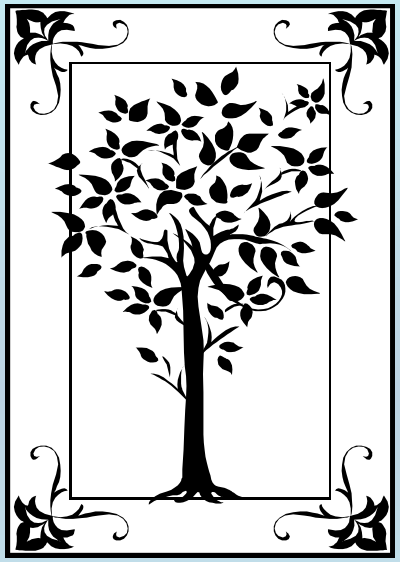
METADATA AND NUMERICAL DATA CAPTURE:
Vapor-Liquid Equilibria: PTxy
(2 component mixture)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Vapor-Liquid Equilibria (2 components)**
PTxy
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 2002, *47*, 1098−1102

Articles

Isobaric Vapor−Liquid Equilibria of Diethyl Carbonate with Four Alkanes at 101.3 kPa

A. Rodríguez, J. Canosa, A. Domínguez, and J. Tojo*

Chemical Engineering Department, Vigo University, 36200 Vigo, Spain

Isobaric vapor−liquid equilibria have been measured for the four binary systems hexane + diethyl carbonate (DEC), DEC + heptane, DEC + octane, and cyclohexane + DEC at 101.3 kPa. The activity coefficients were found to be thermodynamically consistent and were satisfactorily correlated with the Wilson and UNIQUAC equations. They were also compared with results obtained from the application of the ASOG and UNIFAC group contribution methods.

VLE data for **(heptane + diethylcarbonate)** at p = 101.3 kPa

Table 5. Vapor−Liquid Equilibrium Data for the Heptane (1) + DEC (2) System at 101.3 kPa

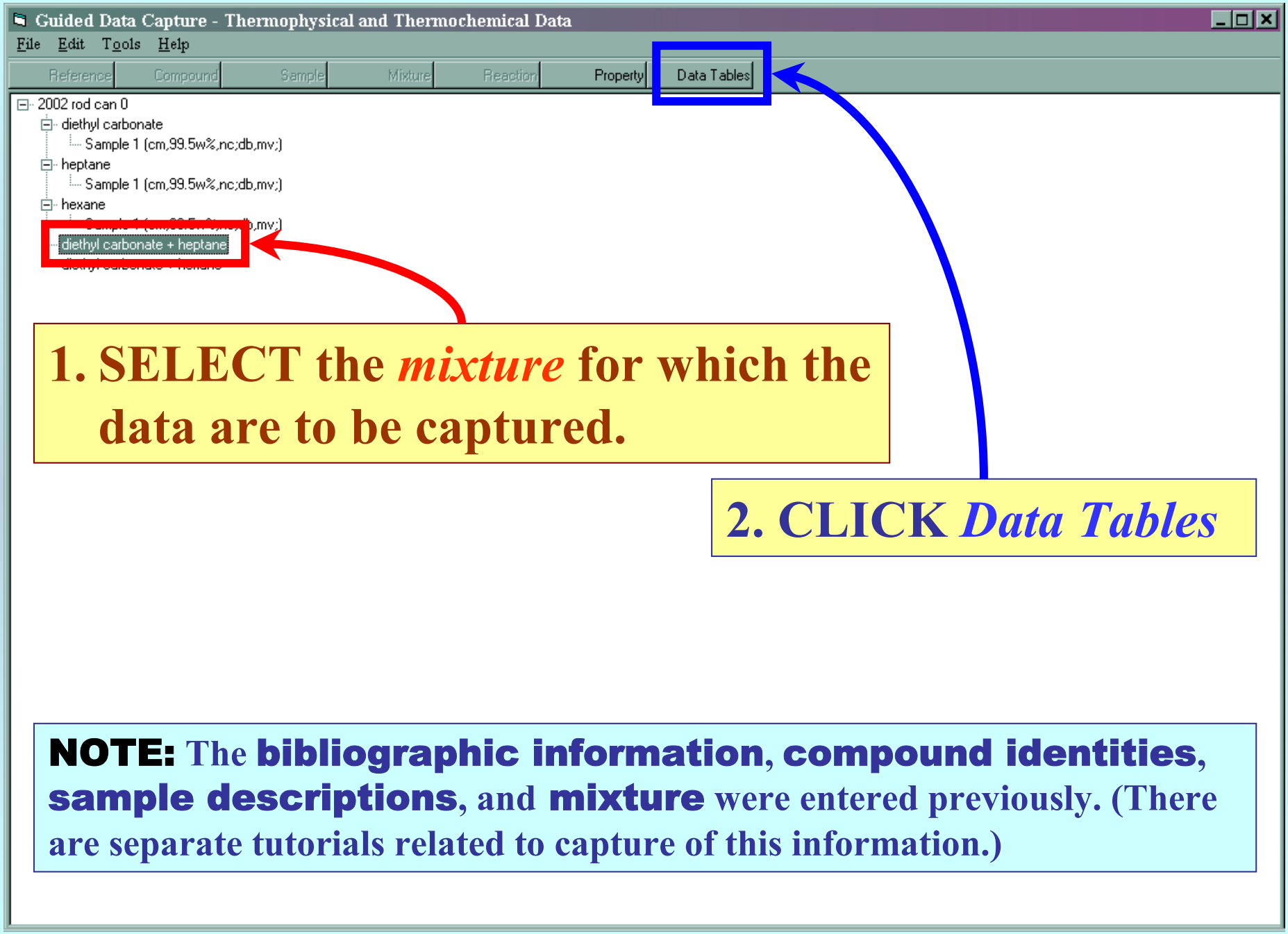
T/K	x	y	γ_1	γ_2
398.17	0.0133	0.0614	2.366	0.975
397.09	0.0213	0.0935	2.309	0.978
394.61	0.0438	0.1677	2.133	0.985
392.20	0.0695	0.2326	1.974	0.999
390.80	0.0858	0.2746	1.951	1.001
389.21	0.1064	0.3160	1.881	1.011
387.08	0.1381	0.3711	1.794	1.027
384.73	0.1782	0.4324	1.718	1.043
383.04	0.2175	0.4775	1.621	1.062
381.48	0.2595	0.5204	1.541	1.081
379.95	0.3083	0.5643	1.463	1.103
379.31	0.3390	0.5833	1.399	1.127
378.21	0.3805	0.6173	1.357	1.143
377.72	0.4039	0.6330	1.328	1.158
376.97	0.4448	0.6580	1.27	1.187
375.97	0.4930	0.6933	1.248	1.204
375.40	0.5322	0.7149	1.211	1.236
374.87	0.5660	0.7336	1.185	1.26
374.48	0.5934	0.7502	1.168	1.284
373.79	0.6514	0.7766	1.122	1.371
373.33	0.6882	0.7980	1.105	1.407
373.05	0.7235	0.8172	1.085	1.450
372.65	0.7658	0.8380	1.063	1.538
372.32	0.8175	0.8649	1.037	1.665
372.14	0.8526	0.8872	1.025	1.732
371.96	0.8833	0.9042	1.013	1.870
371.77	0.9262	0.9352	1.004	2.015
371.62	0.9580	0.9605	1.001	2.169
371.49	0.9774	0.9786	1.004	2.197

This data set is considered here.

Experimental Method:

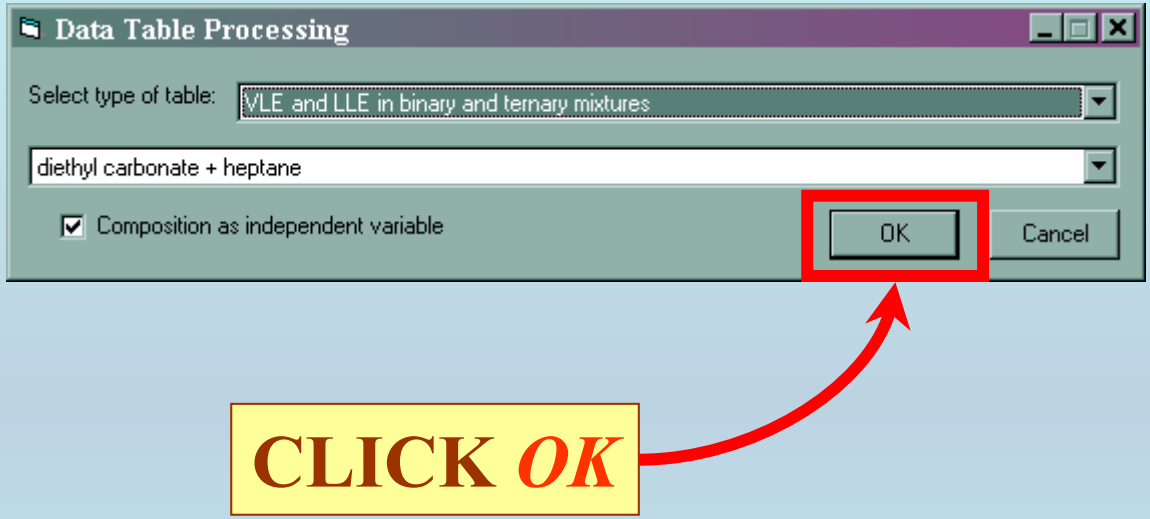
Apparatus and Procedure. A glass Fischer LABODEST VLE apparatus model 602/D, manufactured by Fischer Labor und Verfahrenstechnik (Germany), was used in the equilibrium determinations. The equilibrium vessel was a dynamic recirculating still, equipped with a Cottrell circulation pump. This pump ensures that both liquid and

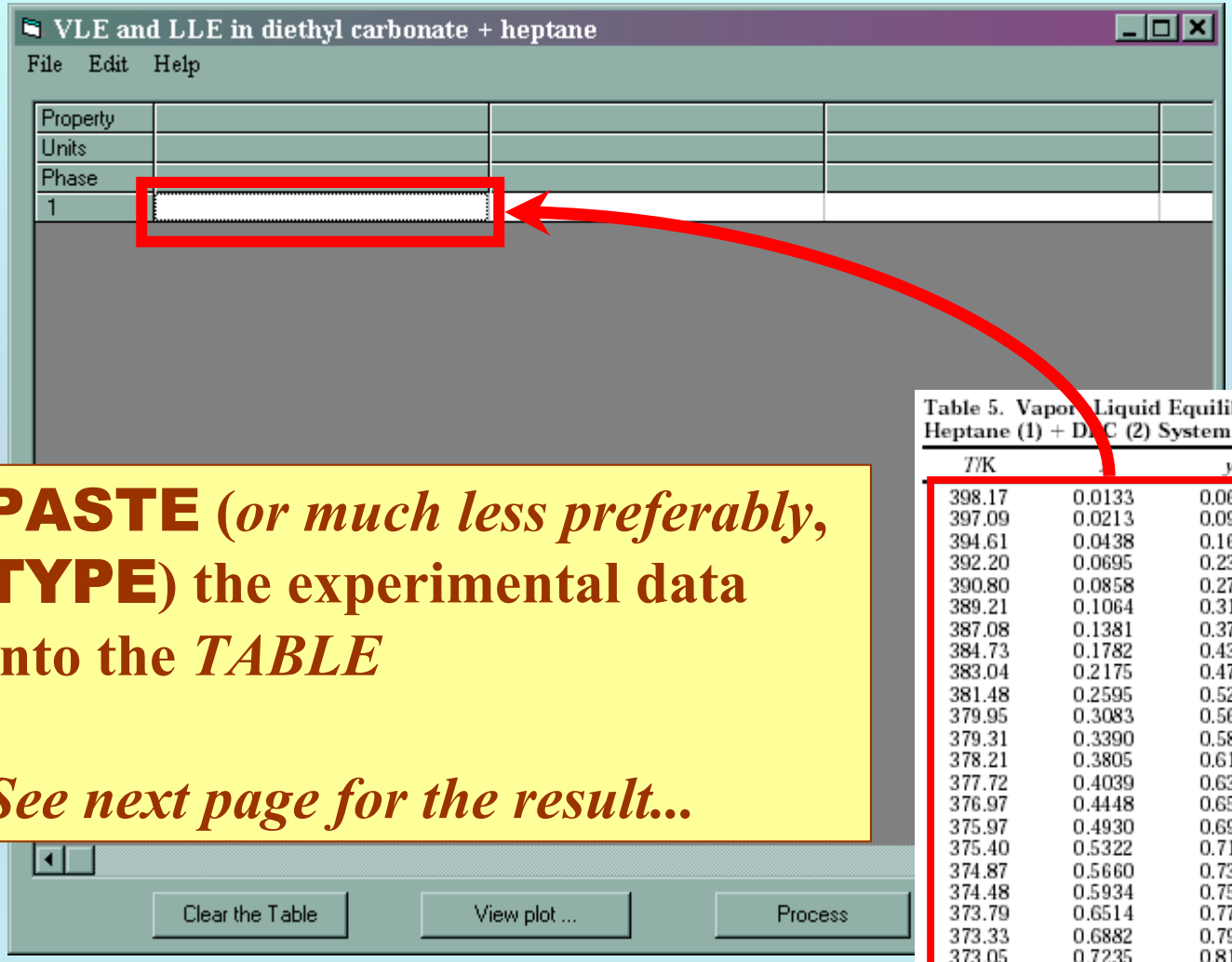
analysis. The composition analysis of both samples was determined using an Anton-Paar DSA-48 digital vibrating tube densimeter. Densimetry was used to establish standard curves for each binary system after the density–composition curves for the mixtures had been plotted. The root-mean-square deviation in the mole fraction was usually <0.001.



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

This form appears:





PASTE (*or much less preferably*, **TYPE**) **the experimental data into the *TABLE***

See next page for the result...

