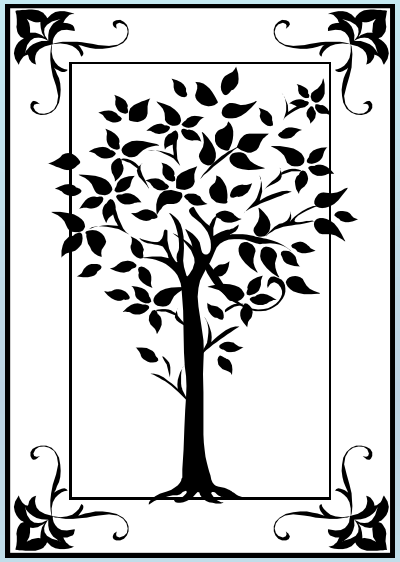
METADATA AND NUMERICAL DATA CAPTURE:
Excess Enthalpy: $H^E_{m,(1 + 23)}$
(3 – Components: *1 component added to binary*)

Guided Data Capture (GDC)



This tutorial decribes
METADATA AND NUMERICAL DATA CAPTURE:
for **3-component:** ***1 component added to binary***
EXCESS ENTHALPY: $H^E_{m,(1 + 23)}$
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:

48 *J. Chem. Eng. Data* 2000, *45*, 48−52

Excess Enthalpies of 2,2,4-Trimethylpentane + Hexane + (Octane or Dodecane) at 298.15 K

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Microcalorimetric measurements of excess molar enthalpies, measured at 298.15 K, are reported for the ternary systems 2,2,4-trimethylpentane (1) + hexane (2) + octane (3) and 2,2,4-trimethylpentane (1) + hexane (2) + dodecane (3). Smooth representations of the results are described and used to construct constant-enthalpy contours on Roozeboom diagrams. It is shown that the Flory theory provides a reasonable correlation of the results.

Excess Enthalpy (H^E) for the ternary system **2,2,4-trimethylpentane + [*hexane + octane*]** at p = 101.3 kPa and T = 298.15 K

Table 3. Experimental Excess Molar Enthalpies $H^E_{m,1+23}$ Measured at 298.15 K, for the Addition of TMP to nC6 + nC8 Mixtures to Form TMP (1) + nC6 (2) + nC8 (3), and Values of $H^E_{m,123}$ Calculated from Eq 1

x_1	$H^E_{m,1+23}$[a]/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}	x_1	$H^E_{m,1+23}$[a]/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}	x_1	$H^E_{m,1+23}$[a]/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}
			$x_2/x_3 = 0.3501$, $H^E_{m,23}$/J·mol^{-1} = 1.64					
0.0499	2.66		0.3997	15.53		0.7000	13.29	
0.0999	5.53		0.4487	15.94		0.7497	11.98	
0.1499	8.12		0.4994	16.20		0.7999	10.09	
0.2001	10.25		0.5501	15.89		0.8498	7.98	
0.2512	12.08		0.6003	15.31		0.9000	5.59	
0.2994	13.58		0.6504	14.58		0.9500	2.93	
0.3498	14.80							
			$x_2/x_3 = 0.9964$, $H^E_{m,23}$/J·mol^{-1} = 1.84					
0.0500	1.63		0.3998	7.50		0.6996	6.17	
0.0999	2.90		0.4498	7.59		0.7496	5.45	
0.1498	4.24		0.4992	7.78		0.7997	4.50	
0.1998	5.26		0.5497	7.42		0.8498	3.65	
0.2497	6.08		0.5998	7.10		0.8999	2.38	
0.2998	6.80		0.6497	6.94		0.9499	1.30	
0.3500	7.22							
			$x_2/x_3 = 3.0000$, $H^E_{m,23}$/J·mol^{-1} = 1.09					
0.0499	−0.22		0.4004	−1.16		0.6998	-1.30	
0.0999	−0.26		0.4497	−1.26		0.7499	-1.36	
0.1500	−0.53		0.4994	−1.60		0.7999	-1.17	
0.1998	−0.58		0.5502	−1.38		0.8498	-0.92	
0.2494	−0.81		0.5999	−1.34		0.9001	-0.67	
0.3002	−0.96		0.6503	−1.49		0.9500	-0.36	
0.3501	−1.10							

This data set is considered here.

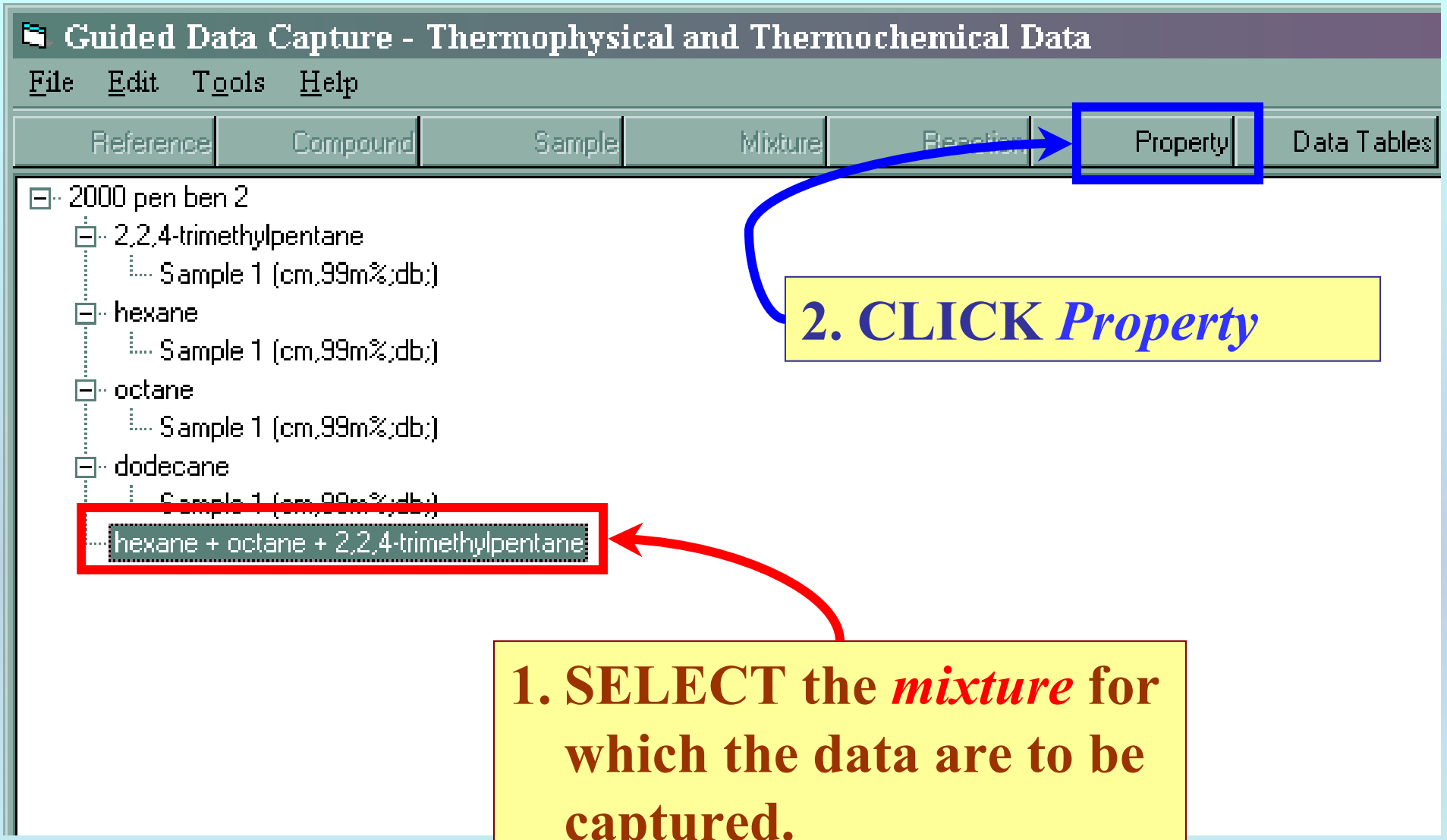
Experimental Method Info:

Excess molar enthalpies, H^E_m, were measured in an LKB-Produkter AB (Bromma, Sweden) flow microcalorimeter (Model 10700-1), thermostated at 298.15 K, maintained within ±0.003 K. Details of the equipment and its operation have been described previously (Tanaka et al., 1975; Kimura et al., 1983). In studying the ternary systems, the excess molar enthalpy $H^E_{m,1+23}$ was determined for several pseudobinary mixtures in which component 1 (TMP) was added to binary mixtures of components 2 (nC6) and 3 (either nC8 or nC12). For this purpose, binaries with fixed mole ratios x_2/x_3 were prepared by mass. The excess molar enthalpy $H^E_{m,123}$ of the ternary mixture was then obtained from the relation

