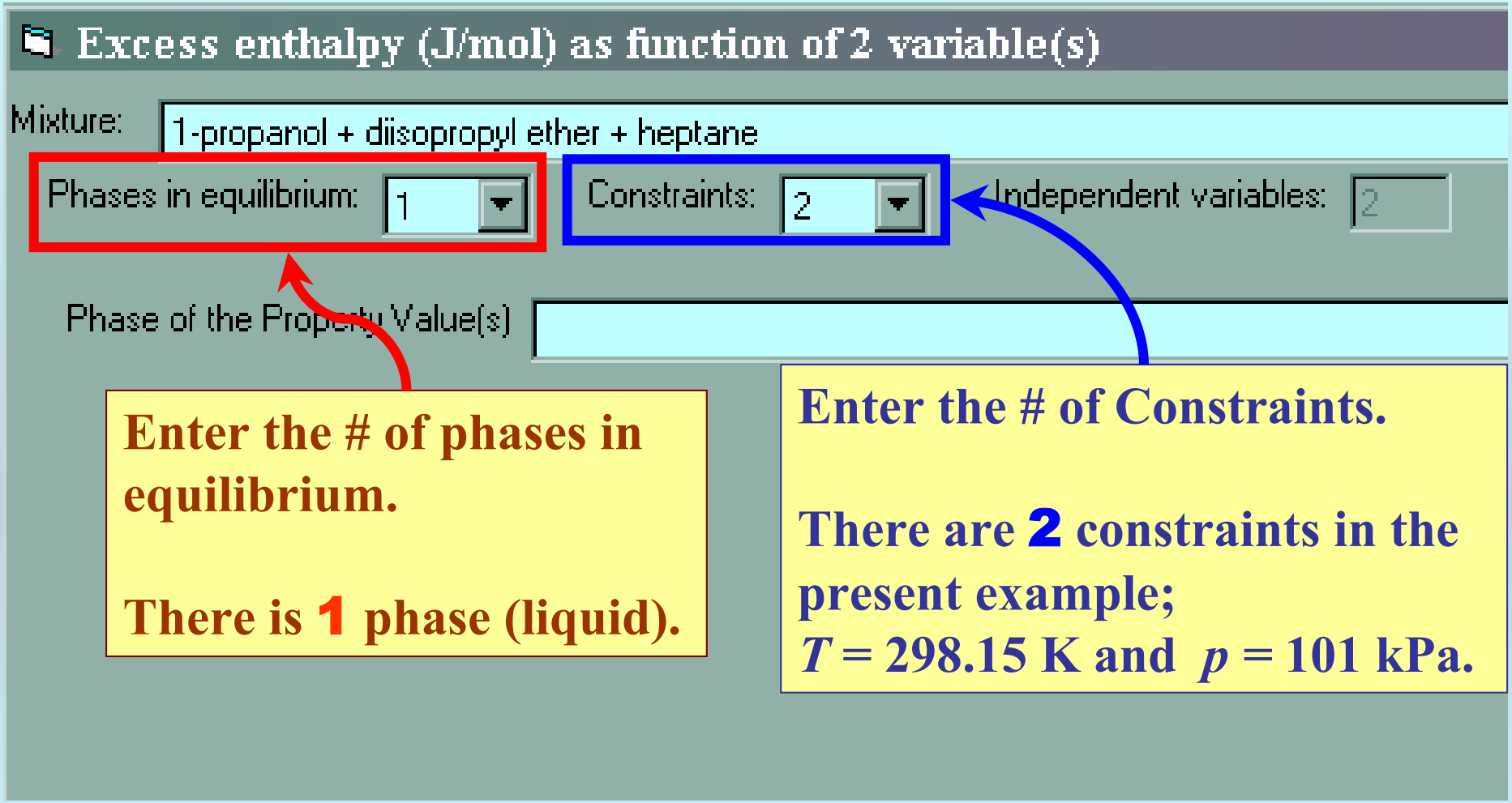


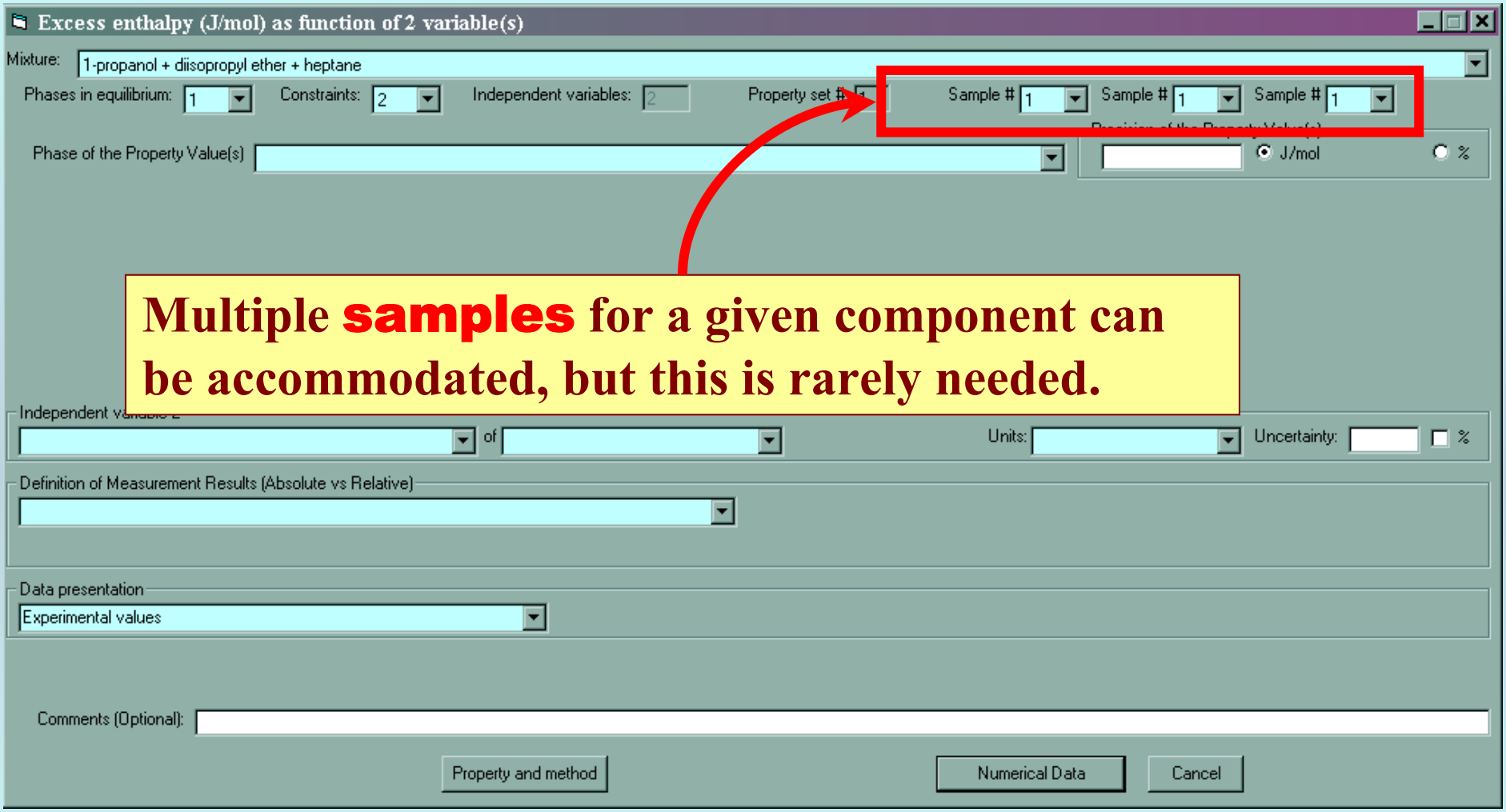
1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