Table 5. Vapor–Liquid Equilibrium Data for the Heptane (1) + DEC (2) System at 101.3 kPa

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375.40	0.5322	0.7149	1.211	1.236
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373.79	0.6514	0.7766	1.122	1.371
373.33	0.6882	0.7980	1.105	1.407
373.05	0.7235	0.8172	1.085	1.450
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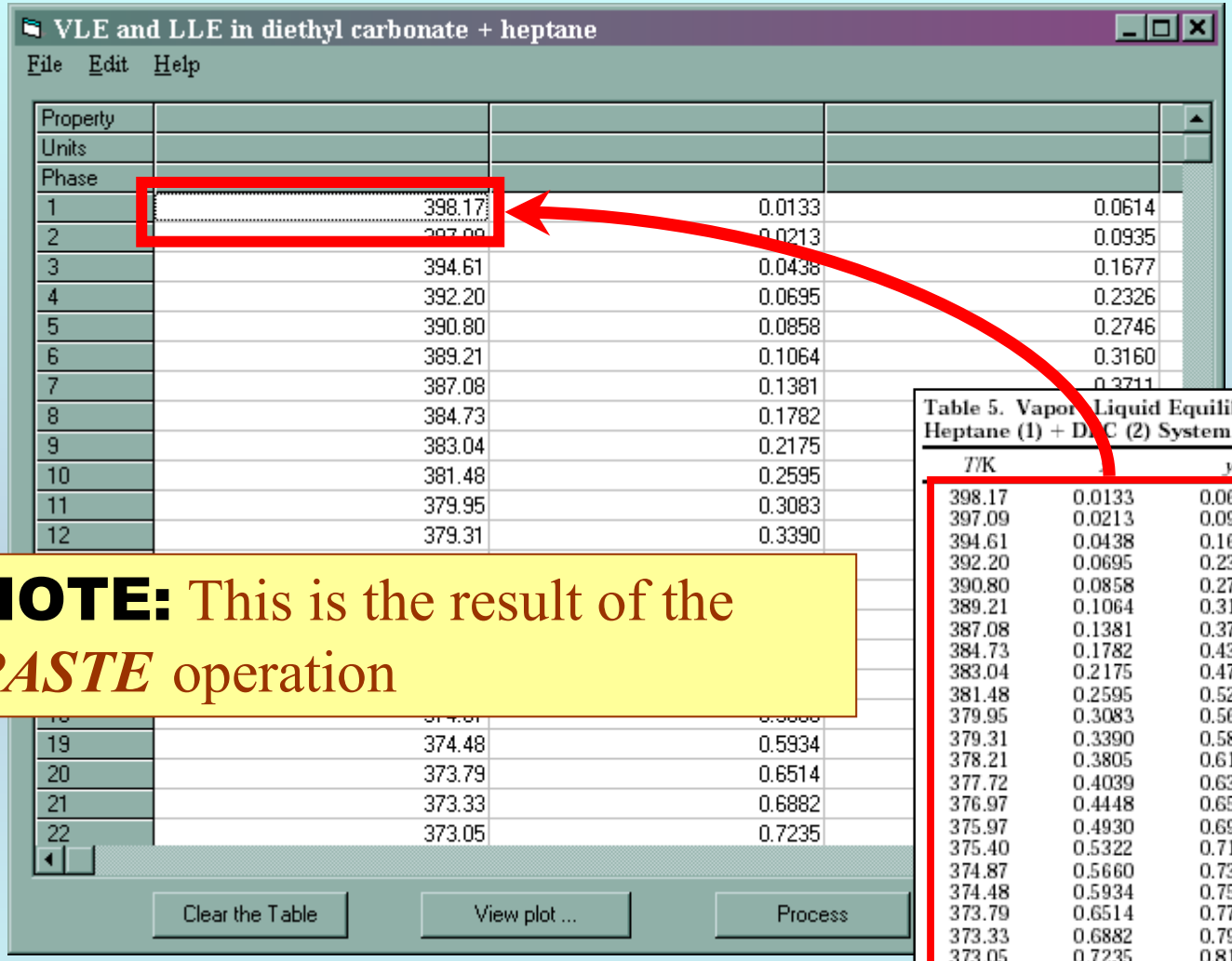

NOTE: This is the result of the ***PASTE*** operation

Table 5. Vapor–Liquid Equilibrium Data for the Heptane (1) + DEC (2) System at 101.3 kPa

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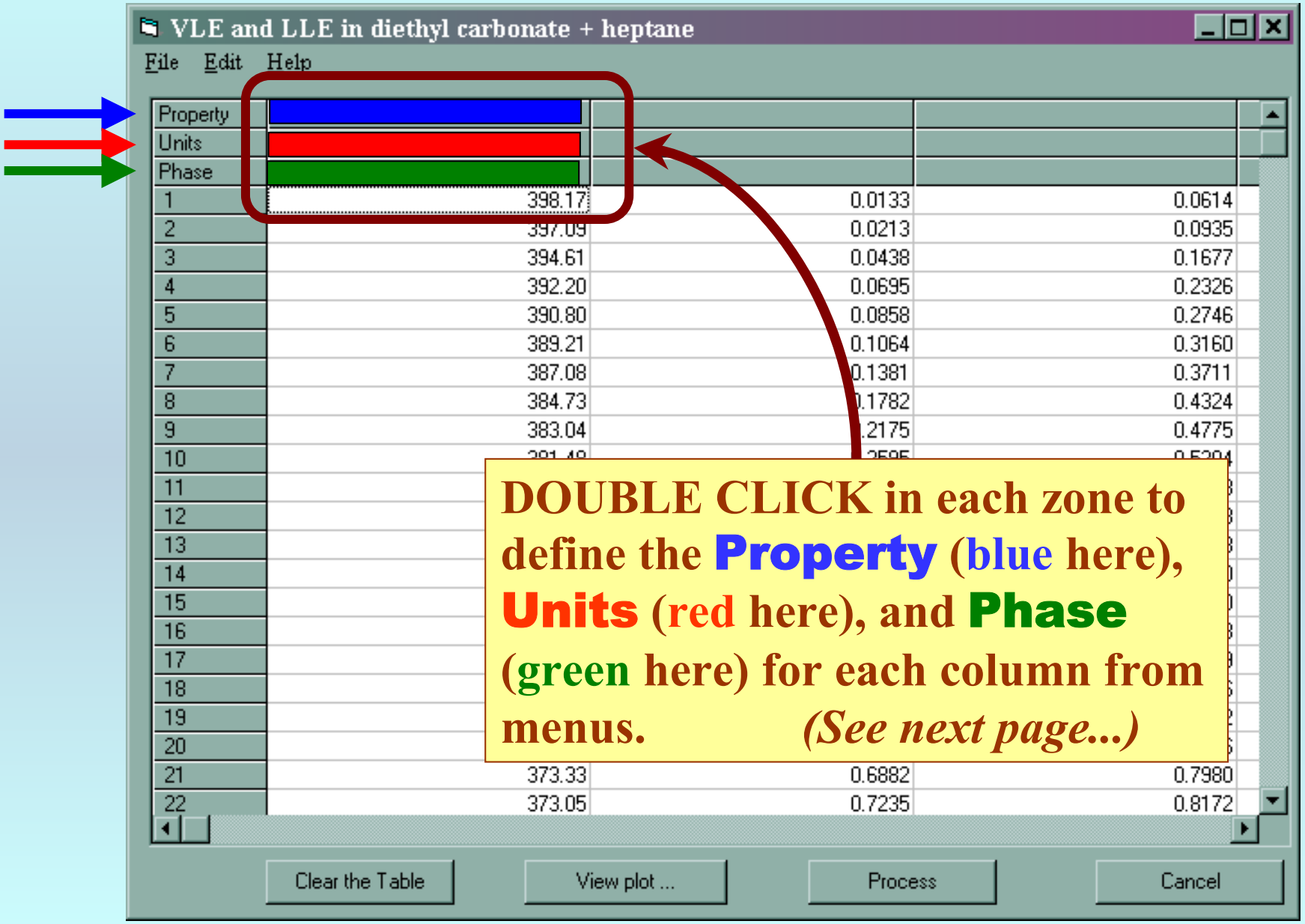
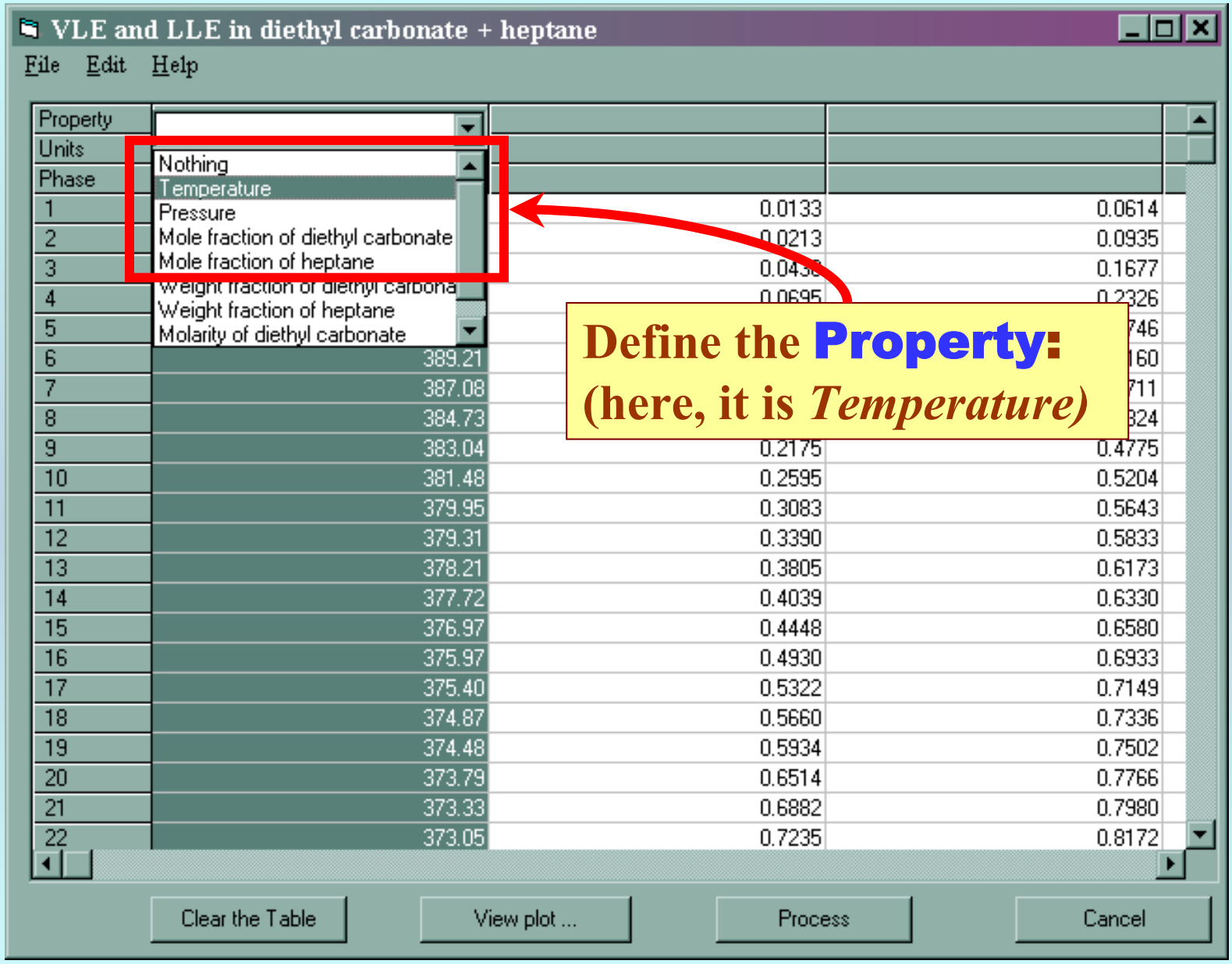
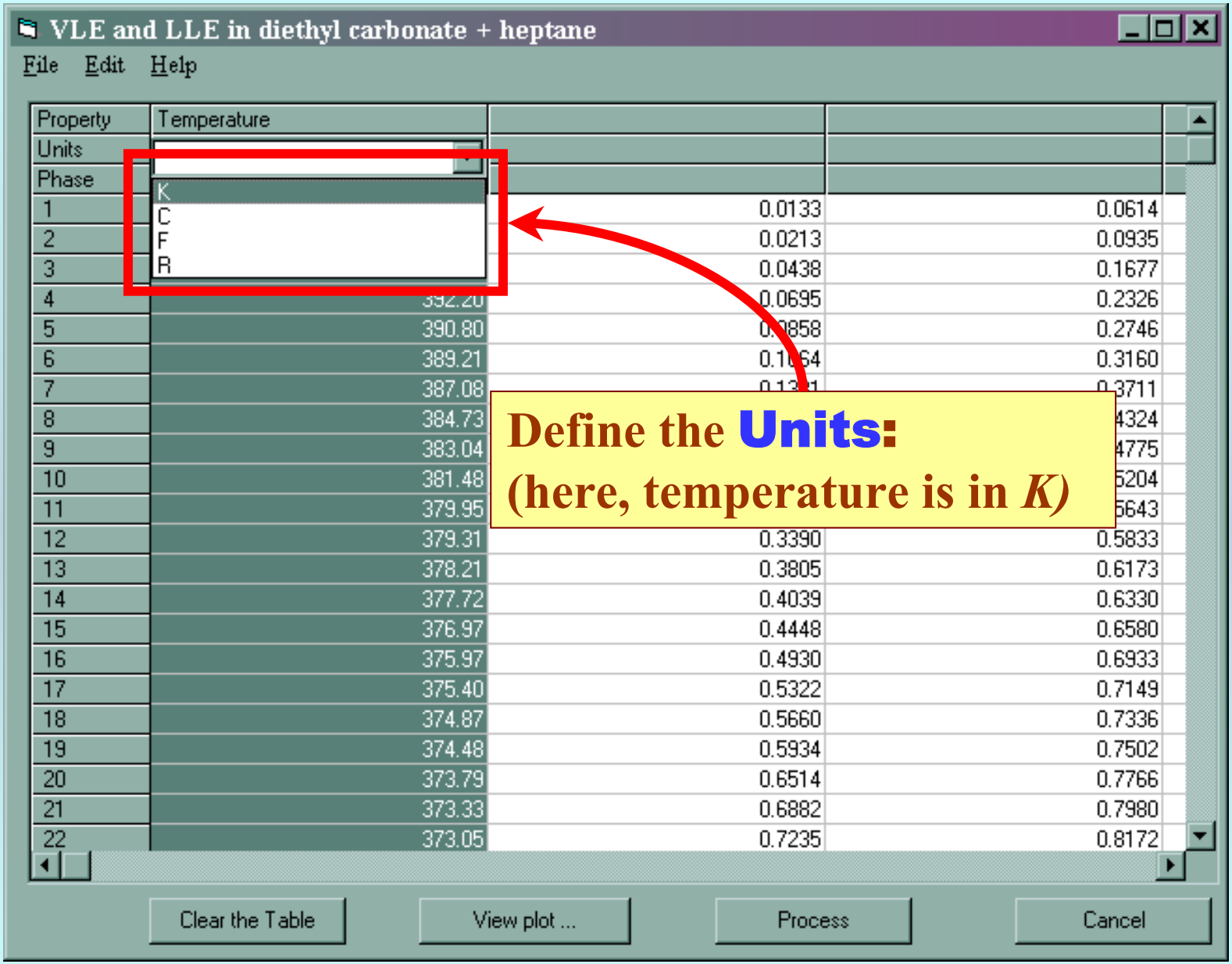
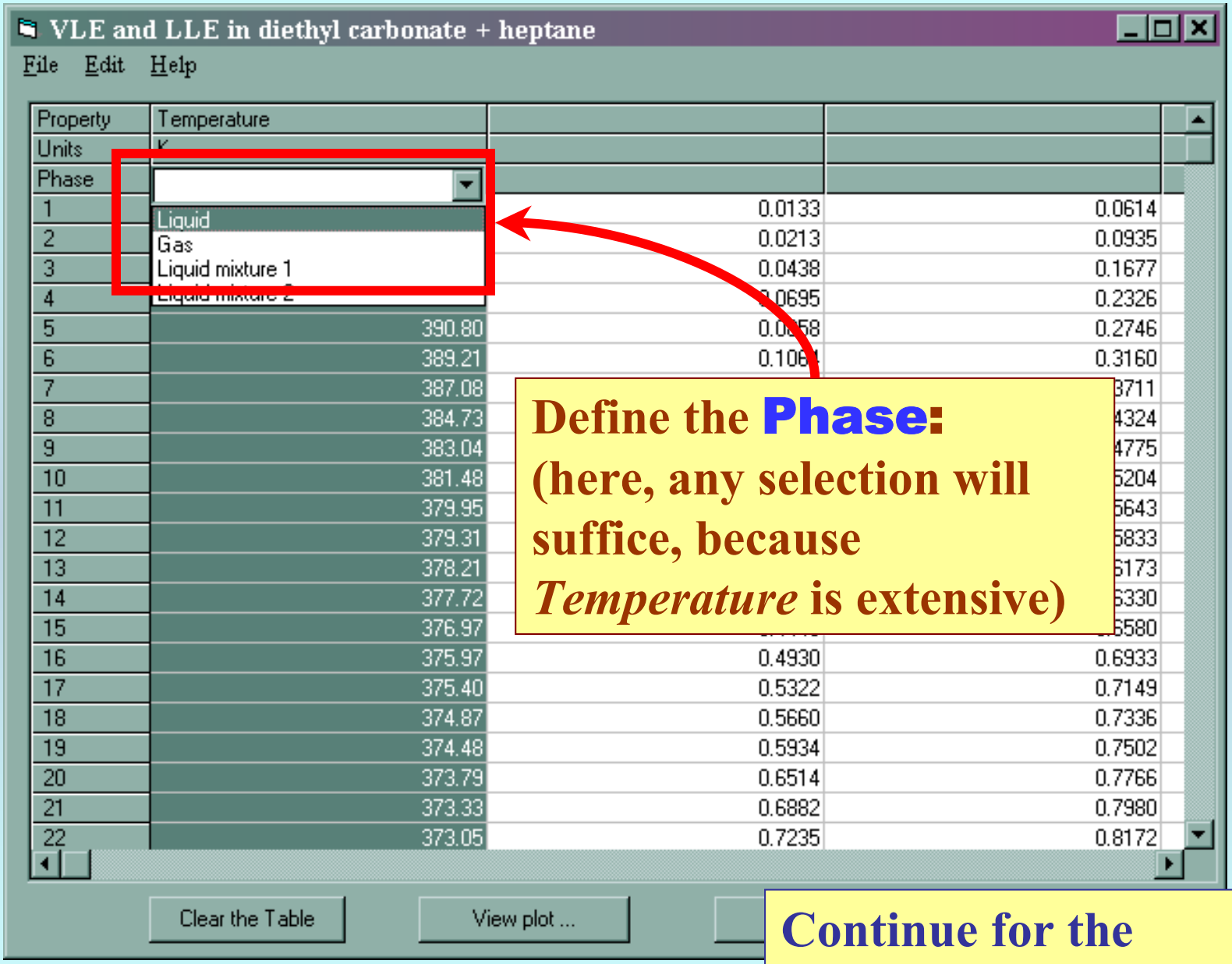
371.49	0.9774	0.9786	1.004	2.197