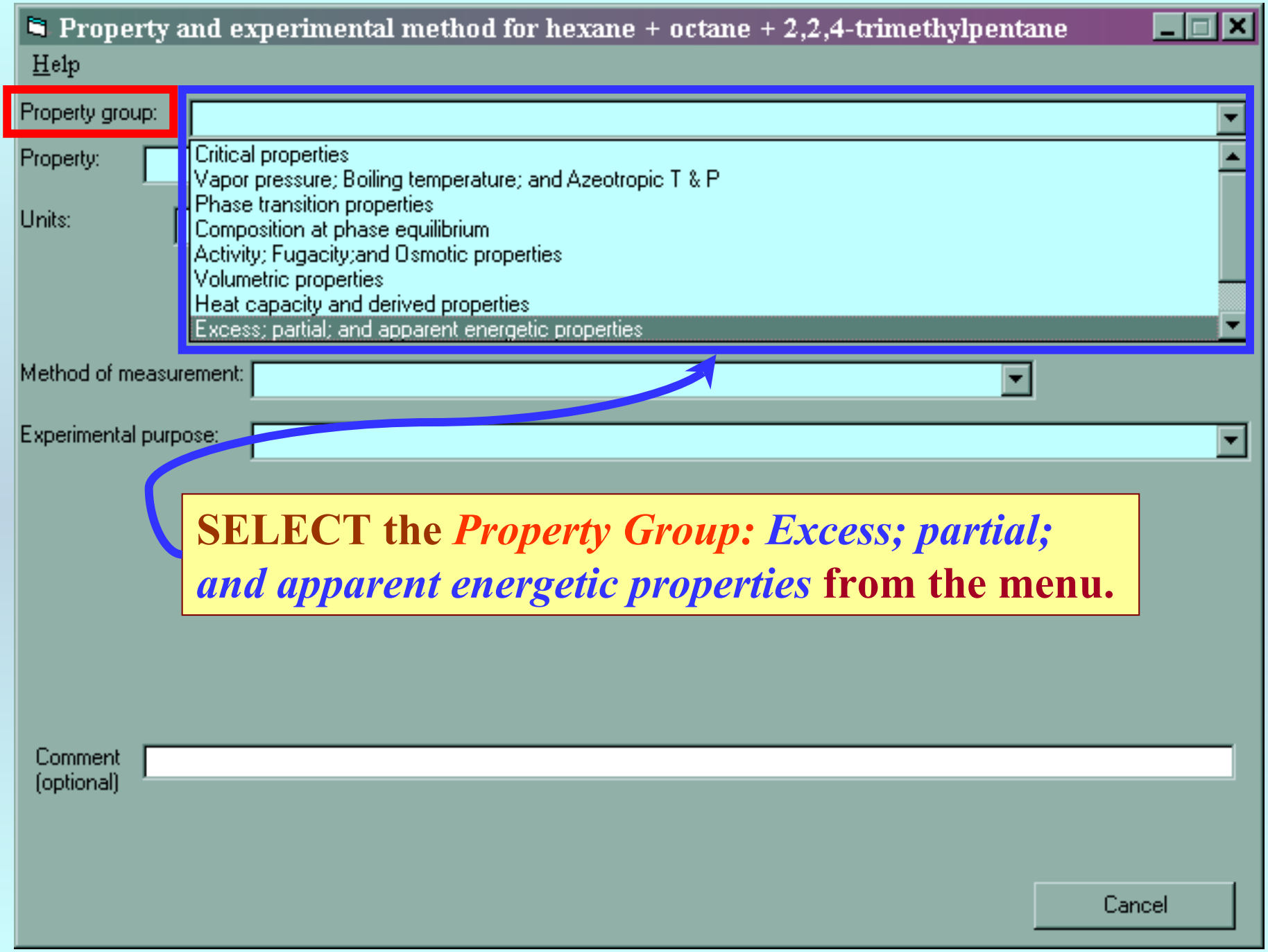
$$H^E_{m,123} = H^E_{m,1+23} + (1 - x_1) H^E_{m,23} \qquad (1)$$

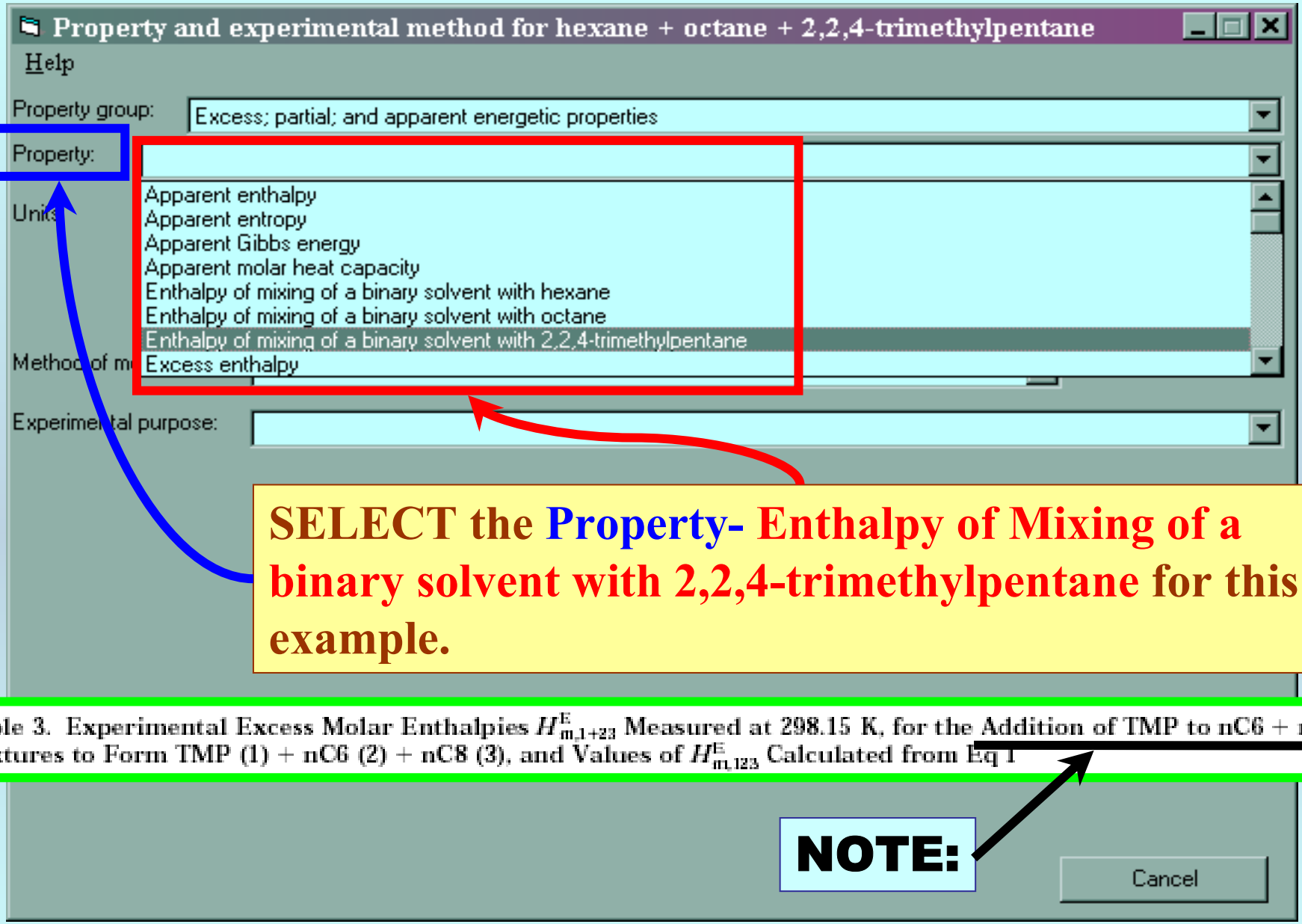
Uncertainty estimates:

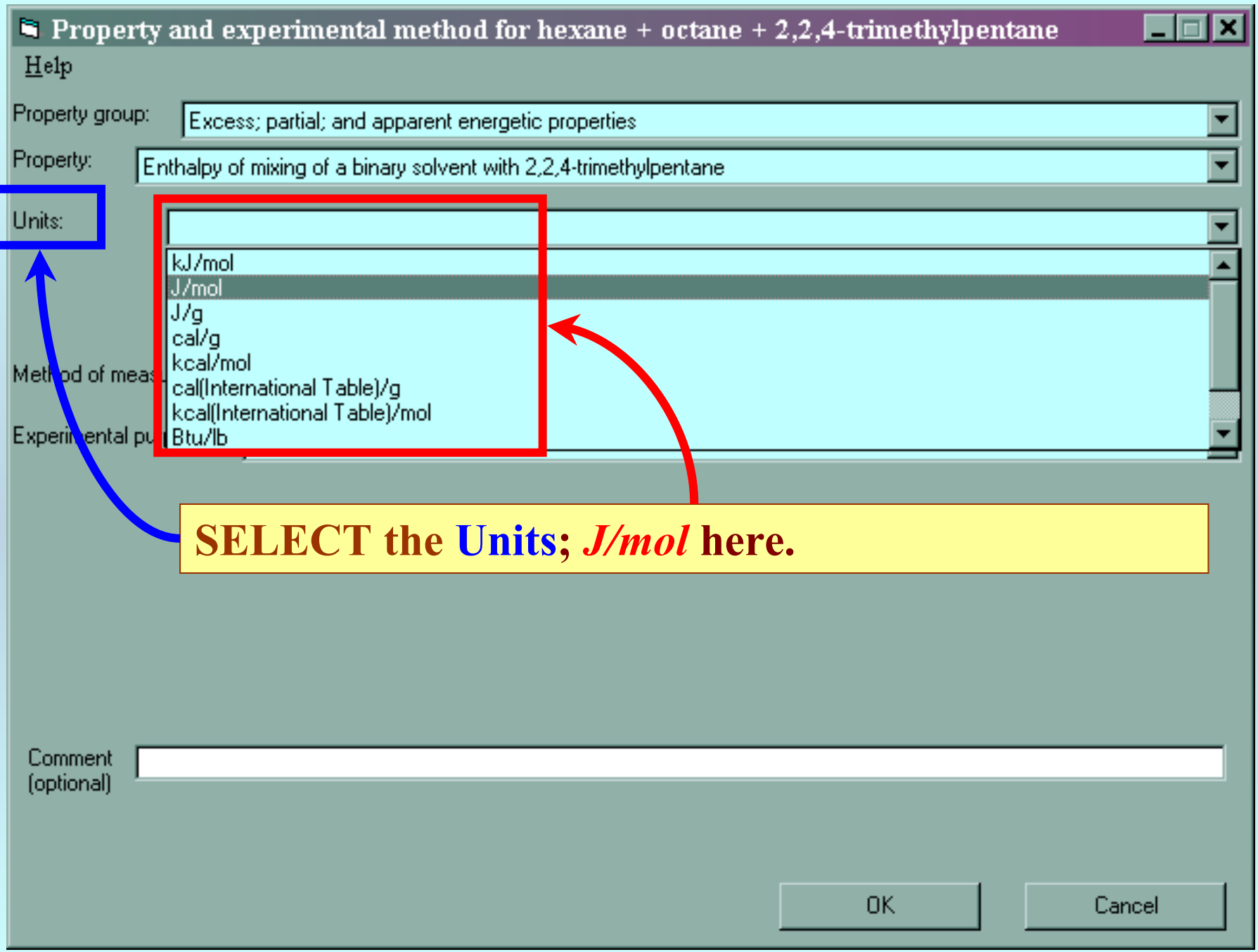
Over most of the mole fraction range, the errors of the excess molar enthalpies and the mole fractions of the final mixtures are estimated to be <0.5% and $< 5 \times 10^{-4}$, respectively.