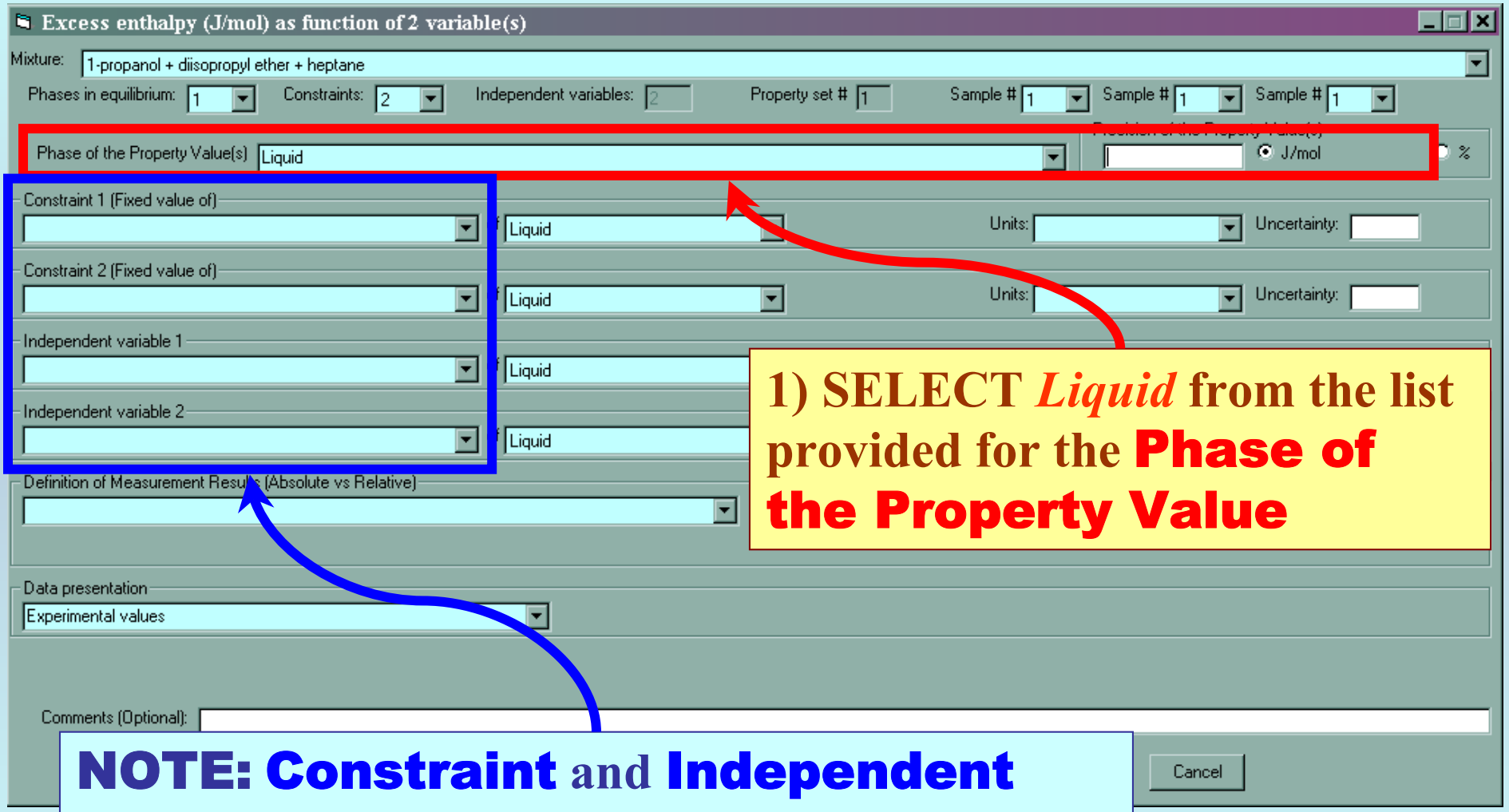
2. SELECT the **Experimental Purpose** from the list provided.