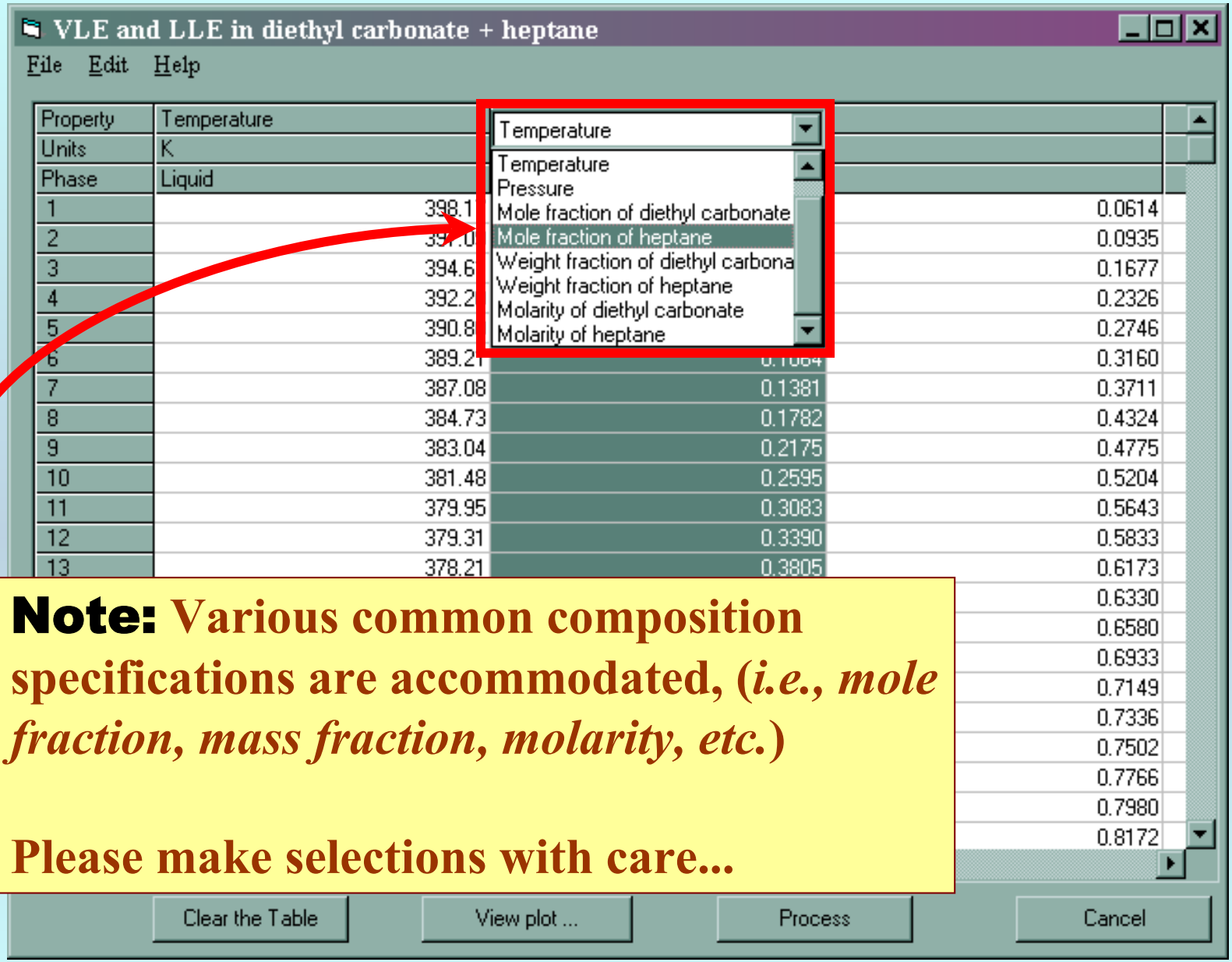
Property, Units, and Phase Definitions:




VLE and LLE in diethyl carbonate + heptane
File
Edit
Help
Property
Units
Phase
Nothing
Temperature
Pressure
Mole fraction of diethyl carbonate
Mole fraction of heptane
Weight fraction of heptane
Molarity of diethyl carbonate
1 0.0133 0.0614
2 0.0213 0.0935
3 0.1677
4
5
6 389.21
7 387.08
8 384.73
9 383.04 0.2175 0.4775
10 381.48 0.2595 0.5204
11 379.95 0.3083 0.5643
12 379.31 0.3390 0.5833
13 378.21 0.3805 0.6173
14 377.72 0.4039 0.6330
15 376.97 0.4448 0.6580
16 375.97 0.4930 0.6933
17 375.40 0.5322 0.7149
18 374.87 0.5660 0.7336
19 374.48 0.5934 0.7502
20 373.79 0.6514 0.7766
21 373.33 0.6882 0.7980
22 373.05 0.7235 0.8172
Clear the Table
View plot ...
Process
Cancel
Define the Property:
(here, it is Temperature)


VLE and LLE in diethyl carbonate + heptane
File
Edit
Help
Property
Temperature
Units
Phase
K
C
F
R
1 0.0133 0.0614
2 0.0213 0.0935
3 0.0438 0.1677
4 0.0695 0.2326
5 390.80 0.2746
6 389.21 0.3160
7 387.08
8 384.73
9 383.04
10 381.48
11 379.95
12 379.31 0.3390 0.5833
13 378.21 0.3805 0.6173
14 377.72 0.4039 0.6330
15 376.97 0.4448 0.6580
16 375.97 0.4930 0.6933
17 375.40 0.5322 0.7149
18 374.87 0.5660 0.7336
19 374.48 0.5934 0.7502
20 373.79 0.6514 0.7766
21 373.33 0.6882 0.7980
22 373.05 0.7235 0.8172
Define the Units:
(here, temperature is in K)
Clear the Table
View plot ...
Process
Cancel