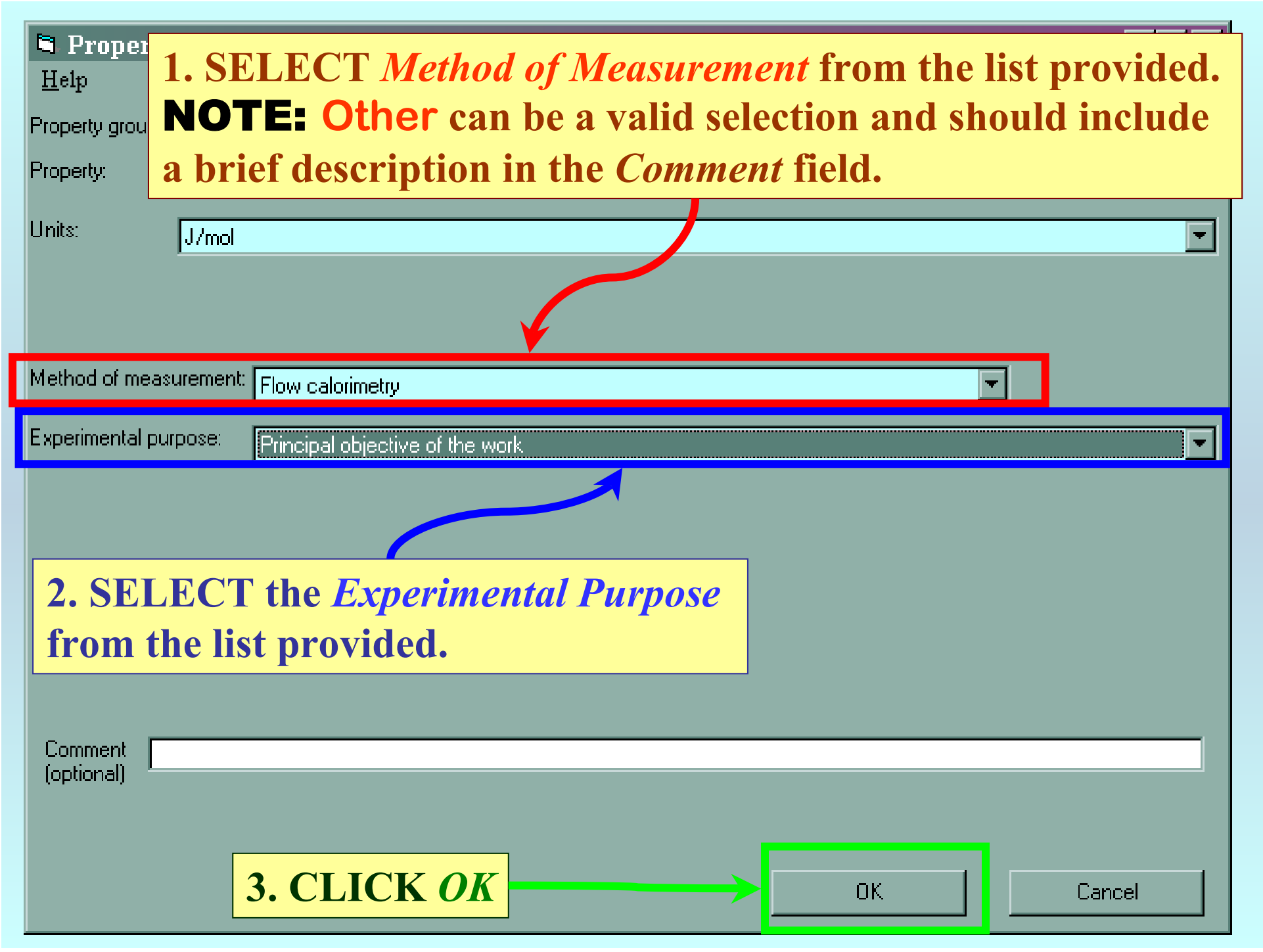


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for hexane + octane + 2,2,4-trimethylpentane
Help
Property group:
Property:
Units:
Critical properties
Vapor pressure; Boiling temperature; and Azeotropic T & P
Phase transition properties
Composition at phase equilibrium
Activity; Fugacity;and Osmotic properties
Volumetric properties
Heat capacity and derived properties
Excess; partial; and apparent energetic properties
Method of measurement:
Experimental purpose:
SELECT the Property Group: Excess; partial; and apparent energetic properties from the menu.
Comment (optional)
Cancel


Property and experimental method for hexane + octane + 2,2,4-trimethylpentane
Help
Property group:
Excess; partial; and apparent energetic properties
Property:
Apparent enthalpy
Apparent entropy
Apparent Gibbs energy
Apparent molar heat capacity
Enthalpy of mixing of a binary solvent with hexane
Enthalpy of mixing of a binary solvent with octane
Enthalpy of mixing of a binary solvent with 2,2,4-trimethylpentane
Excess enthalpy
Experimental purpose:
SELECT the Property- Enthalpy of Mixing of a binary solvent with 2,2,4-trimethylpentane for this example.
Table 3. Experimental Excess Molar Enthalpies $H^{E}_{m,1+23}$ Measured at 298.15 K, for the Addition of TMP to nC6 + nC8 Mixtures to Form TMP (1) + nC6 (2) + nC8 (3), and Values of $H^{E}_{m,123}$ Calculated from Eq 1
NOTE:
Cancel


Property and experimental method for hexane + octane + 2,2,4-trimethylpentane
Help
Property group:
Excess; partial; and apparent energetic properties
Property:
Enthalpy of mixing of a binary solvent with 2,2,4-trimethylpentane
Units:
kJ/mol
J/mol
J/g
cal/g
kcal/mol
cal(International Table)/g
kcal(International Table)/mol
Btu/lb
SELECT the Units; J/mol here.
Comment (optional)
OK
Cancel