3. CLICK *OK*

SELECTION of # of Phases in Equilibrium and # of Constraints




Excess enthalpy (J/mol) as function of 2 variable(s)
Mixture:
1-propanol + diisopropyl ether + heptane
Phases in equilibrium:
1
Constraints:
2
Independent variables:
2
Property set #
1
Sample #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
J/mol
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
of
Units:
Uncertainty:
%
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel

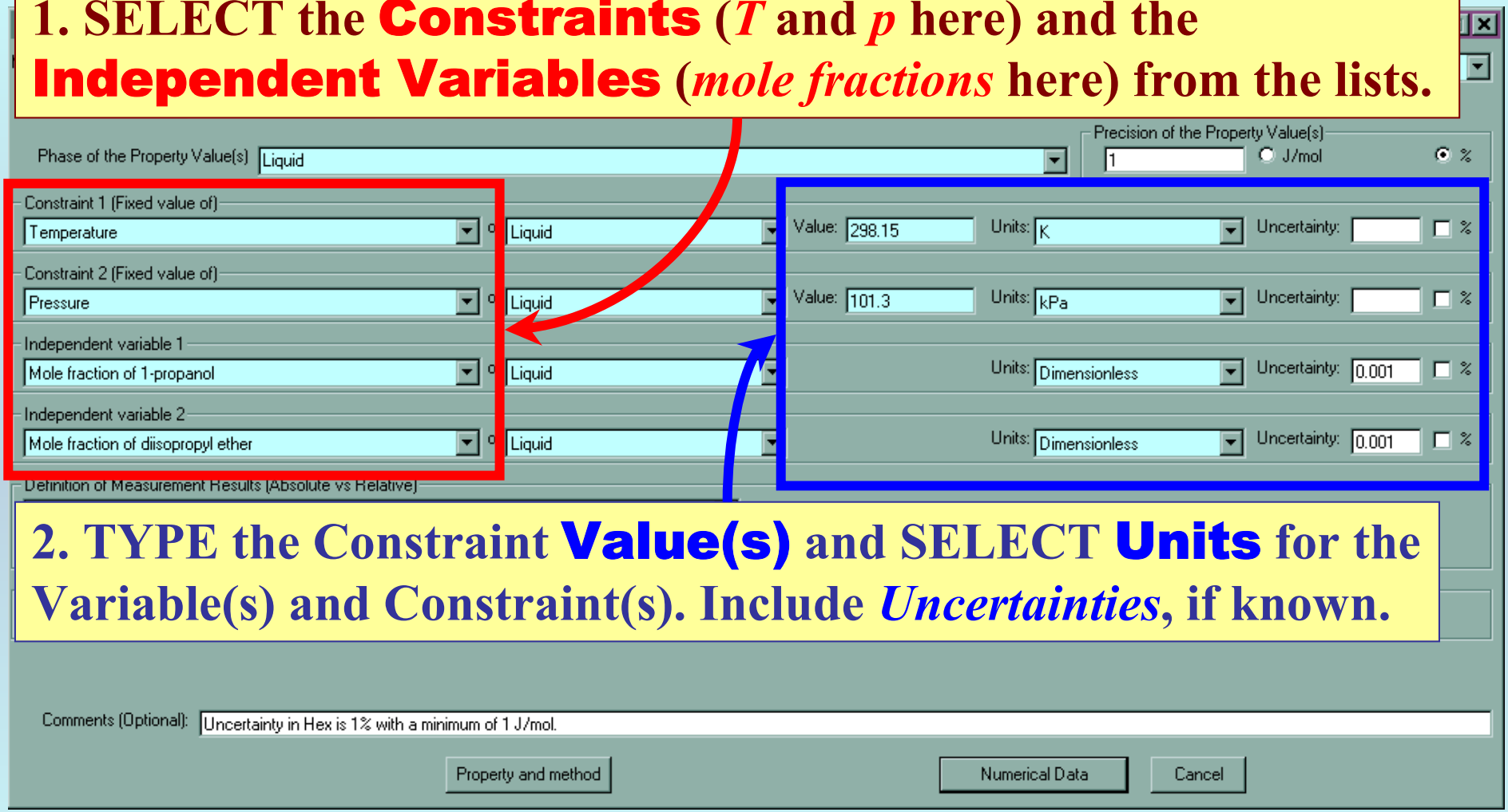


1) SELECT *Liquid* from the list provided for the **Phase of the Property Value**

NOTE: Constraint and **Independent Variable** field(s) appear automatically based on the entries and the Gibbs Phase Rule.