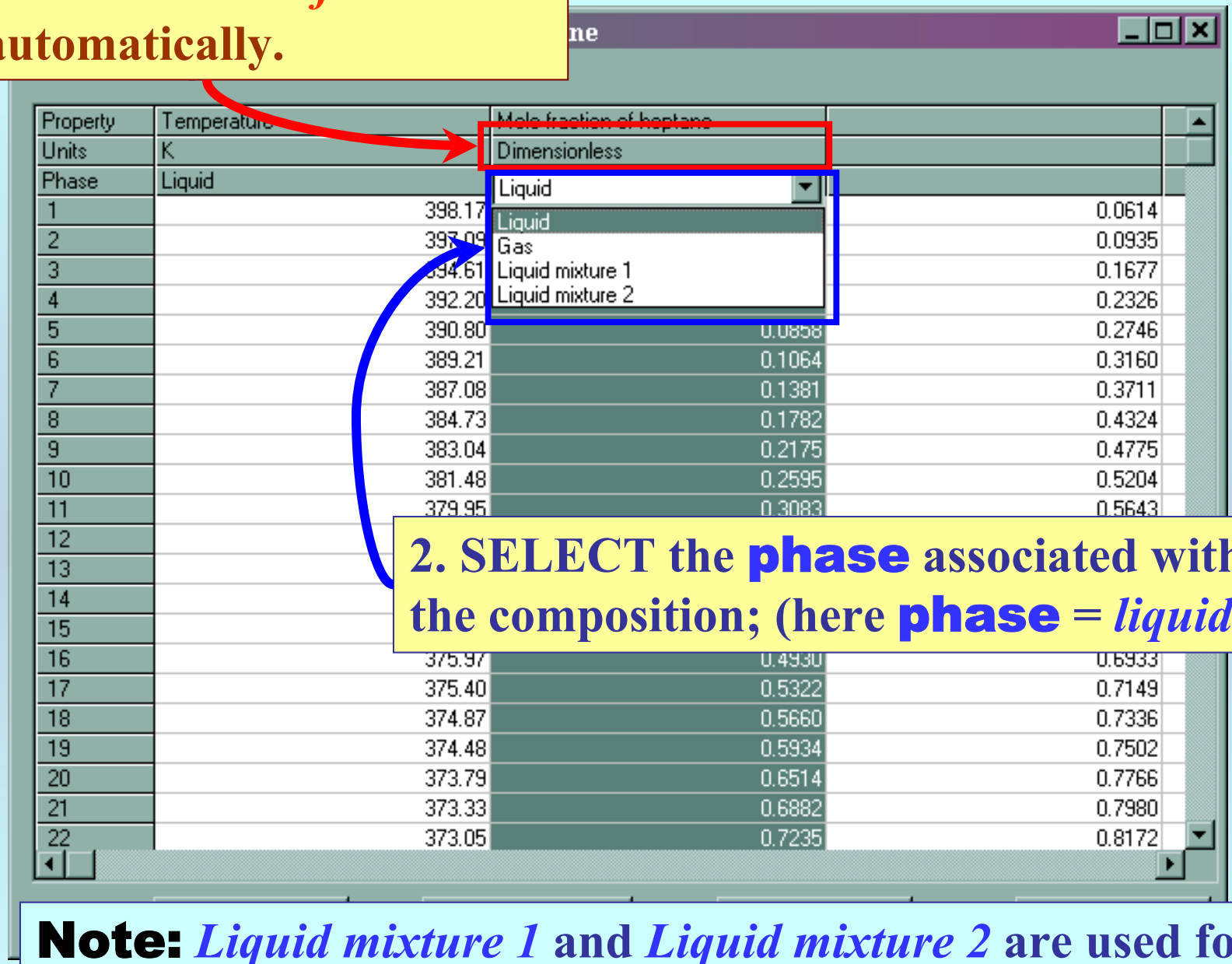

VLE and LLE in diethyl carbonate + heptane
File Edit Help
Property
Temperature
Units
K
Phase
Liquid
Gas
Liquid mixture 1
Liquid mixture 2
1 0.0133 0.0614
2 0.0213 0.0935
3 0.0438 0.1677
4 0.0695 0.2326
5 390.80 0.0858 0.2746
6 389.21 0.1064 0.3160
7 387.08 3711
8 384.73 4324
9 383.04 4775
10 381.48 5204
11 379.95 5643
12 379.31 5833
13 378.21 6173
14 377.72 6330
15 376.97 6580
16 375.97 0.4930 0.6933
17 375.40 0.5322 0.7149
18 374.87 0.5660 0.7336
19 374.48 0.5934 0.7502
20 373.79 0.6514 0.7766
21 373.33 0.6882 0.7980
22 373.05 0.7235 0.8172
Clear the Table
View plot ...
Define the Phase:
(here, any selection will suffice, because
Temperature is extensive)
Continue for the remaining columns...



Note: Various common composition specifications are accommodated, (*i.e., mole fraction, mass fraction, molarity, etc.*)

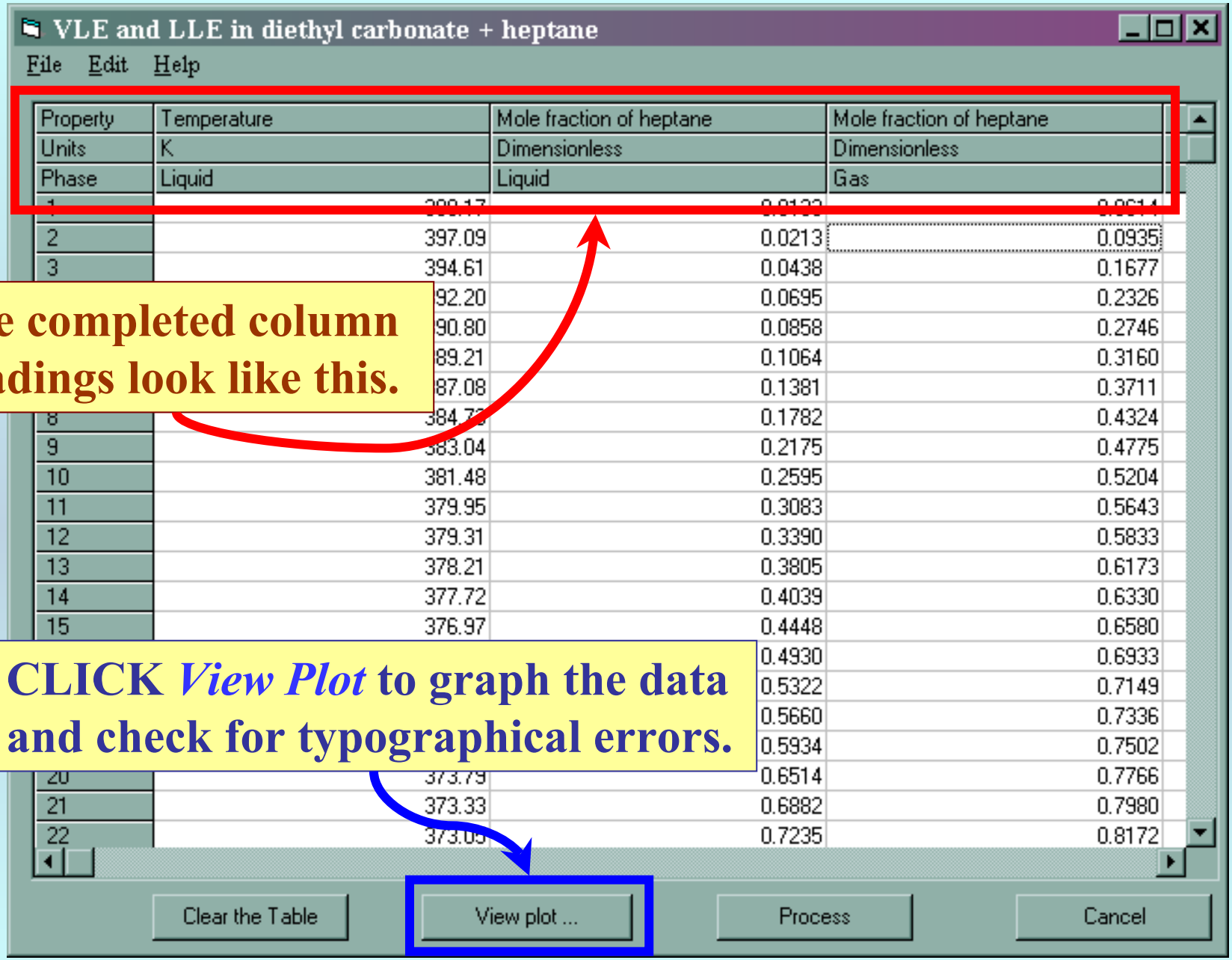
Please make selections with care...

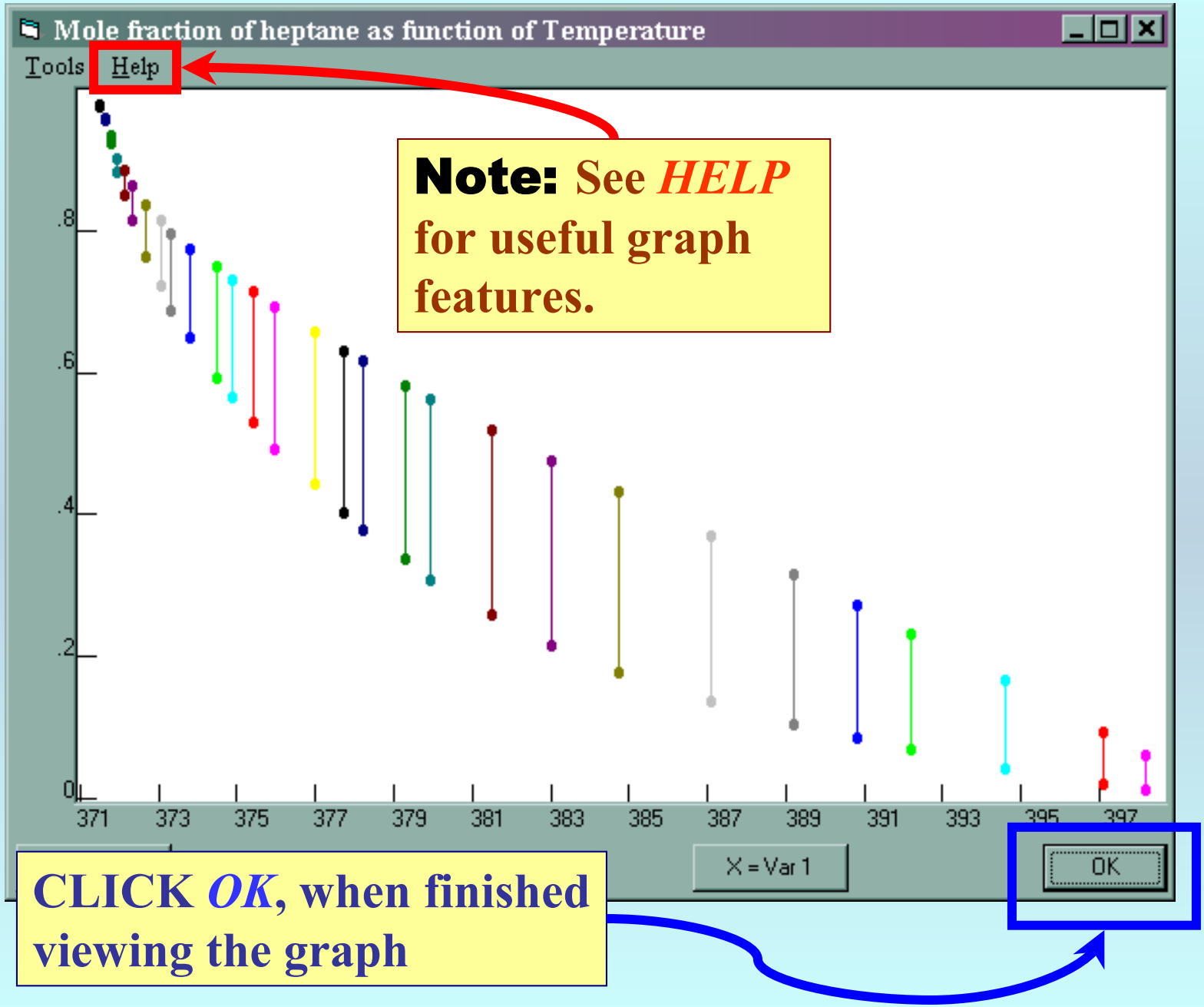
1. The **unit** for *mole fraction* is filled automatically.

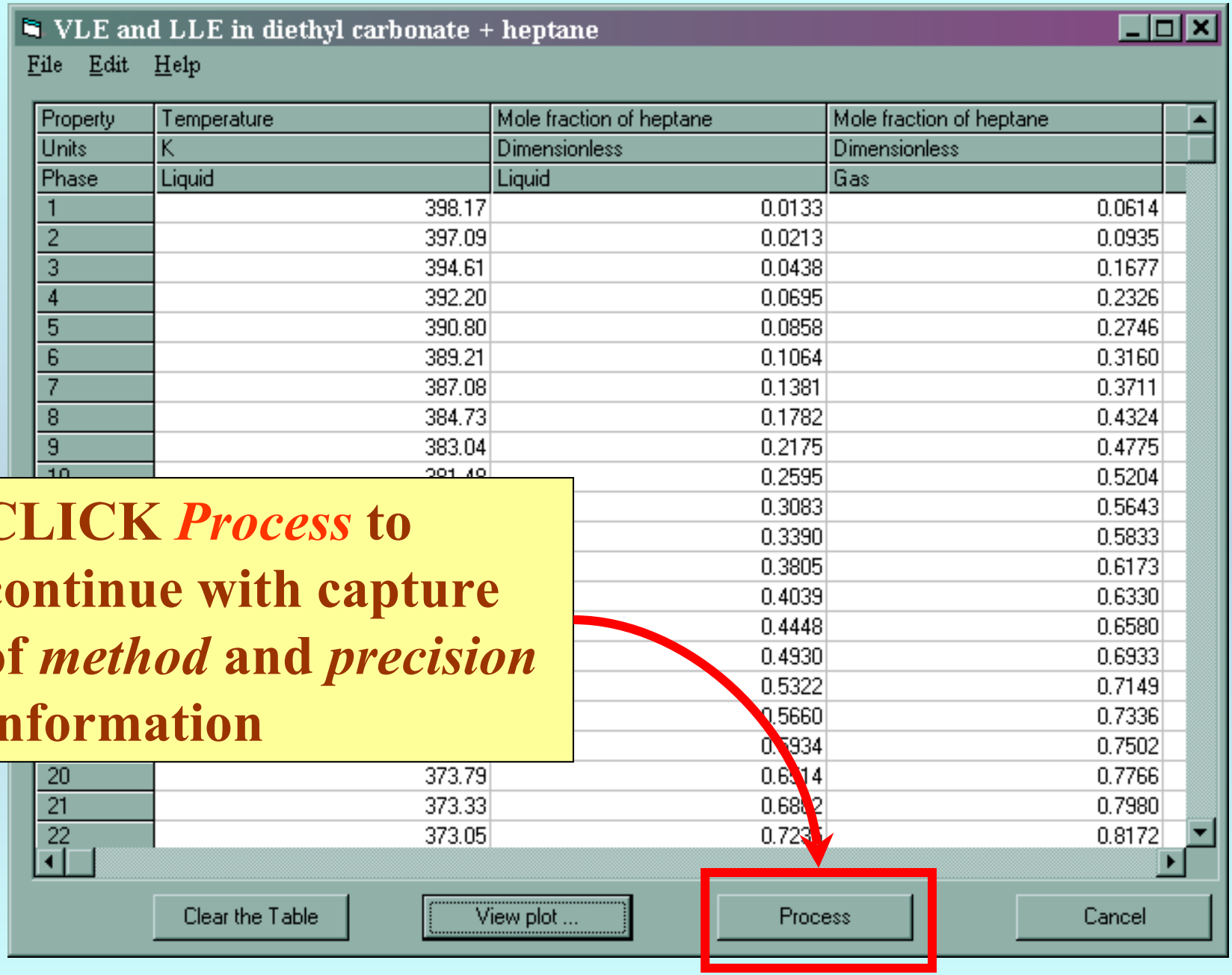


2. SELECT the **phase** associated with the composition; (here **phase** = *liquid*)

Note: *Liquid mixture 1* and *Liquid mixture 2* are used for LLE data, and are not applicable in this example.