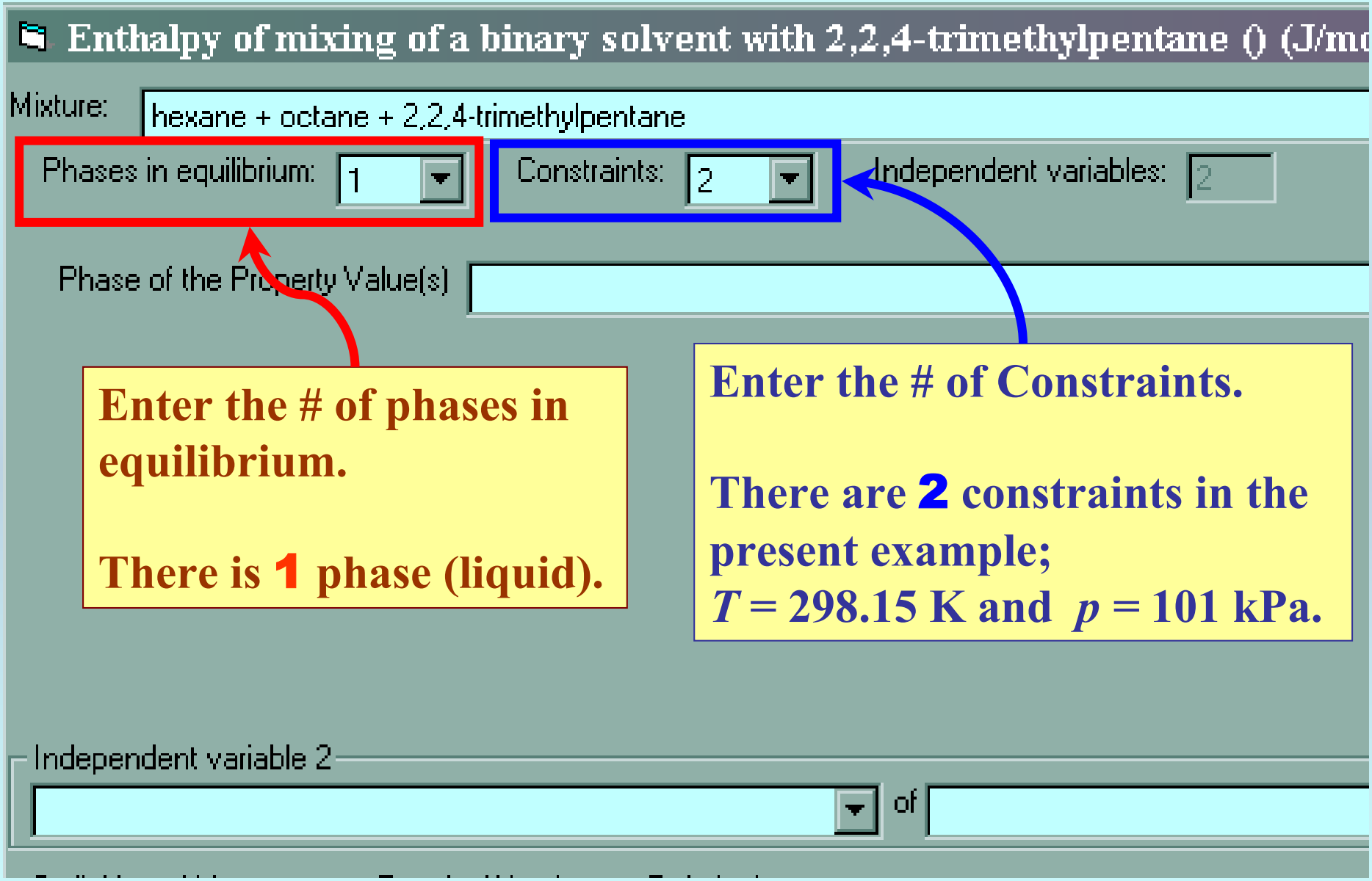


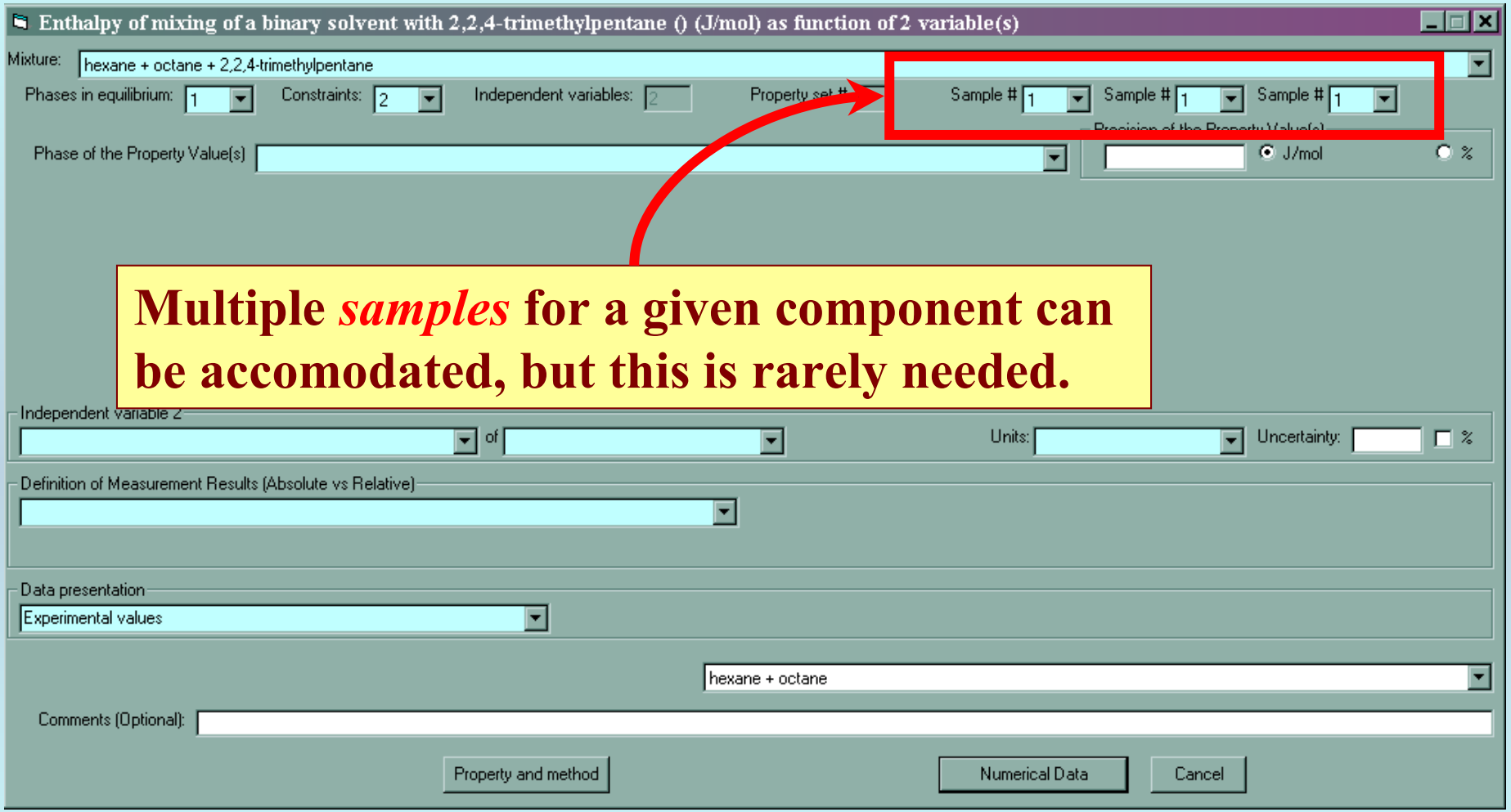
1. SELECT *Method of Measurement* from the list provided.
NOTE: Other can be a valid selection and should include a brief description in the *Comment* field.

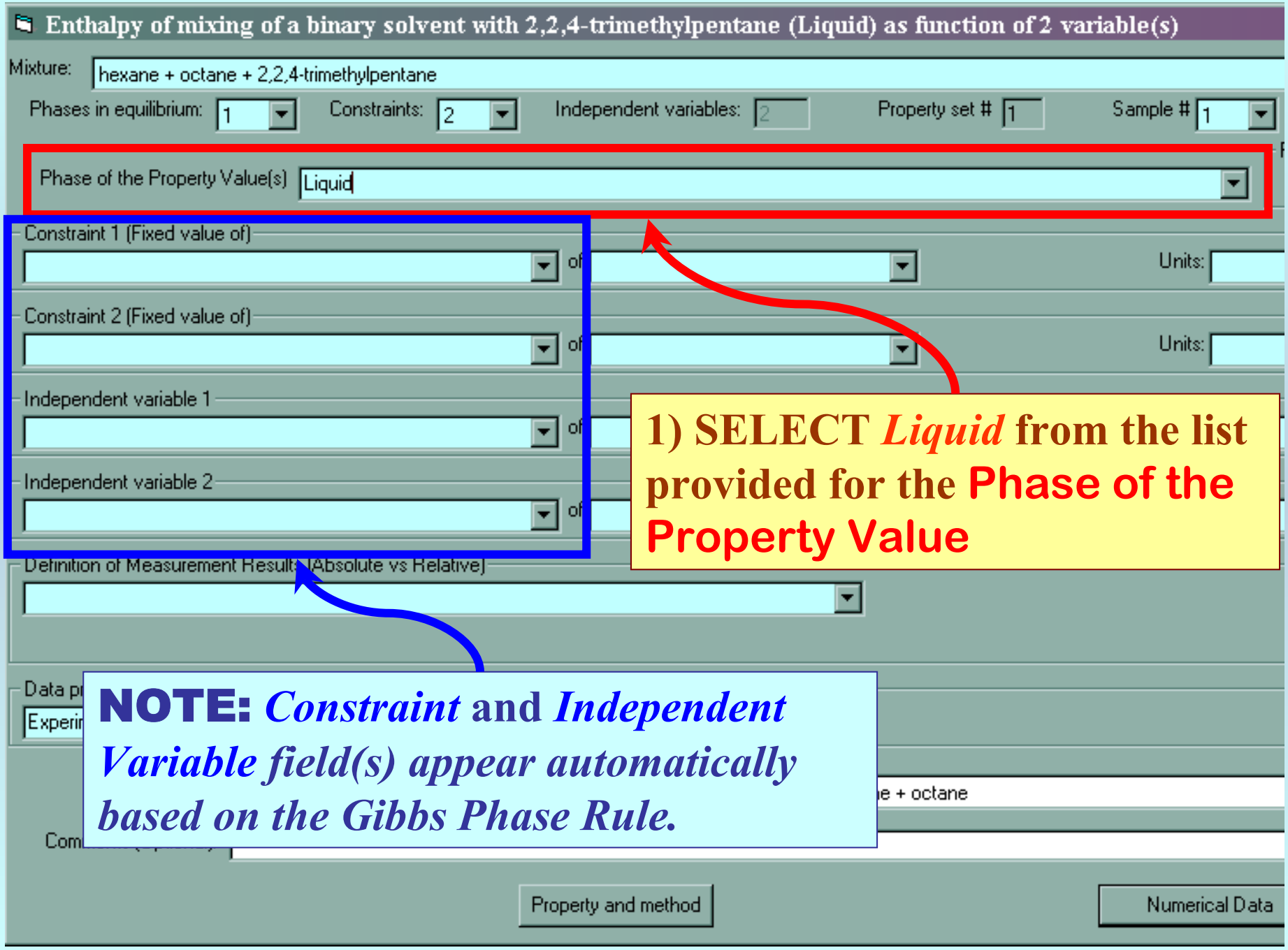
2. SELECT the *Experimental Purpose* from the list provided.

3. CLICK *OK*

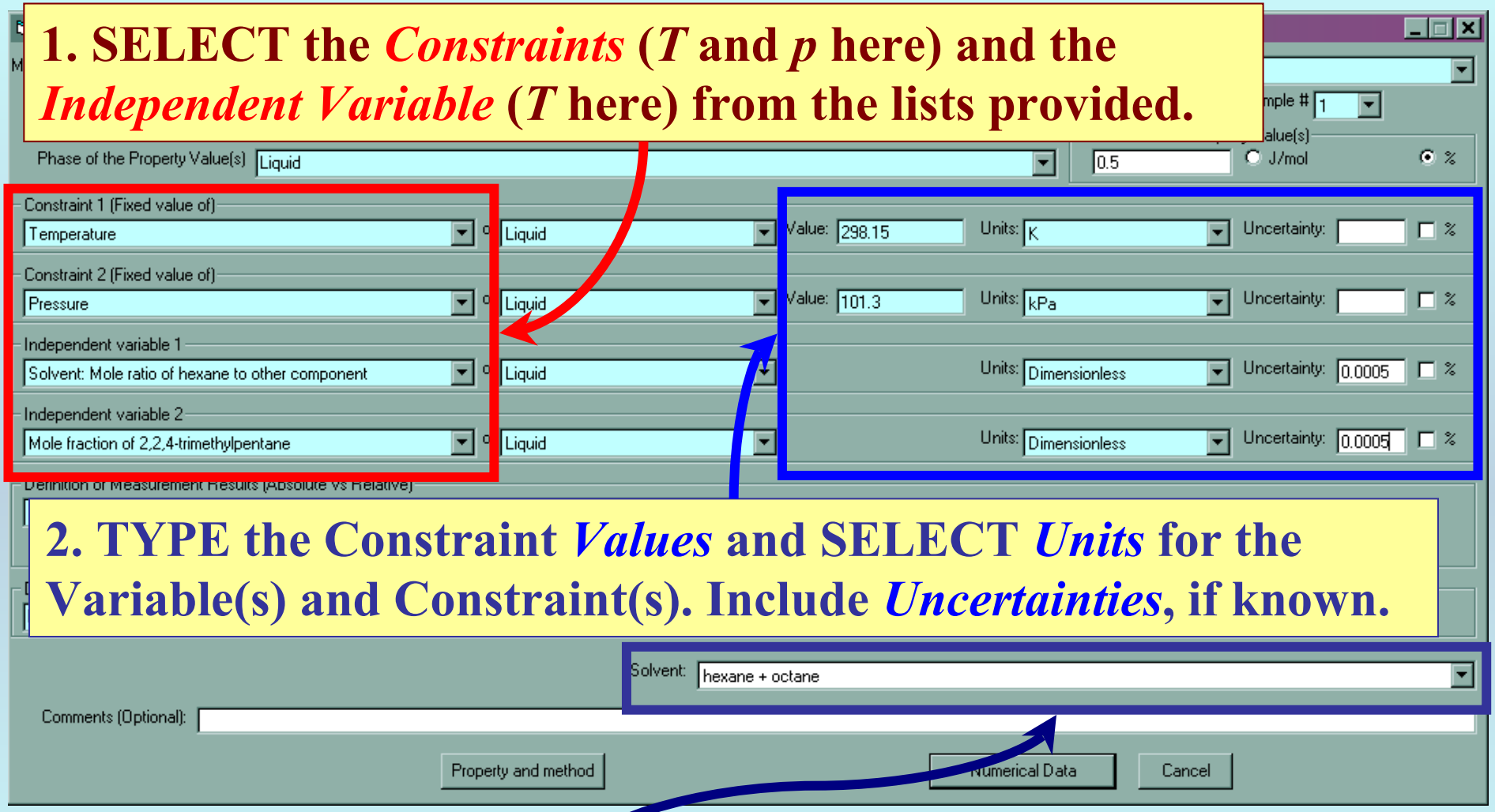
SELECTION of # of Phases in Equilibrium and # of Constraints