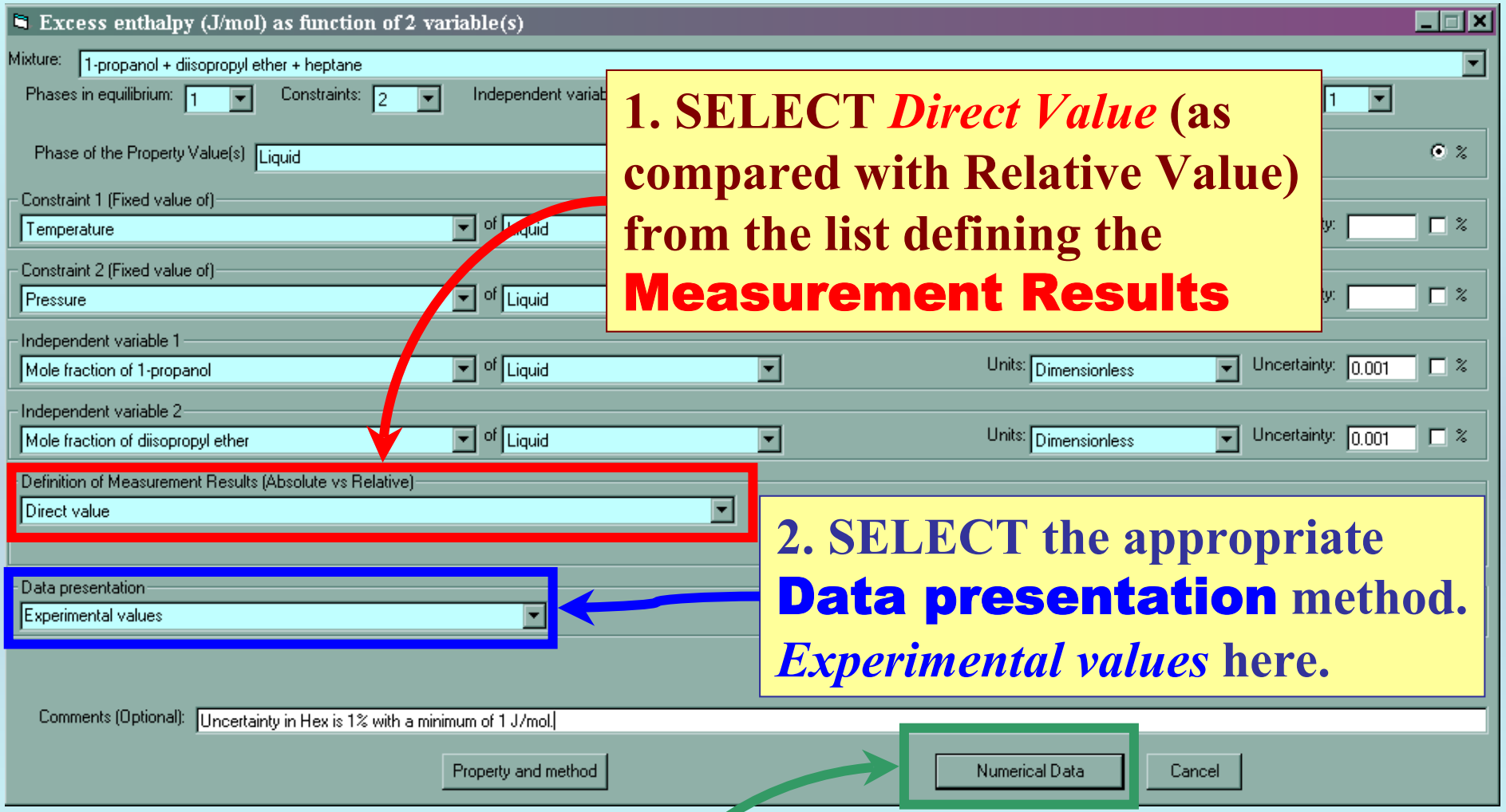
Specification of constraints, constraint values, and constraint units

1. SELECT the Constraints (*T* and *p* here) and the Independent Variables (*mole fractions* here) from the lists.



2. TYPE the Constraint Value(s) 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*

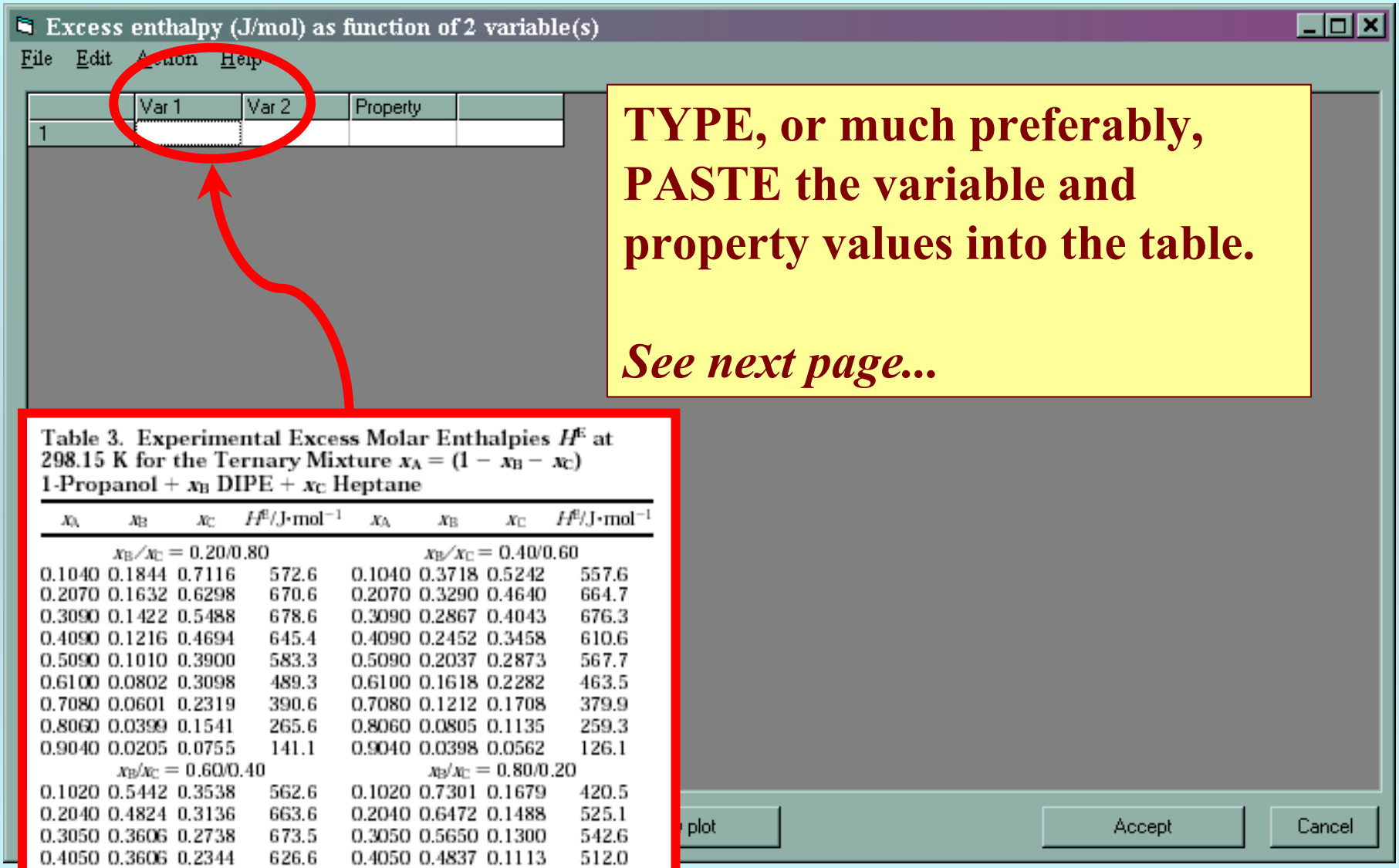


Table 3. Experimental Excess Molar Enthalpies H^E at 298.15 K for the Ternary Mixture $x_A = (1 - x_B - x_C)$ 1-Propanol + x_B DIPE + x_C Heptane