VLE and LLE in diethyl carbonate + heptane
File Edit Help
Property | Temperature | Mole fraction of heptane | Mole fraction of heptane
Units | K | Dimensionless | Dimensionless
Phase | Liquid | Liquid | Gas
2 397.09 0.0213 0.0935
3 394.61 0.0438 0.1677
92.20 0.0695 0.2326
90.80 0.0858 0.2746
89.21 0.1064 0.3160
87.08 0.1381 0.3711
0.1782 0.4324
9 383.04 0.2175 0.4775
10 381.48 0.2595 0.5204
11 379.95 0.3083 0.5643
12 379.31 0.3390 0.5833
13 378.21 0.3805 0.6173
14 377.72 0.4039 0.6330
15 376.97 0.4448 0.6580
0.4930 0.6933
0.5322 0.7149
0.5660 0.7336
0.5934 0.7502
0.6514 0.7766
21 373.33 0.6882 0.7980
22 0.7235 0.8172
The completed column headings look like this.
CLICK View Plot to graph the data and check for typographical errors.
Clear the Table
View plot ...
Process
Cancel

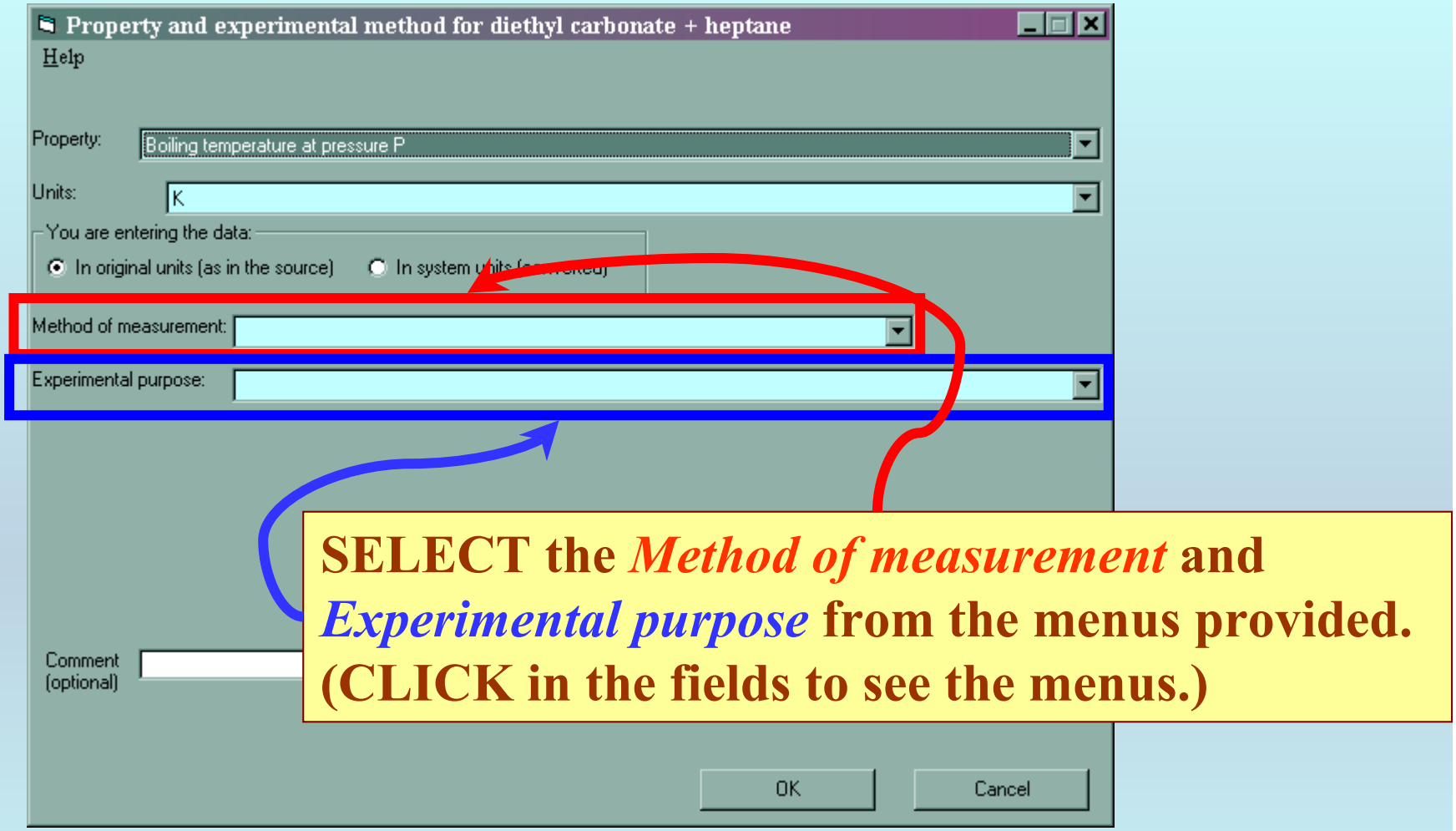

Mole fraction of heptane as function of Temperature
Tools
Help
Note: See HELP for useful graph features.
.8
.6
.4
.2
0
371
373
375
377
379
381
383
385
387
389
391
393
395
397
X = Var 1
OK
CLICK OK, when finished viewing the graph



CLICK *Process* to continue with capture of *method* and *precision* information

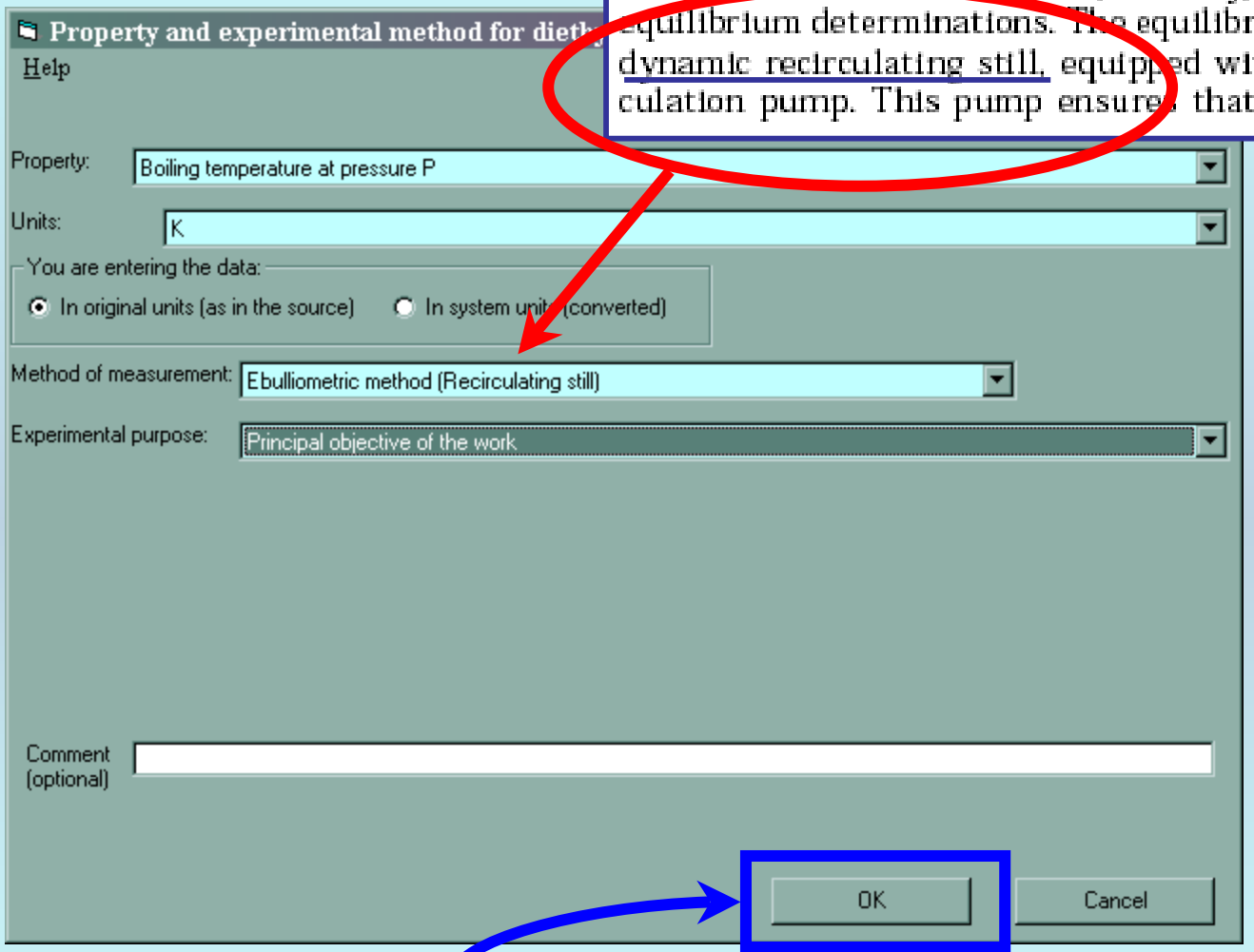
NOTE: The GDC software *automatically* divides the entered table of VLE data into an appropriate number of separate data sets (*two in the present example*) based on the Gibbs Phase rule.

The following screens capture information concerning the experimental methods and precisions for the data.


Property and experimental method for diethyl carbonate + heptane
Help
Property:
Boiling temperature at pressure P
Units:
K
You are entering the data:
In original units (as in the source)
Method of measurement:
Experimental purpose:
Comment (optional)
OK
Cancel
SELECT the Method of measurement and Experimental purpose from the menus provided. (CLICK in the fields to see the menus.)

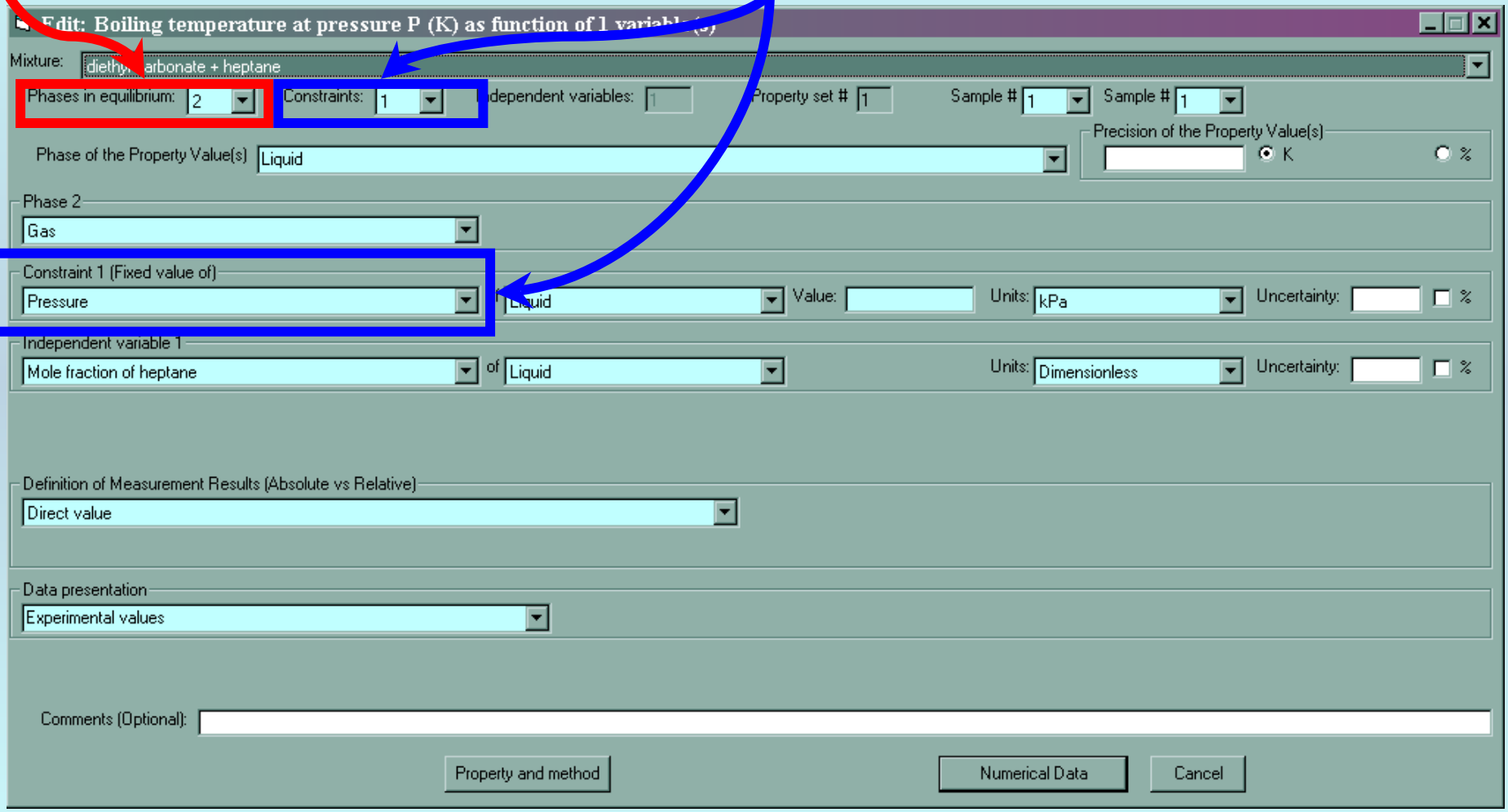
Experimental Method:

Apparatus and Procedure. A glass Fischer LABODEST VLE apparatus model 602/D, manufactured by Fischer Labor und Verfahrenstechnik (Germany), was used in the equilibrium determinations. The equilibrium vessel was a dynamic recirculating still, equipped with a Cottrell circulation pump. This pump ensures that both liquid and