Enthalpy of mixing of a binary solvent with 2,2,4-trimethylpentane () (J/mol) as function of 2 variable(s)
Mixture:
hexane + octane + 2,2,4-trimethylpentane
Phases in equilibrium:
1
Constraints:
2
Independent variables:
2
Property set #
Sample #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
J/mol
%
Multiple samples for a given component can be accomodated, but this is rarely needed.
Independent variable 2
of
Units:
Uncertainty:
%
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
hexane + octane
Comments (Optional):
Property and method
Numerical Data
Cancel


Enthalpy of mixing of a binary solvent with 2,2,4-trimethylpentane (Liquid) as function of 2 variable(s)
Mixture:
hexane + octane + 2,2,4-trimethylpentane
Phases in equilibrium:
1
Constraints:
2
Independent variables:
2
Property set #
1
Sample #
1
Phase of the Property Value(s)
Liquid
Constraint 1 (Fixed value of)
of
Units:
Constraint 2 (Fixed value of)
of
Units:
Independent variable 1
of
Independent variable 2
of
Definition of Measurement Result (Absolute vs 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.
e + octane
Property and method
Numerical Data

Specification of constraints, constraint values, and constraint units



NOTE: The solvent (here, **hexane+octane**) is identified automatically by the software

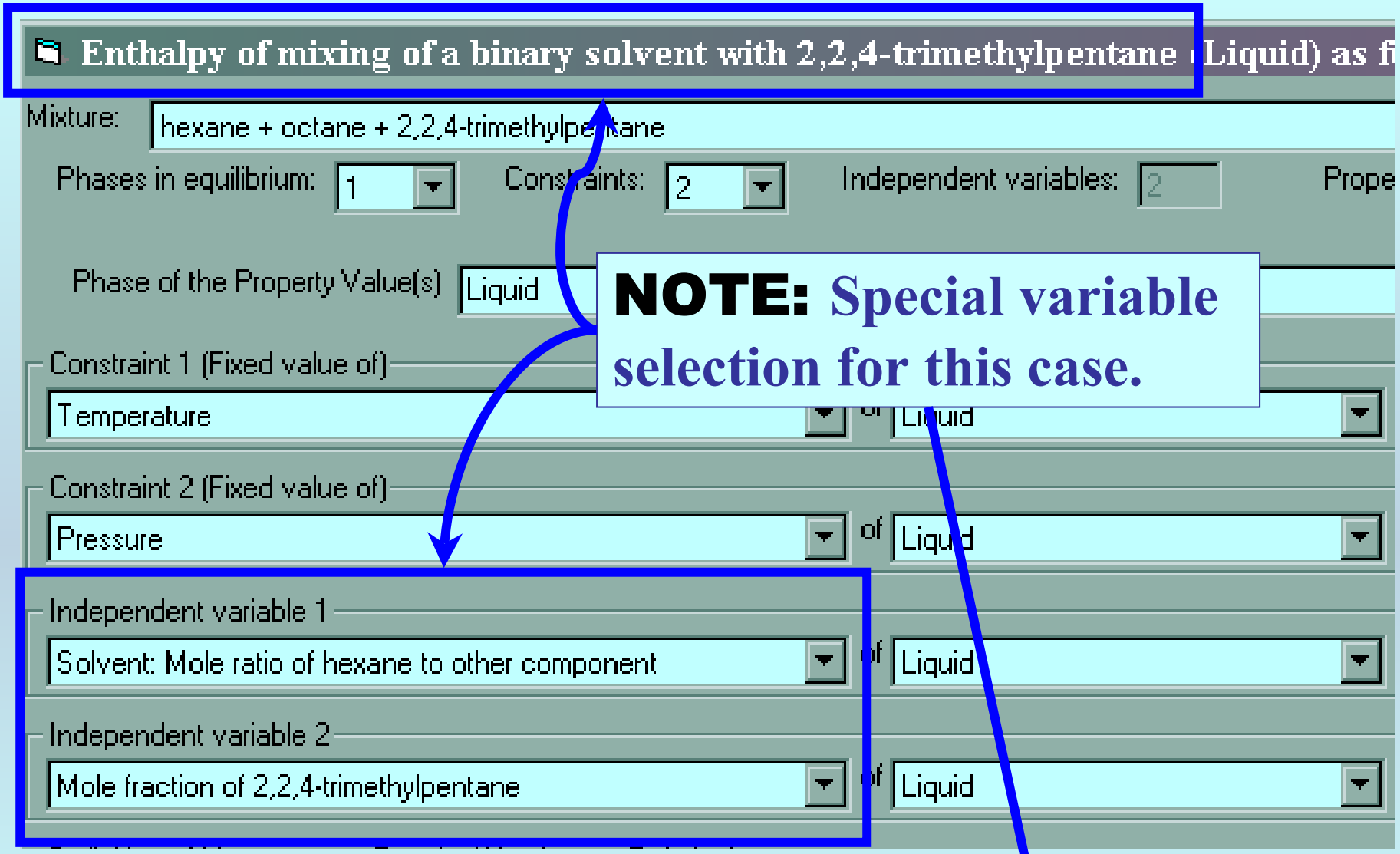
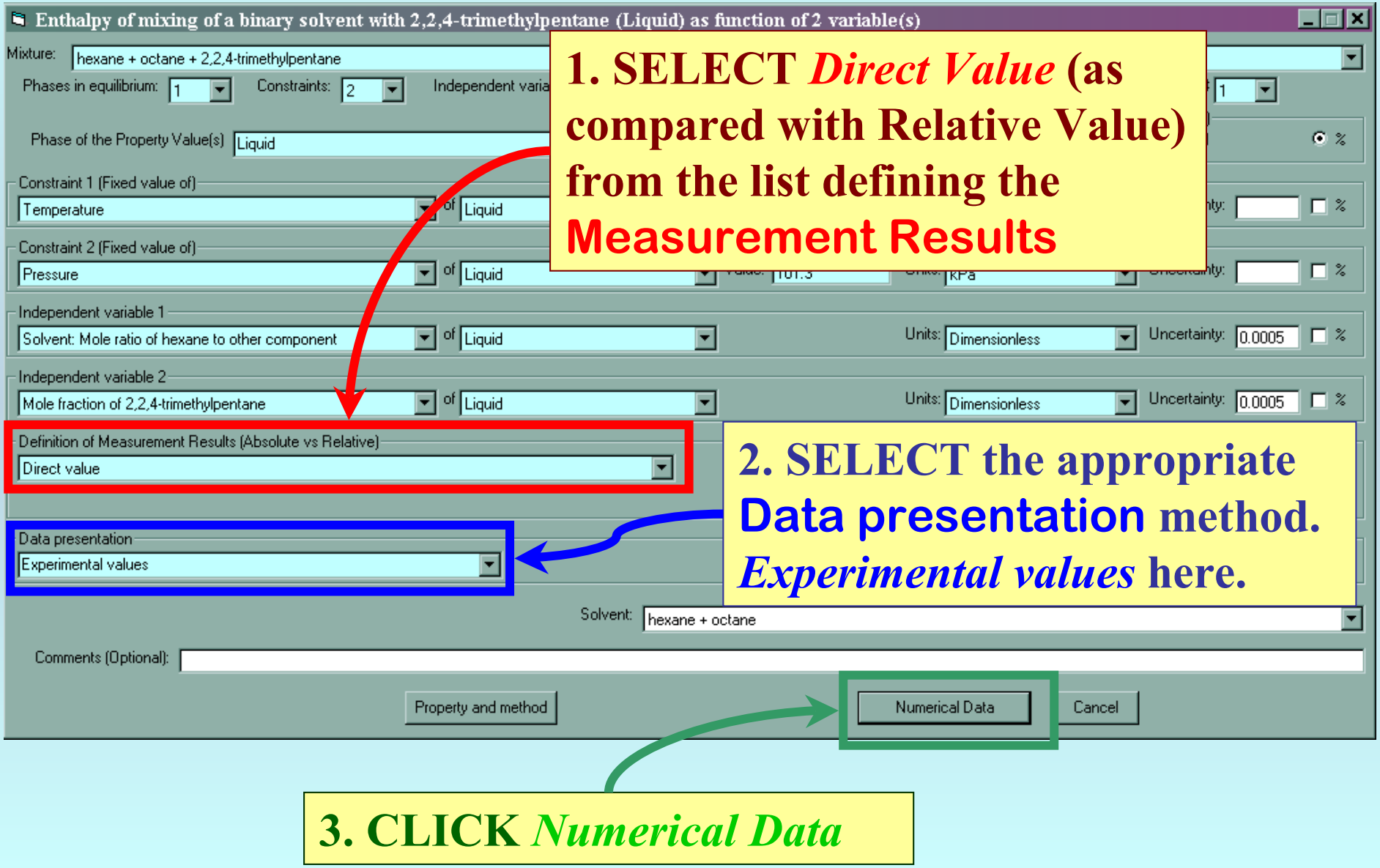
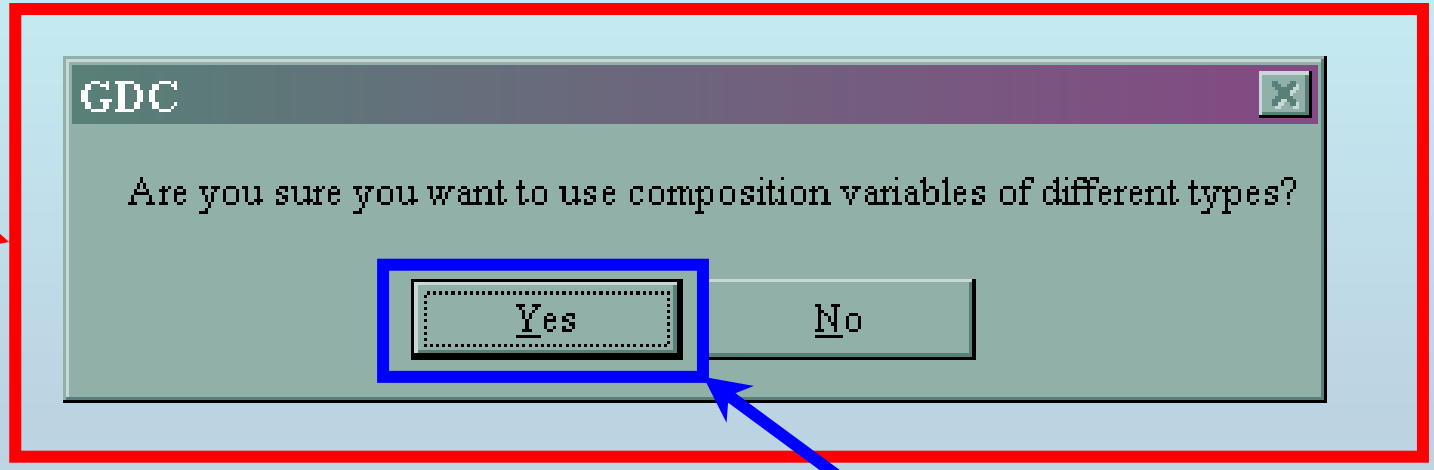