x_A	x_B	x_C	H^E/J·mol^{-1}	x_A	x_B	x_C	H^E/J·mol^{-1}
$x_B/x_C = 0.20/0.80$				$x_B/x_C = 0.40/0.60$			
0.1040	0.1844	0.7116	572.6	0.1040	0.3718	0.5242	557.6
0.2070	0.1632	0.6298	670.6	0.2070	0.3290	0.4640	664.7
0.3090	0.1422	0.5488	678.6	0.3090	0.2867	0.4043	676.3
0.4090	0.1216	0.4694	645.4	0.4090	0.2452	0.3458	610.6
0.5090	0.1010	0.3900	583.3	0.5090	0.2037	0.2873	567.7
0.6100	0.0802	0.3098	489.3	0.6100	0.1618	0.2282	463.5
0.7080	0.0601	0.2319	390.6	0.7080	0.1212	0.1708	379.9
0.8060	0.0399	0.1541	265.6	0.8060	0.0805	0.1135	259.3
0.9040	0.0205	0.0755	141.1	0.9040	0.0398	0.0562	126.1
$x_B/x_C = 0.60/0.40$				$x_B/x_C = 0.80/0.20$			
0.1020	0.5442	0.3538	562.6	0.1020	0.7301	0.1679	420.5
0.2040	0.4824	0.3136	663.6	0.2040	0.6472	0.1488	525.1
0.3050	0.3606	0.2738	673.5	0.3050	0.5650	0.1300	542.6
0.4050	0.3606	0.2344	626.6	0.4050	0.4837	0.1113	512.0
0.5050	0.3000	0.1950	554.5	0.5050	0.4024	0.0926	450.9
0.6050	0.2394	0.1556	456.5	0.6050	0.3211	0.0739	366.3
0.7040	0.1794	0.1166	341.9	0.7040	0.2407	0.0553	267.9
0.8030	0.1194	0.0776	223.5	0.8030	0.1602	0.0368	167.0
0.9020	0.0594	0.0386	108.9	0.9020	0.0797	0.0183	71.2

Excess enthalpy (J/mol) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	0.1040	0.1844	572.6
2	0.2070	0.1632	670.6
3	0.3090	0.1422	678.6
4	0.4090	0.1216	645.4
5	0.5090	0.1010	583.3
6	0.6100	0.0802	489.3
7	0.7080	0.0601	390.6
8	0.8060	0.0399	265.6
9	0.9040	0.0205	141.1
10	0.1040	0.3718	557.6
11	0.2070	0.3290	664.7
12	0.3090	0.2867	676.3
13	0.4090	0.2452	610.6
14	0.5090	0.2037	567.7
15	0.6100	0.1618	4
16	0.7080	0.1212	379.9
17	0.8060	0.0805	259.3
18	0.9040	0.0398	126.1
19	0.1020	0.5442	562.6
20	0.2040	0.4824	663.6
21	0.3050	0.3606	673.5
22	0.4050	0.3606	626.6
23	0.5050	0.3000	554.5
24	0.6050	0.2394	456.5
25	0.7040	0.1794	341.9