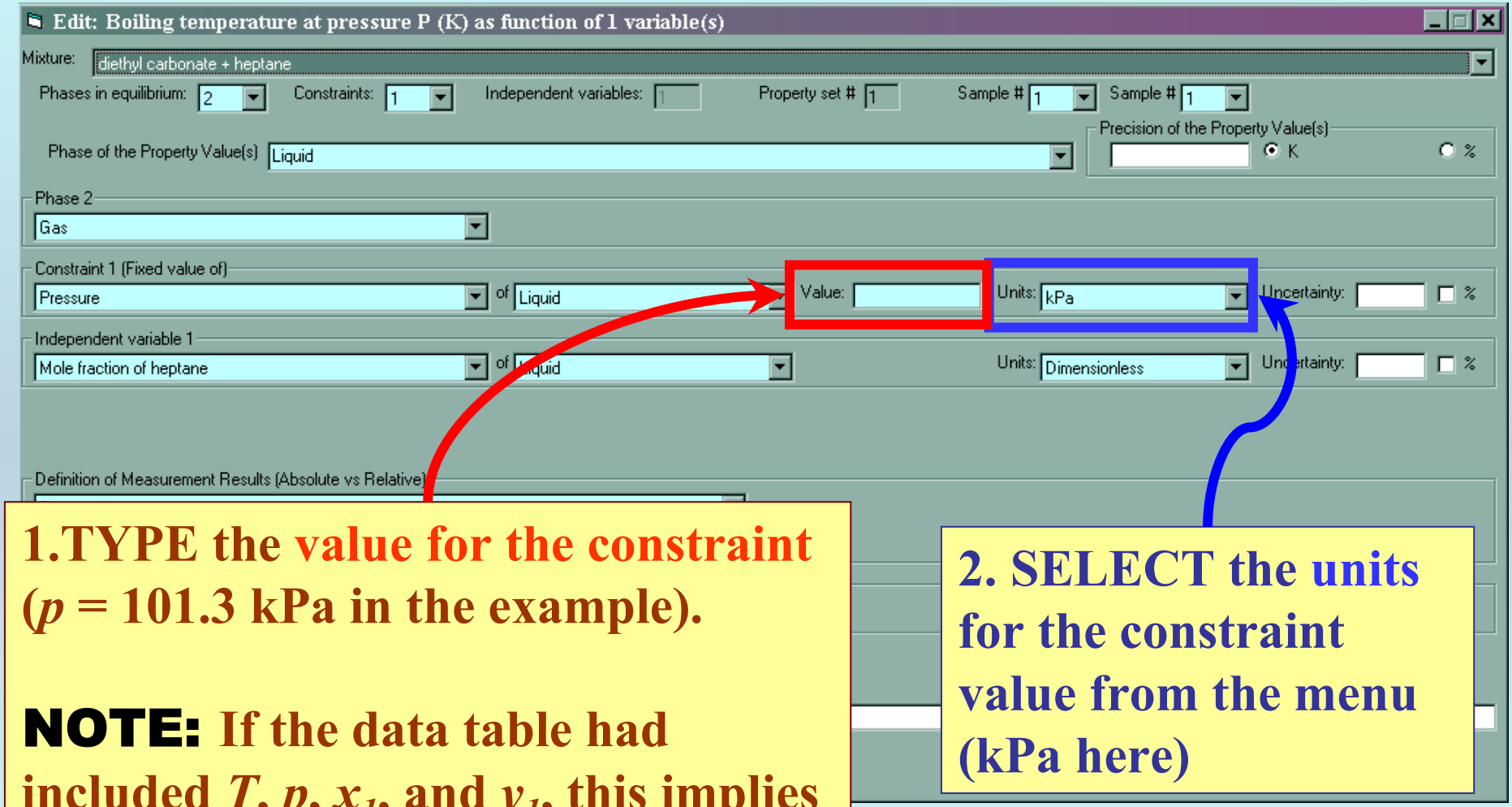


CLICK *OK*

NOTE: Based on the information pasted into the original table, the GDC software determines the # of *phases in equilibrium* and *constraints*. These fields are defined by the program.



Continue with tutorial...



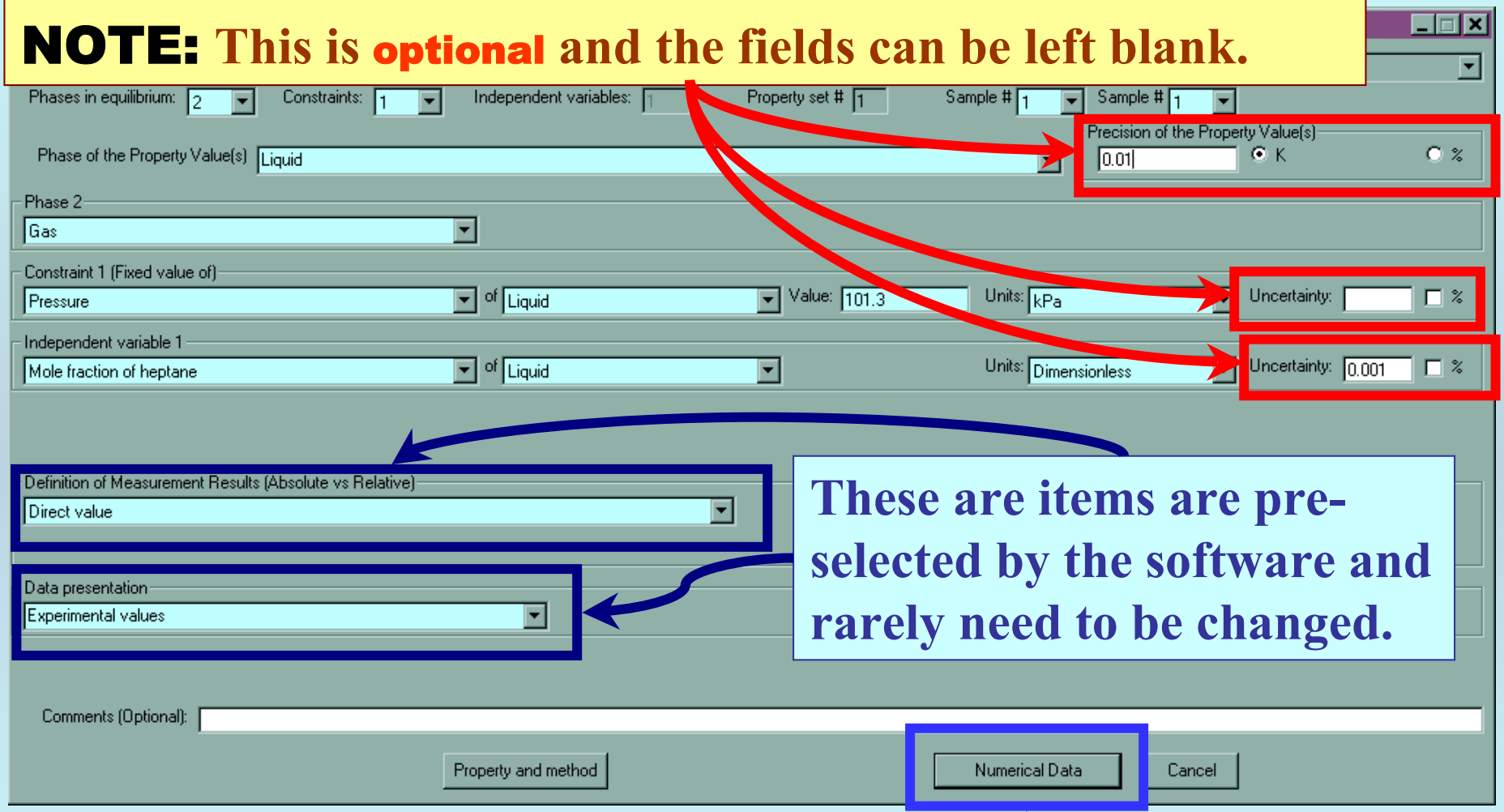
1.TYPE the value for the constraint (p = 101.3 kPa in the example).

NOTE: If the data table had included T, p, x_1, and y_1, this implies that there were no constraints, and p would be listed as a variable, also.

2. SELECT the units for the constraint value from the menu (kPa here)

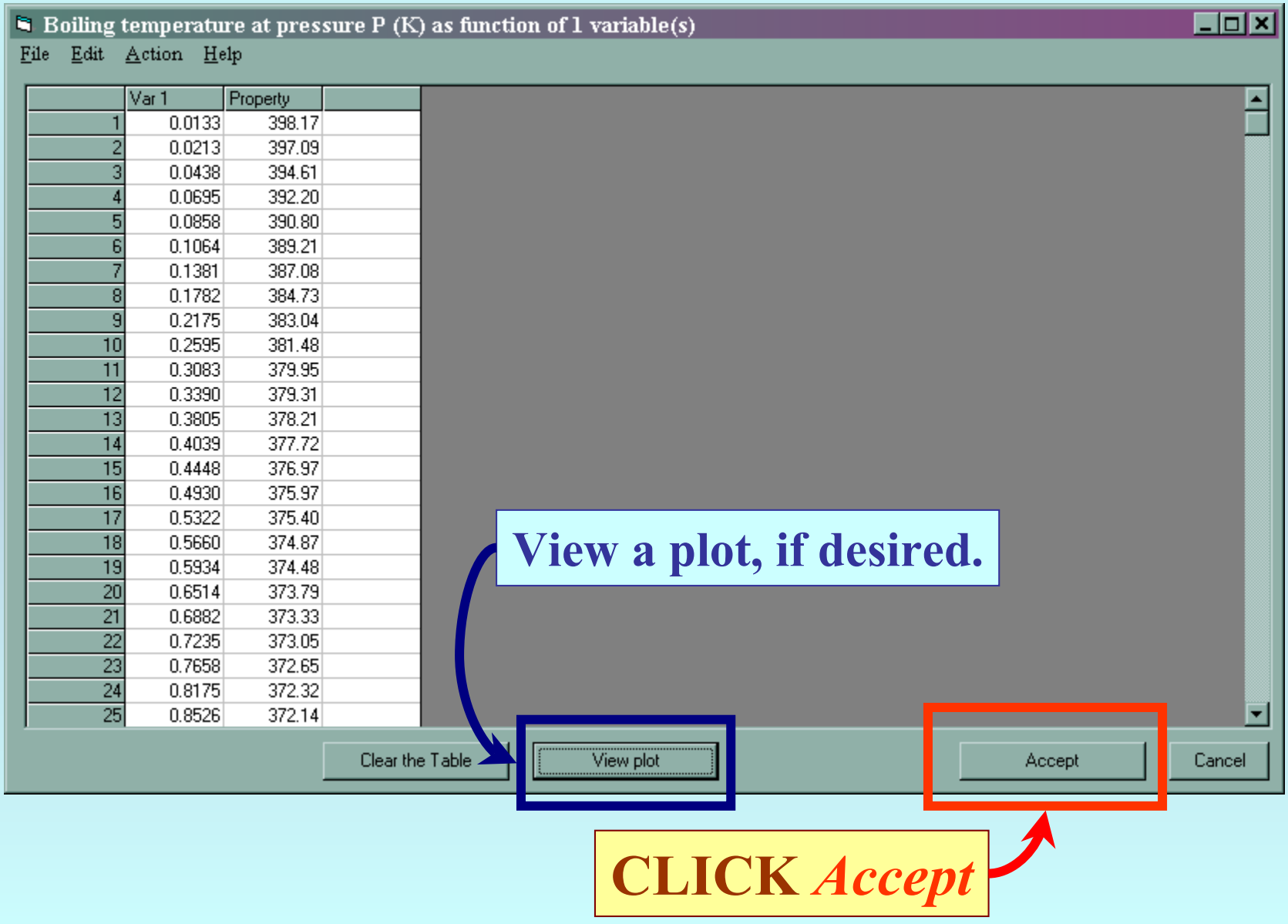
1. TYPE estimated precisions for the *property*, *constraint*, and *independent-variable value(s)*.

NOTE: This is **optional** and the fields can be left blank.