Table 3. Experimental Excess Molar Enthalpies $H^{E}_{m,1+23}$ Measured at 298.15 K, for the Addition of TMP to nC6 + nC8 Mixtures to Form TMP (1) + nC6 (2) + nC8 (3), and Values of $H^{E}_{m,123}$ Calculated from Eq 1

Measurement definition and Data presentation



1. This form will appear. The purpose is to minimize typographical errors.



2. CLICK *Yes*, here.

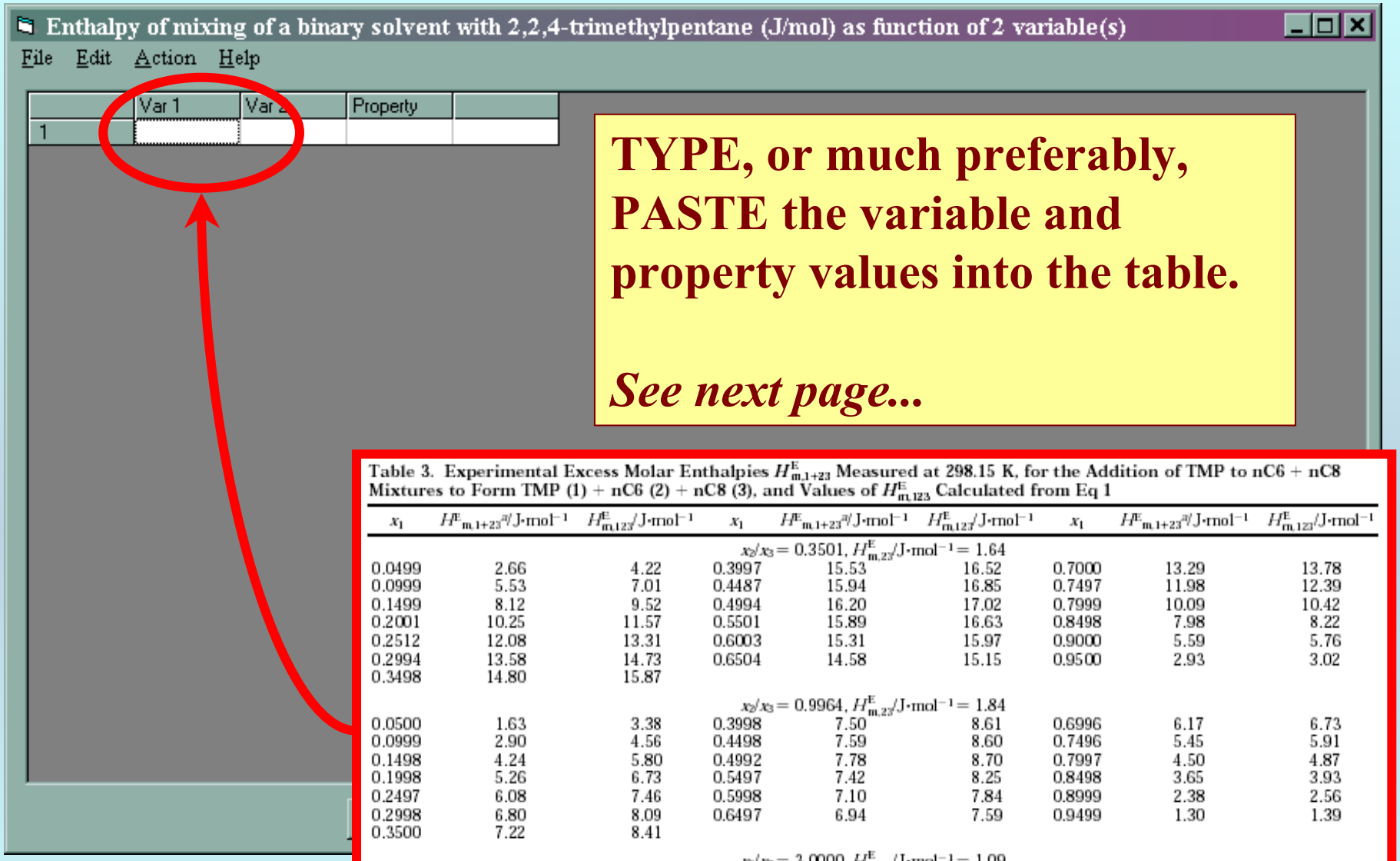


Table 3. Experimental Excess Molar Enthalpies $H^E_{m,1+23}$ Measured at 298.15 K, for the Addition of TMP to nC6 + nC8 Mixtures to Form TMP (1) + nC6 (2) + nC8 (3), and Values of $H^E_{m,123}$ Calculated from Eq 1

x_1	$H^E_{m,1+23}$[a]/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}	x_1	$H^E_{m,1+23}$[a]/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}	x_1	$H^E_{m,1+23}$[a]/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}
			$x_2/x_3 = 0.3501$, $H^E_{m,23}$/J·mol^{-1} = 1.64					
0.0499	2.66	4.22	0.3997	15.53	16.52	0.7000	13.29	13.78
0.0999	5.53	7.01	0.4487	15.94	16.85	0.7497	11.98	12.39
0.1499	8.12	9.52	0.4994	16.20	17.02	0.7999	10.09	10.42
0.2001	10.25	11.57	0.5501	15.89	16.63	0.8498	7.98	8.22
0.2512	12.08	13.31	0.6003	15.31	15.97	0.9000	5.59	5.76
0.2994	13.58	14.73	0.6504	14.58	15.15	0.9500	2.93	3.02
0.3498	14.80	15.87						
			$x_2/x_3 = 0.9964$, $H^E_{m,23}$/J·mol^{-1} = 1.84					
0.0500	1.63	3.38	0.3998	7.50	8.61	0.6996	6.17	6.73
0.0999	2.90	4.56	0.4498	7.59	8.60	0.7496	5.45	5.91
0.1498	4.24	5.80	0.4992	7.78	8.70	0.7997	4.50	4.87
0.1998	5.26	6.73	0.5497	7.42	8.25	0.8498	3.65	3.93
0.2497	6.08	7.46	0.5998	7.10	7.84	0.8999	2.38	2.56
0.2998	6.80	8.09	0.6497	6.94	7.59	0.9499	1.30	1.39
0.3500	7.22	8.41						
			$x_2/x_3 = 3.0000$, $H^E_{m,23}$/J·mol^{-1} = 1.09					
0.0499	−0.22	0.82	0.4004	−1.16	−0.50	0.6998	-1.30	-0.98
0.0999	−0.26	0.72	0.4497	−1.26	−0.66	0.7499	-1.36	-1.09
0.1500	−0.53	0.40	0.4994	−1.60	−1.06	0.7999	-1.17	-0.95
0.1998	−0.58	0.29	0.5502	−1.38	−0.88	0.8498	-0.92	-0.76
0.2494	−0.81	0.01	0.5999	−1.34	−0.90	0.9001	-0.67	-0.56
0.3002	−0.96	−0.19	0.6503	−1.49	−1.11	0.9500	-0.36	-0.31
0.3501	−1.10	−0.39						

Enthalpy of mixing of a binary solvent with 2,2,4-trimethylpentane (J/mol) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property	
1	0.3501	0.0499	2.66	4.22
2	0.3501	0.0999	5.53	7.01
3	0.3501	0.1499	8.12	9.52
4	0.3501	0.2001	10.25	11.57
5	0.3501	0.2512	12.08	13.31
6	0.3501	0.2994	13.58	14.73
7	0.3501	0.3498		
8	0.3501	0.3997		
9	0.3501	0.4487		
10	0.3501	0.4994		
11	0.3501	0.5501		
12	0.3501	0.6003		
13	0.3501	0.6504		
14	0.3501	0.7		
15	0.3501			
16	0.3501			
17	0.3501			
18	0.3501	0.9		
19	0.3501	0.9500		
20	0.9964	0.0500		
21	0.9964	0.0999		
22	0.9964	0.1498		
23	0.9964	0.1998		
24	0.9964	0.2497		
25	0.9964	0.2998		