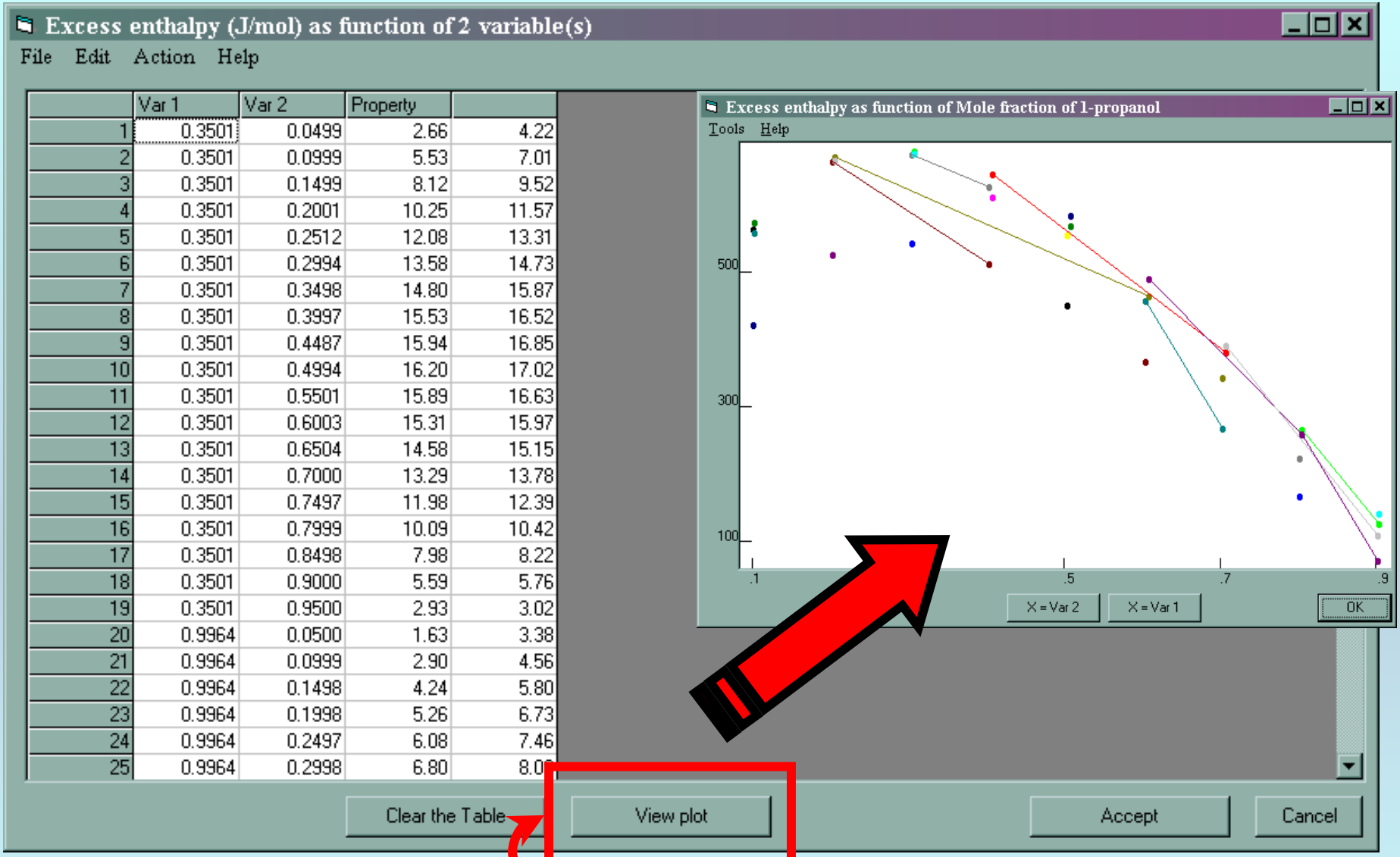
Clear the Table

Cancel

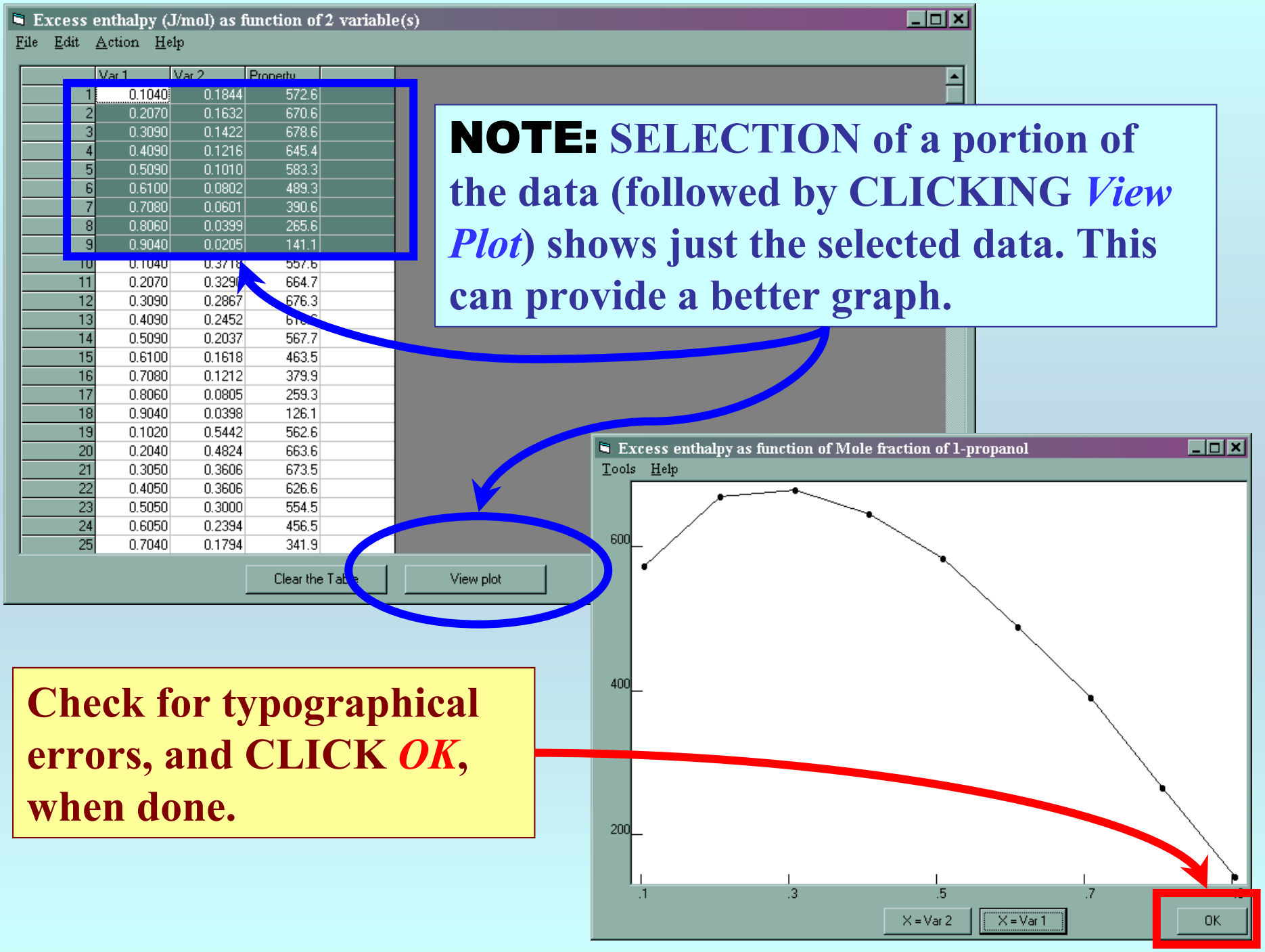
Table 3. Experimental Excess Molar Enthalpies H^E at 298.15 K for the Ternary Mixture $x_A = (1 - x_B - x_C)$ 1-Propanol + x_B DIPE + x_C Heptane