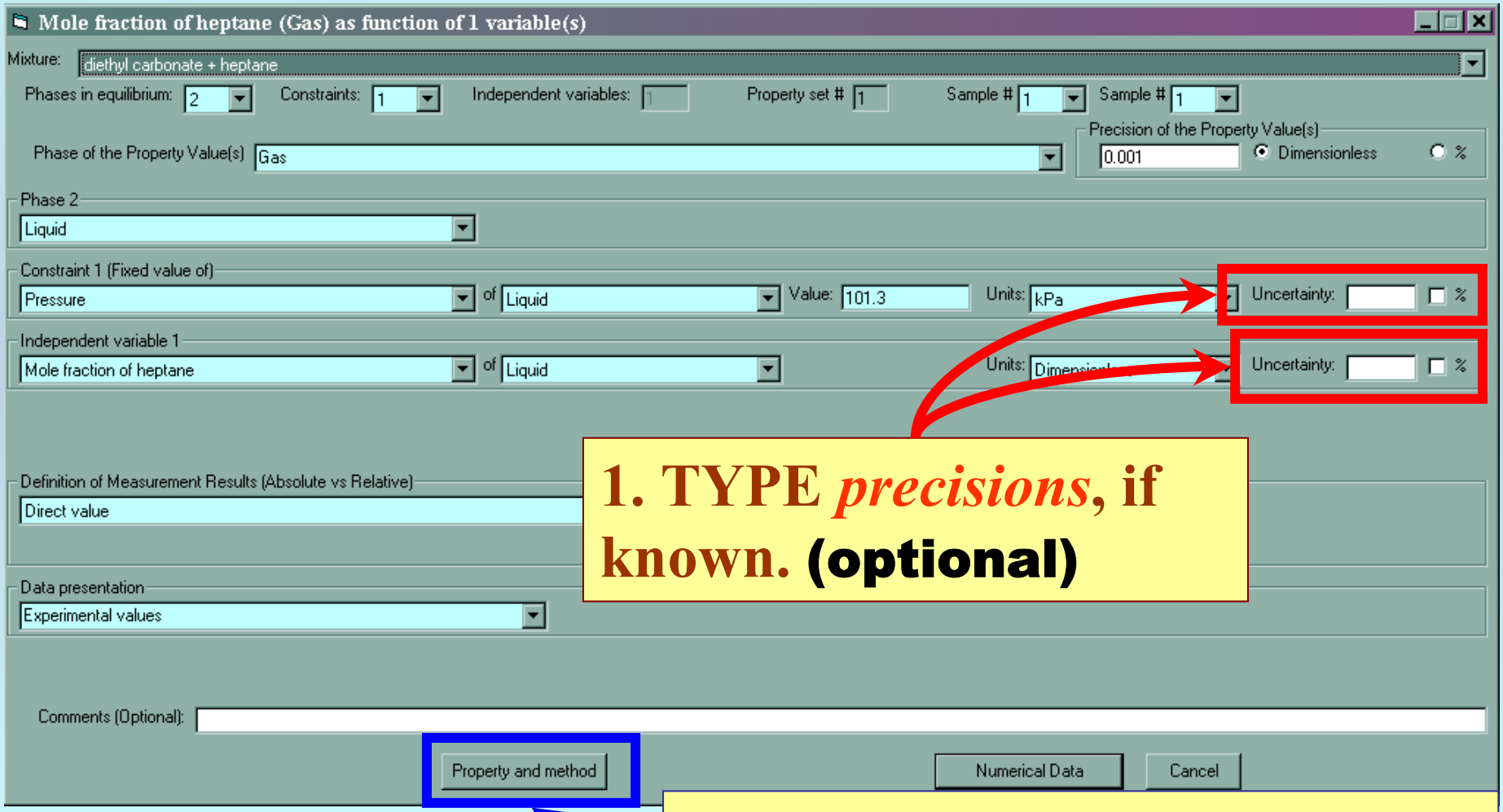
These are items are pre-selected by the software and rarely need to be changed.

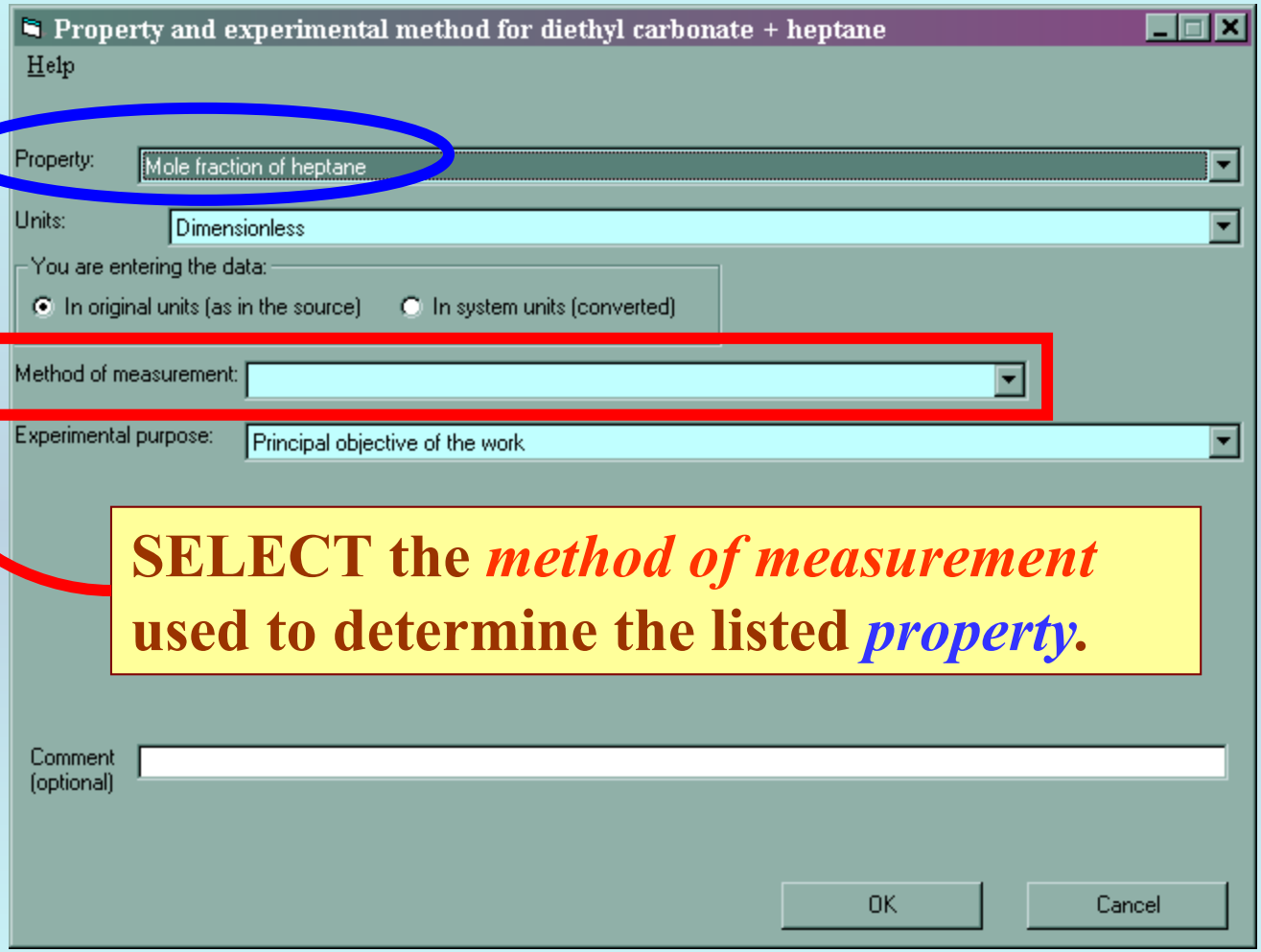
2. CLICK *Numerical Data*


Boiling temperature at pressure P (K) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 0.0133 398.17
2 0.0213 397.09
3 0.0438 394.61
4 0.0695 392.20
5 0.0858 390.80
6 0.1064 389.21
7 0.1381 387.08
8 0.1782 384.73
9 0.2175 383.04
10 0.2595 381.48
11 0.3083 379.95
12 0.3390 379.31
13 0.3805 378.21
14 0.4039 377.72
15 0.4448 376.97
16 0.4930 375.97
17 0.5322 375.40
18 0.5660 374.87
19 0.5934 374.48
20 0.6514 373.79
21 0.6882 373.33
22 0.7235 373.05
23 0.7658 372.65
24 0.8175 372.32
25 0.8526 372.14
Clear the Table
View plot
Accept
Cancel
View a plot, if desired.
CLICK Accept

Continue with data capture for the second dataset obtained based upon the VLE data table.

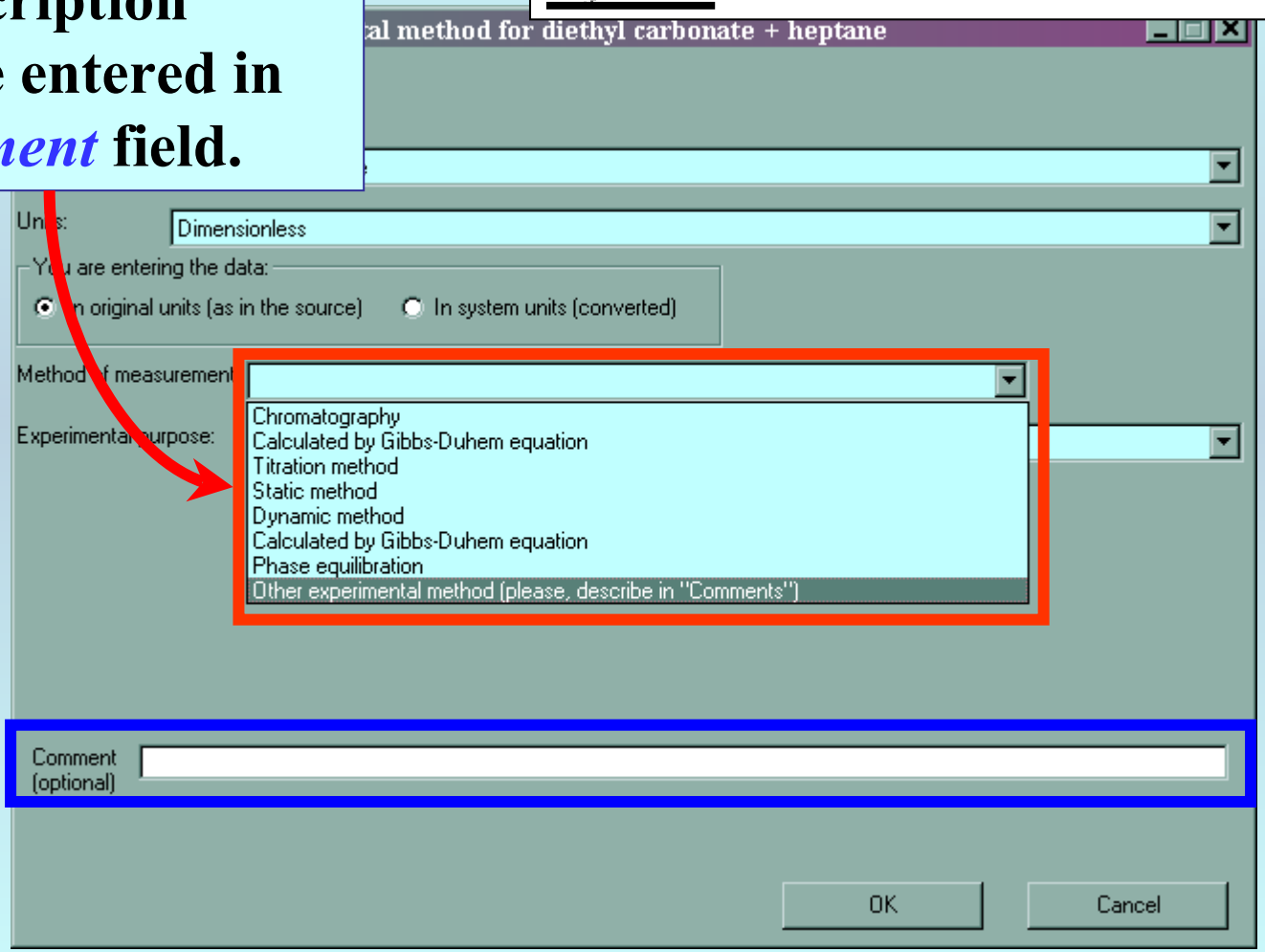
NOTE: **Most fields are filled automatically by the software.**

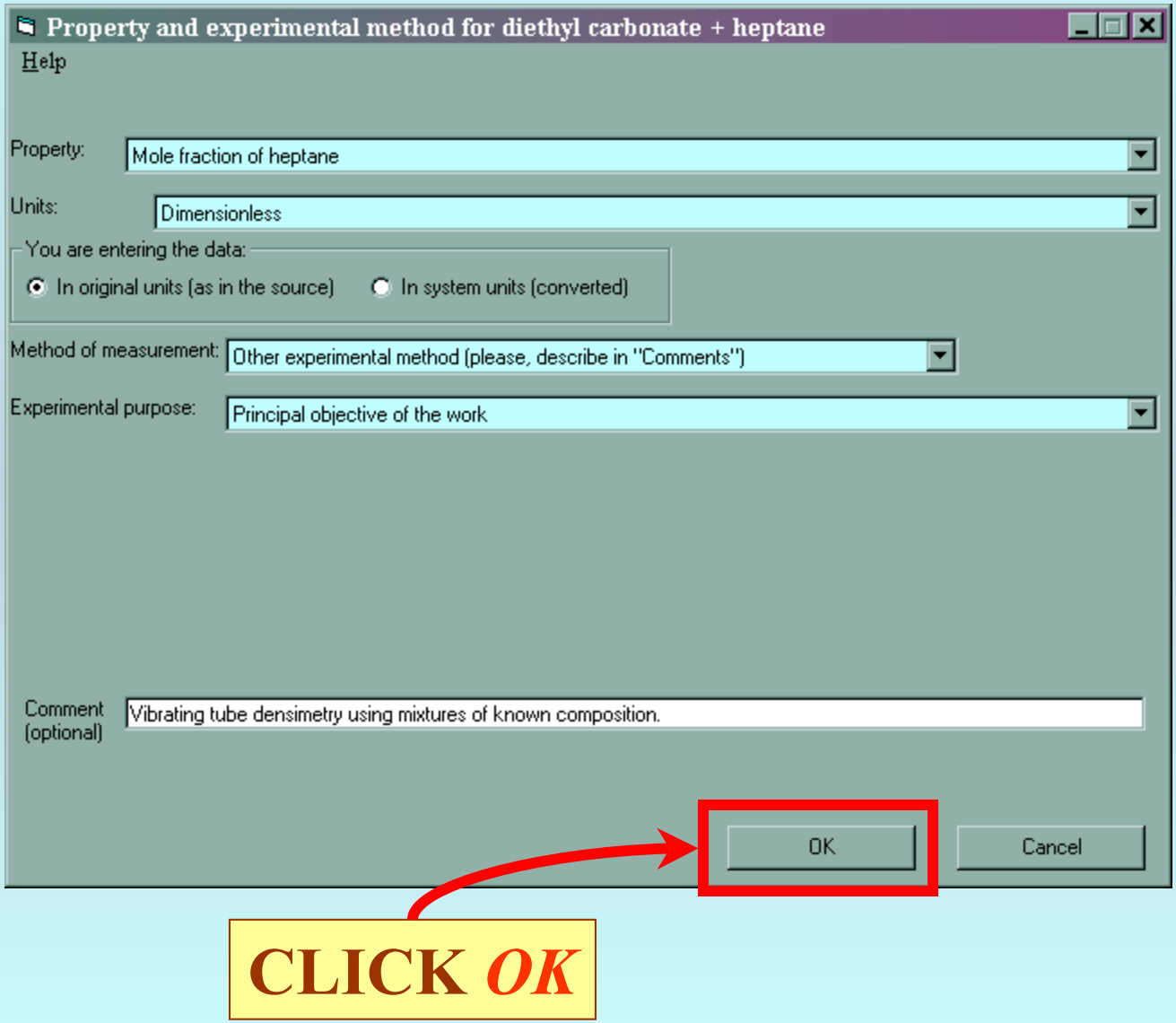



Property and experimental method for diethyl carbonate + heptane
Help
Property:
Mole fraction of heptane
Units:
Dimensionless
You are entering the data:
In original units (as in the source)
In system units (converted)
Method of measurement:
Experimental purpose:
Principal objective of the work
SELECT the method of measurement used to determine the listed property.
Comment (optional)
OK
Cancel