Table 3. Experimental Excess Molar Enthalpies $H^E_{m,1+23}$ Measured at 298.15 K, for the Addition of TMP to nC6 + nC8 Mixtures to Form TMP (1) + nC6 (2) + nC8 (3), and Values of $H^E_{m,123}$ Calculated from Eq 1

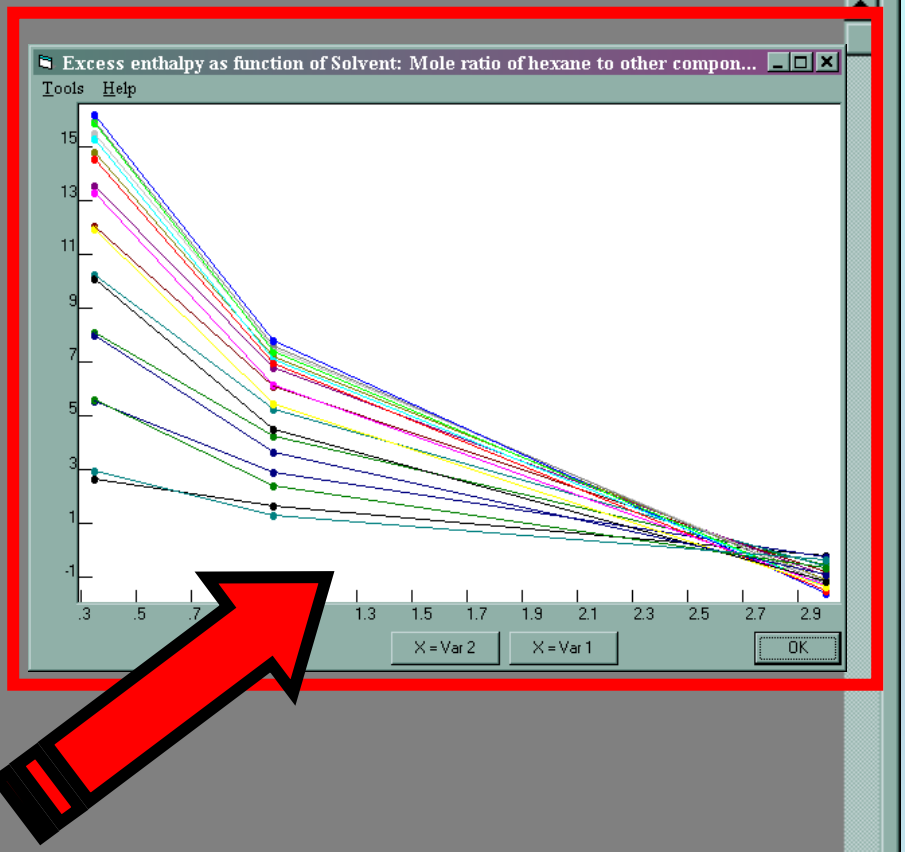
x_1	$H^E_{m,1+23}$/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}	x_1	$H^E_{m,1+23}$/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}	x_1	$H^E_{m,1+23}$/J·mol^{-1}	$H^E_{m,123}$/J·mol^{-1}
			$x_2/x_3 = 0.3501$, $H^E_{m,23}$/J·mol^{-1} = 1.64					
0.0499	2.66	4.22	0.3997	15.53	16.52	0.7000	13.29	13.78
0.0999	5.53	7.01	0.4487	15.94	16.85	0.7497	11.98	12.39
0.1499	8.12	9.52	0.4994	16.20	17.02	0.7999	10.09	10.42
0.2001	10.25	11.57	0.5501	15.89	16.63	0.8498	7.98	8.22
0.2512	12.08	13.31	0.6003	15.31	15.97	0.9000	5.59	5.76
		14.73	0.6504	14.58	15.15	0.9500	2.93	3.02
		15.87						
			$x_2/x_3 = 0.9964$, $H^E_{m,23}$/J·mol^{-1} = 1.84					
0.0500	1.63	3.38	0.3998	7.50	8.61	0.6996	6.17	6.73
0.0999	2.90	4.56	0.4498	7.59	8.60	0.7496	5.45	5.91
0.1498	4.24	5.80	0.4992	7.78	8.70	0.7997	4.50	4.87
0.1998	5.26	6.73	0.5497	7.42	8.25	0.8498	3.65	3.93
0.2497	6.08	7.46	0.5998	7.10	7.84	0.8999	2.38	2.56
0.2998	6.80	8.09	0.6497	6.94	7.59	0.9499	1.30	1.39
0.3500	7.22	8.41						
			$x_2/x_3 = 3.0000$, $H^E_{m,23}$/J·mol^{-1} = 1.09					
0.0499	−0.22	0.82	0.4004	−1.16	−0.50	0.6998	-1.30	-0.98
0.0999	−0.26	0.72	0.4497	−1.26	−0.66	0.7499	-1.36	-1.09
0.1500	−0.53	0.40	0.4994	−1.60	−1.06	0.7999	-1.17	-0.95
0.1998	−0.58	0.29	0.5502	−1.38	−0.88	0.8498	-0.92	-0.76
0.2494	−0.81	0.01	0.5999	−1.34	−0.90	0.9001	-0.67	-0.56
0.3002	−0.96	−0.19	0.6503	−1.49	−1.11	0.9500	-0.36	-0.31
0.3501	−1.10	−0.39						

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.)