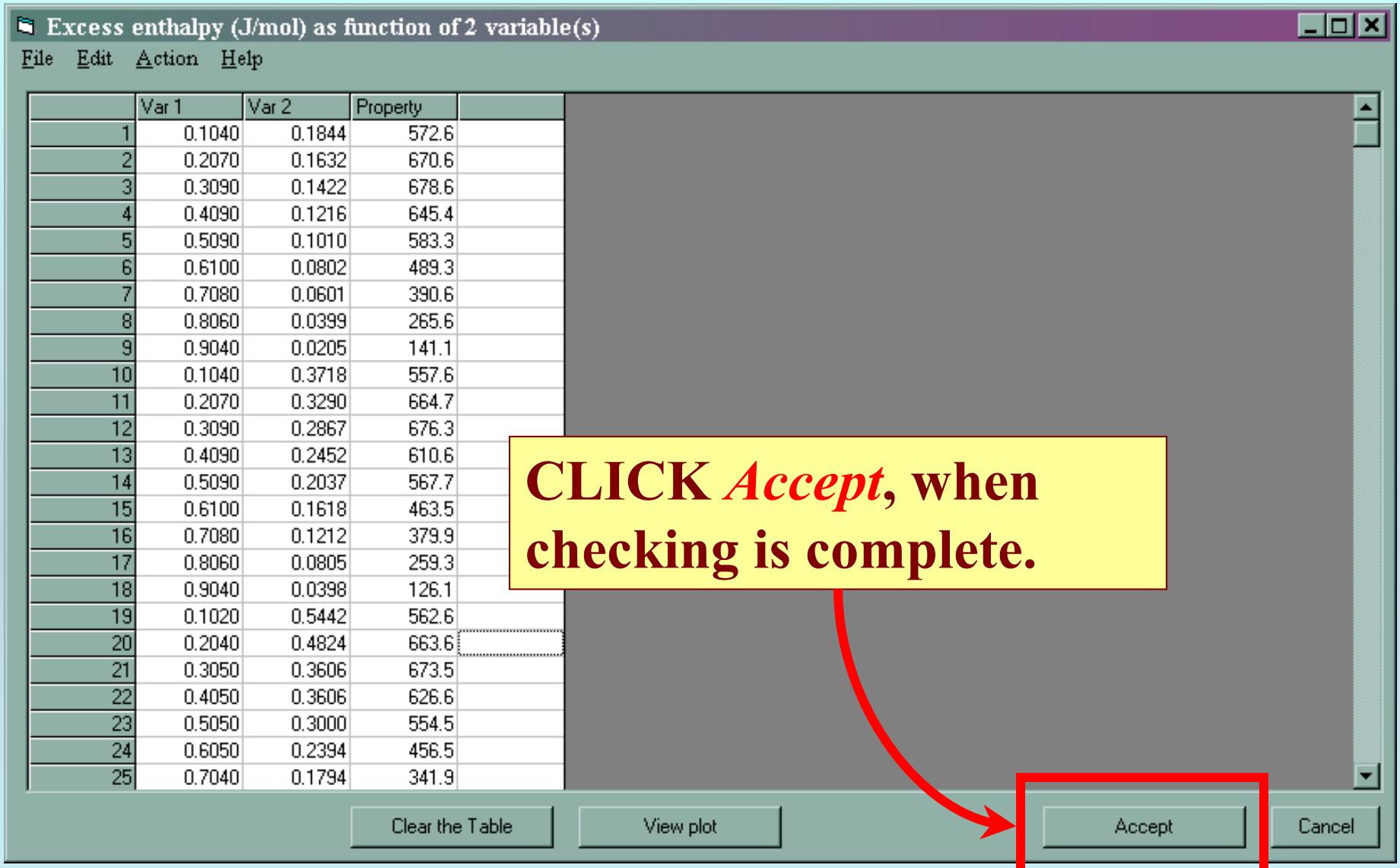
x_A	x_B	x_C	H^E/J·mol^{-1}	x_A	x_B	x_C	H^E/J·mol^{-1}
	~~x_B/x_C = 0.20/0.80~~				~~x_B/x_C = 0.40/0.60~~		
0.1040	0.1844		572.6	0.1040	0.3718		557.6
0.2070	0.1632		670.6	0.2070	0.3290		664.7
0.3090	0.1422		678.6	0.3090	0.2867		676.3
0.4090	0.1216		645.4	0.4090	0.2452		610.6
0.5090	0.1010		583.3	0.5090	0.2037		567.7
0.6100	0.0802		489.3	0.6100	0.1618		463.5
0.7080	0.0601		390.6	0.7080	0.1212		379.9
0.8060	0.0399		265.6	0.8060	0.0805		259.3
0.9040	0.0205		141.1	0.9040	0.0398		126.1
	x_B/x_C = 0.60/0.40				~~x_B/x_C = 0.80/0.20~~		
0.1020	0.5442		562.6	0.1020	0.7301		420.5
0.2040	0.4824		663.6	0.2040	0.6472		525.1
0.3050	0.3606		673.5	0.3050	0.5650		542.6
0.4050	0.3606		626.6	0.4050	0.4837		512.0
0.5050	0.3000		554.5	0.5050	0.4024		450.9
0.6050	0.2394		456.5	0.6050	0.3211		366.3
0.7040	0.1794		341.9	0.7040	0.2407		267.9
0.8030	0.1194		223.5	0.8030	0.1602		167.0
0.9020	0.0594		108.9	0.9020	0.0797		71.2