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

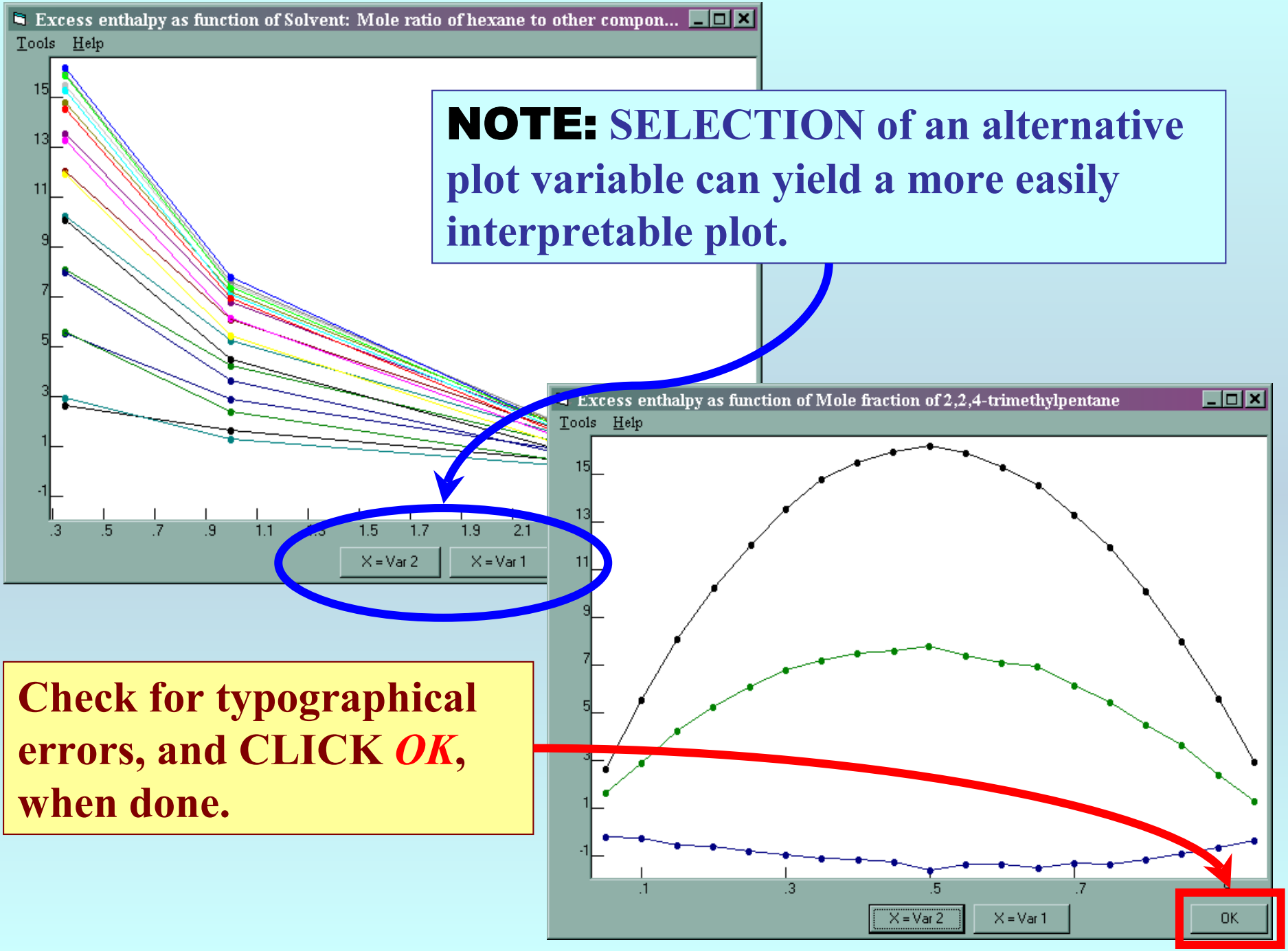
File Edit Action Help

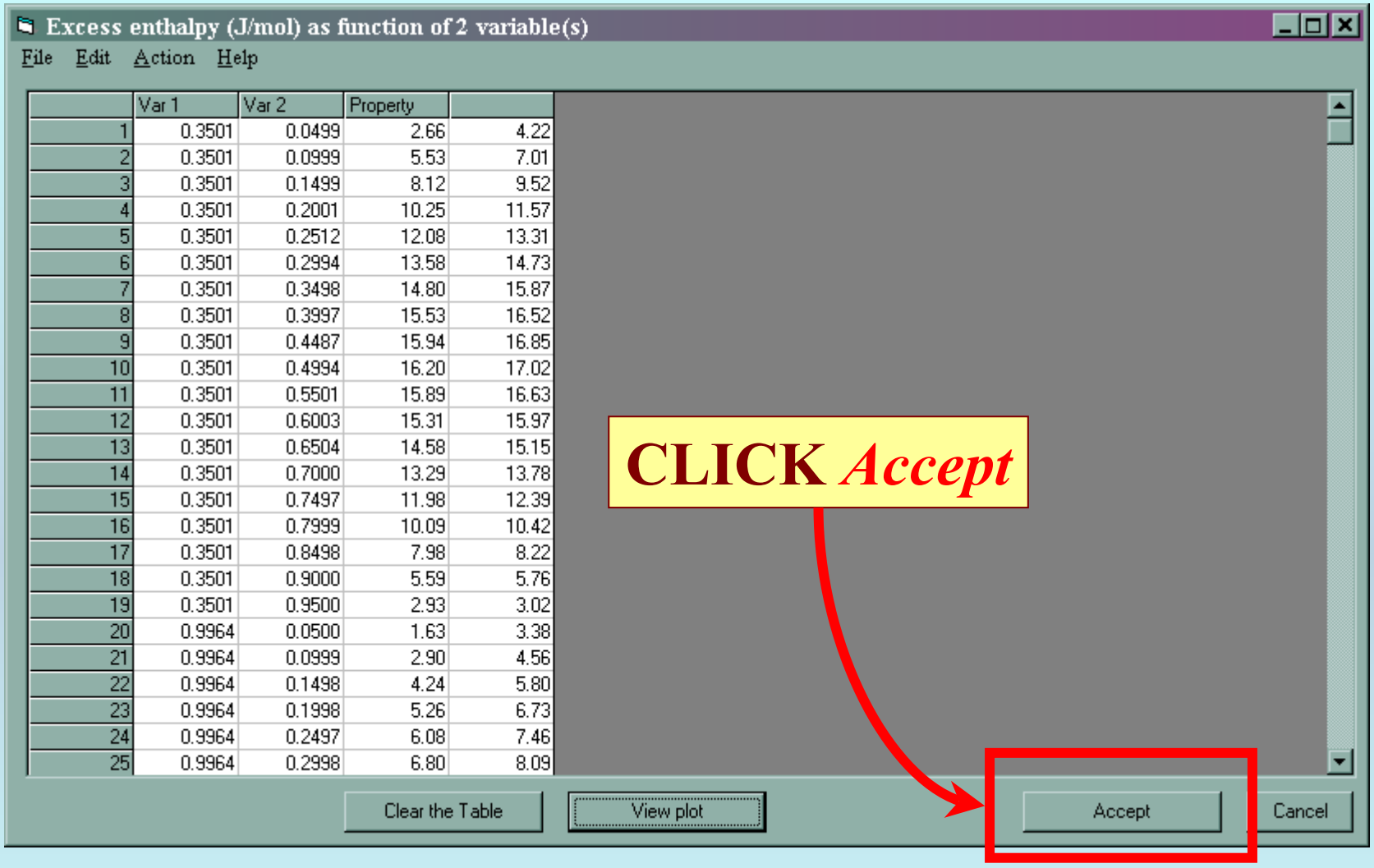
	Var 1	Var 2	Property	
1	0.3501	0.0499	2.66	4.22
2	0.3501	0.0999	5.53	7.01
3	0.3501	0.1499	8.12	9.52
4	0.3501	0.2001	10.25	11.57
5	0.3501	0.2512	12.08	13.31
6	0.3501	0.2994	13.58	14.73
7	0.3501	0.3498	14.80	15.87
8	0.3501	0.3997	15.53	16.52
9	0.3501	0.4487	15.94	16.85
10	0.3501	0.4994	16.20	17.02
11	0.3501	0.5501	15.89	16.63
12	0.3501	0.6003	15.31	15.97
13	0.3501	0.6504	14.58	15.15
14	0.3501	0.7000	13.29	13.78
15	0.3501	0.7497	11.98	12.39
16	0.3501	0.7999	10.09	10.42
17	0.3501	0.8498	7.98	8.22
18	0.3501	0.9000	5.59	5.76
19	0.3501	0.9500	2.93	3.02
20	0.9964	0.0500	1.63	3.38
21	0.9964	0.0999	2.90	4.56
22	0.9964	0.1498	4.24	5.80
23	0.9964	0.1998	5.26	6.73
24	0.9964	0.2497	6.08	7.46
25	0.9964	0.2998	6.80	8.0

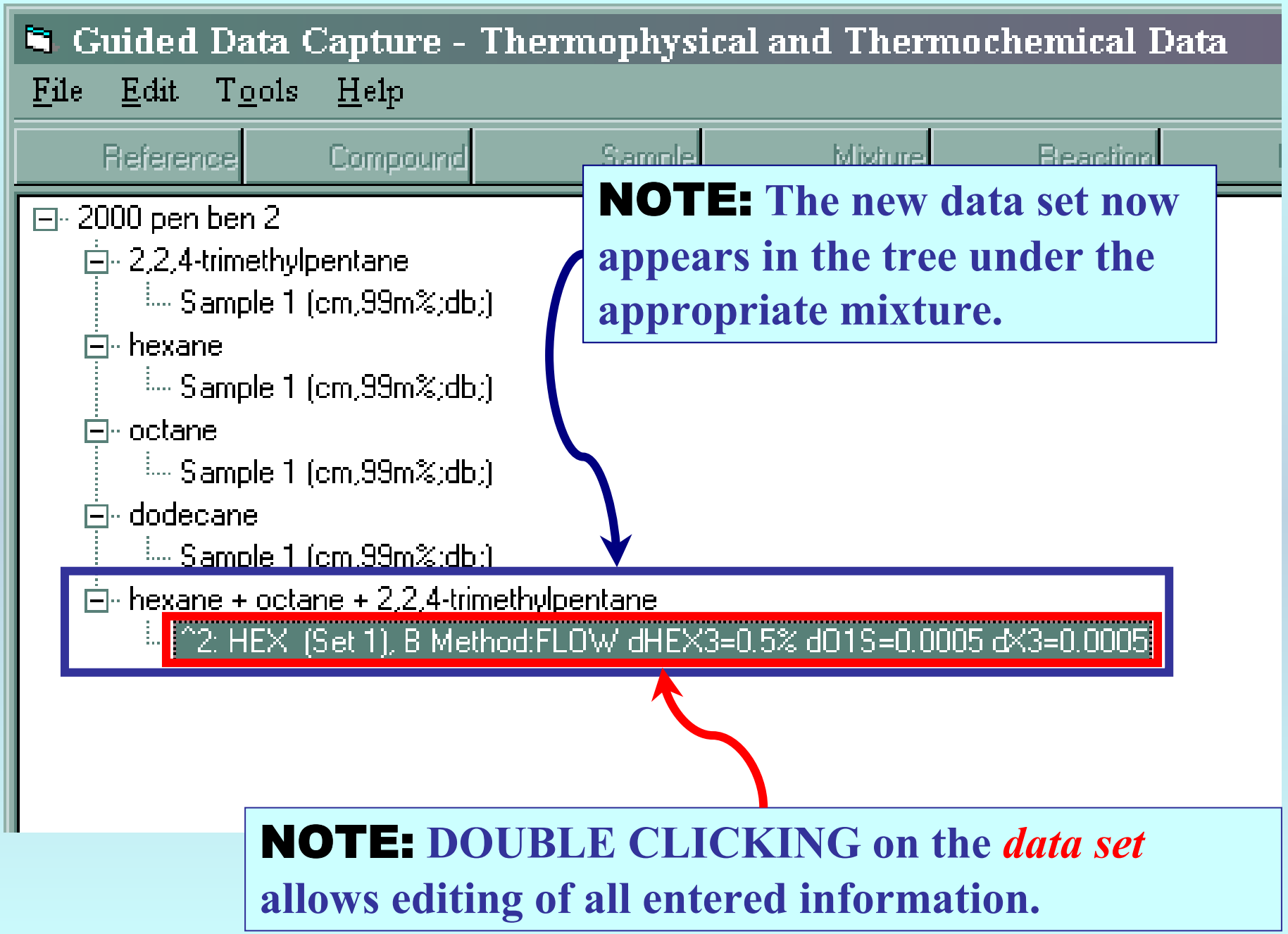


Clear the Table | View plot | Accept | Cancel

CLICK *View plot* to see a graphical representation of the data. *See next page...*


Excess enthalpy as function of Solvent: Mole ratio of hexane to other compon...
Tools Help
15
13
11
9
7
5
3
1
-1
.3 .5 .7 .9 1.1 1.5 1.7 1.9 2.1
X = Var 2
X = Var 1
NOTE: SELECTION of an alternative plot variable can yield a more easily interpretable plot.
Excess enthalpy as function of Mole fraction of 2,2,4-trimethylpentane
Tools Help
15
13
11
9
7
5
1
-1
.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 0.3501 0.0499 2.66 4.22
2 0.3501 0.0999 5.53 7.01
3 0.3501 0.1499 8.12 9.52
4 0.3501 0.2001 10.25 11.57
5 0.3501 0.2512 12.08 13.31
6 0.3501 0.2994 13.58 14.73
7 0.3501 0.3498 14.80 15.87
8 0.3501 0.3997 15.53 16.52
9 0.3501 0.4487 15.94 16.85
10 0.3501 0.4994 16.20 17.02
11 0.3501 0.5501 15.89 16.63
12 0.3501 0.6003 15.31 15.97
13 0.3501 0.6504 14.58 15.15
14 0.3501 0.7000 13.29 13.78
15 0.3501 0.7497 11.98 12.39
16 0.3501 0.7999 10.09 10.42
17 0.3501 0.8498 7.98 8.22
18 0.3501 0.9000 5.59 5.76
19 0.3501 0.9500 2.93 3.02
20 0.9964 0.0500 1.63 3.38
21 0.9964 0.0999 2.90 4.56
22 0.9964 0.1498 4.24 5.80
23 0.9964 0.1998 5.26 6.73
24 0.9964 0.2497 6.08 7.46
25 0.9964 0.2998 6.80 8.09
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction
2000 pen ben 2
2,2,4-trimethylpentane
Sample 1 (cm,99m%;db;)
hexane
Sample 1 (cm,99m%;db;)
octane
Sample 1 (cm,99m%;db;)
dodecane
Sample 1 (cm,99m%;db;)
hexane + octane + 2,2,4-trimethylpentane
^2: HEX (Set 1), B Method:FLOW dHEX3=0.5% dO1S=0.0005 dX3=0.0005
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.**