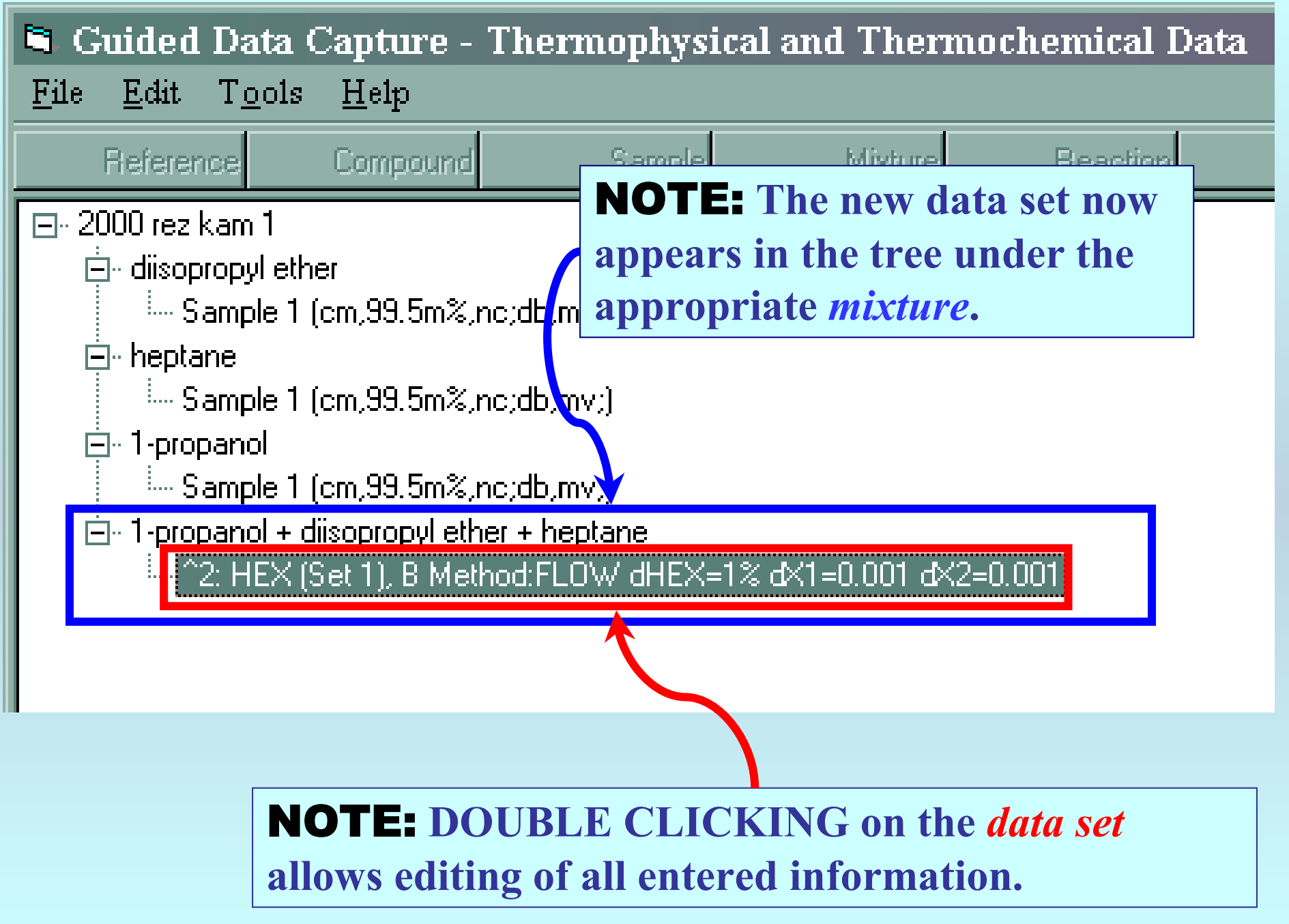
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)



CLICK *View plot* to see an automatic graphical representation of the data. *NOT very helpful in this case!* See next page...


Excess enthalpy (J/mol) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 0.1040 0.1844 572.6
2 0.2070 0.1632 670.6
3 0.3090 0.1422 678.6
4 0.4090 0.1216 645.4
5 0.5090 0.1010 583.3
6 0.6100 0.0802 489.3
7 0.7080 0.0601 390.6
8 0.8060 0.0399 265.6
9 0.9040 0.0205 141.1
11 0.2070 664.7
12 0.3090 0.2867 676.3
13 0.4090 0.2452
14 0.5090 0.2037 567.7
15 0.6100 0.1618 463.5
16 0.7080 0.1212 379.9
17 0.8060 0.0805 259.3
18 0.9040 0.0398 126.1
19 0.1020 0.5442 562.6
20 0.2040 0.4824 663.6
21 0.3050 0.3606 673.5
22 0.4050 0.3606 626.6
23 0.5050 0.3000 554.5
24 0.6050 0.2394 456.5
25 0.7040 0.1794 341.9
Clear the Table
View plot
NOTE: SELECTION of a portion of the data (followed by CLICKING View Plot) shows just the selected data. This can provide a better graph.
Excess enthalpy as function of Mole fraction of 1-propanol
Tools Help
600
400
200
.1
.3
.5
.7
X = Var 2
X = Var 1
OK
Check for typographical errors, and CLICK OK, when done.


Excess enthalpy (J/mol) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 0.1040 0.1844 572.6
2 0.2070 0.1632 670.6
3 0.3090 0.1422 678.6
4 0.4090 0.1216 645.4
5 0.5090 0.1010 583.3
6 0.6100 0.0802 489.3
7 0.7080 0.0601 390.6
8 0.8060 0.0399 265.6
9 0.9040 0.0205 141.1
10 0.1040 0.3718 557.6
11 0.2070 0.3290 664.7
12 0.3090 0.2867 676.3
13 0.4090 0.2452 610.6
14 0.5090 0.2037 567.7
15 0.6100 0.1618 463.5
16 0.7080 0.1212 379.9
17 0.8060 0.0805 259.3
18 0.9040 0.0398 126.1
19 0.1020 0.5442 562.6
20 0.2040 0.4824 663.6
21 0.3050 0.3606 673.5
22 0.4050 0.3606 626.6
23 0.5050 0.3000 554.5
24 0.6050 0.2394 456.5
25 0.7040 0.1794 341.9
CLICK Accept, when checking is complete.
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction
2000 rez kam 1
diisopropyl ether
Sample 1 (cm,99.5m%,nc;db,m
heptane
Sample 1 (cm,99.5m%,nc;db,mv;)
1-propanol
Sample 1 (cm,99.5m%,nc;db,mv;)
1-propanol + diisopropyl ether + heptane
^2: HEX (Set 1), B Method:FLOW dHEX=1% dX1=0.001 dX2=0.001
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.**