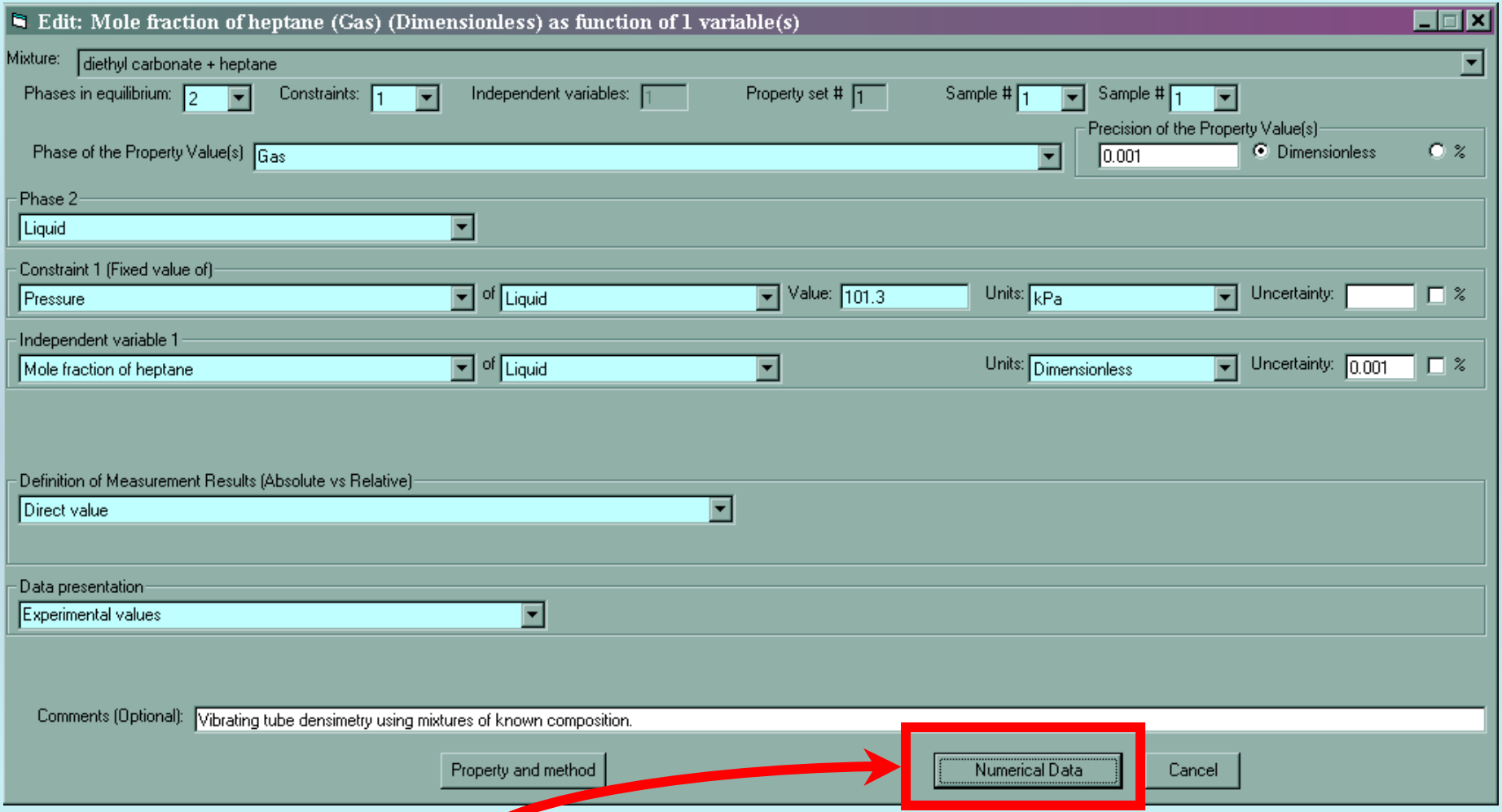
NOTE: ***Other*** **is an appropriate selection for the example, and a brief description should be entered in the** ***Comment*** **field.**

analysis. The composition analysis of both samples was determined using an Anton-Paar DSA-48 digital vibrating tube densimeter. Densimetry was used to establish standard curves for each binary system after the density–composition curves for the mixtures had been plotted. The root-mean-square deviation in the mole fraction was usually <0.001.

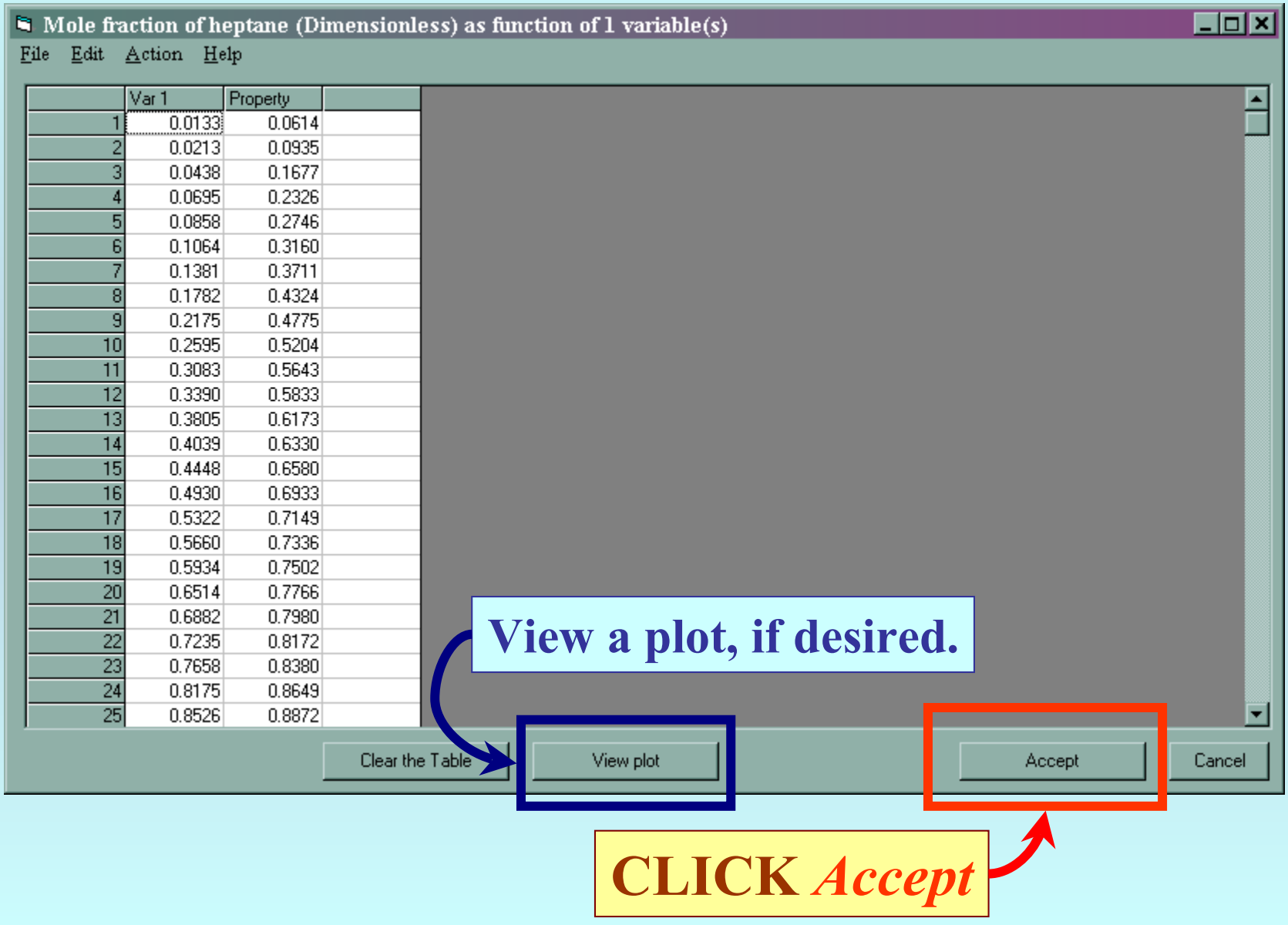


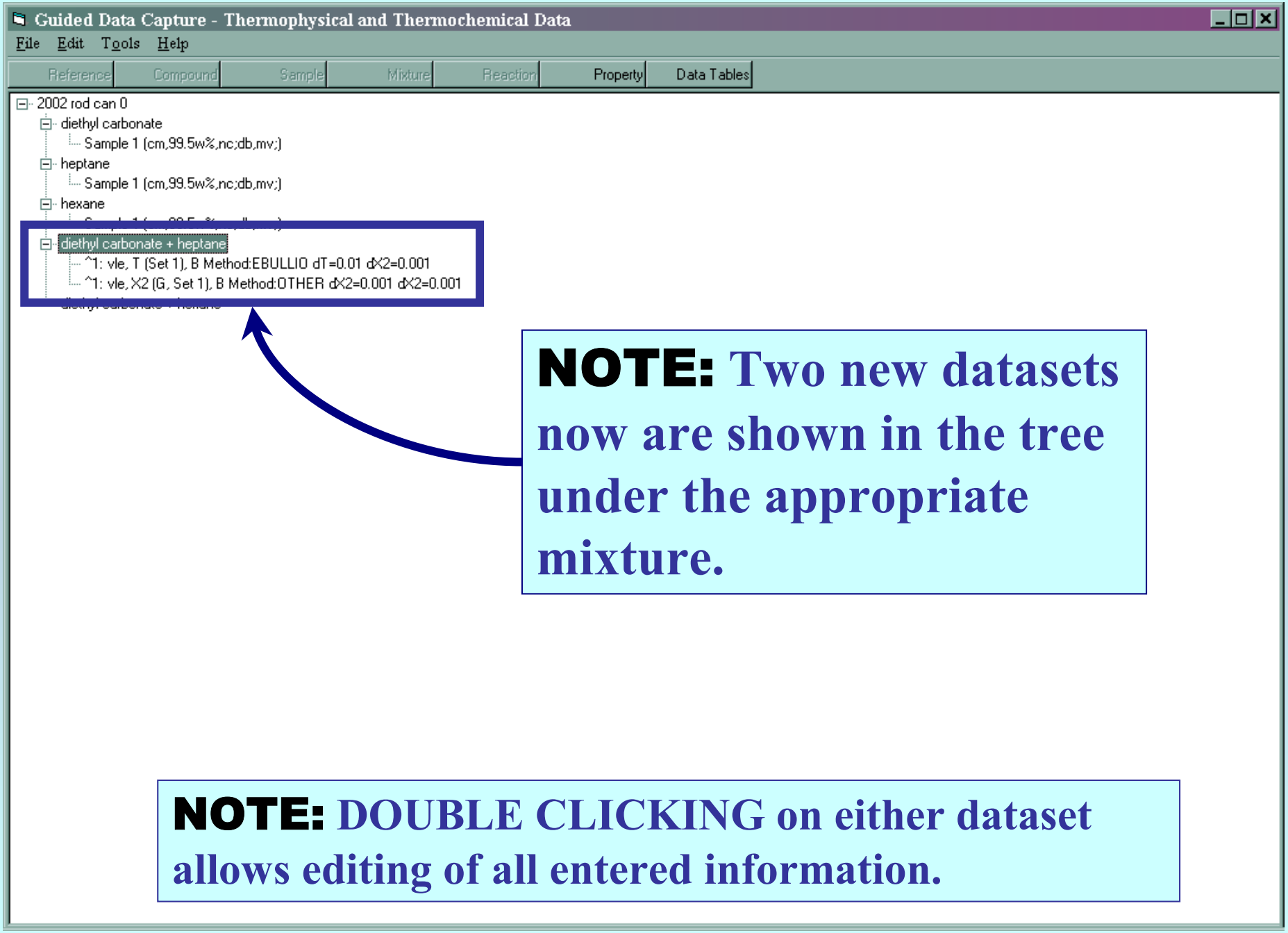

Property and experimental method for diethyl carbonate + heptane
Help
Property:
Mole fraction of heptane
Units:
Dimensionless
You are entering the data:
In original units (as in the source)
In system units (converted)
Method of measurement:
Other experimental method (please, describe in "Comments")
Experimental purpose:
Principal objective of the work
Comment (optional)
Vibrating tube densimetry using mixtures of known composition.
OK
Cancel
CLICK OK

You are returned to the previous screen.
Check that entries are complete...



CLICK *Numerical Data*


Mole fraction of heptane (Dimensionless) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 0.0133 0.0614
2 0.0213 0.0935
3 0.0438 0.1677
4 0.0695 0.2326
5 0.0858 0.2746
6 0.1064 0.3160
7 0.1381 0.3711
8 0.1782 0.4324
9 0.2175 0.4775
10 0.2595 0.5204
11 0.3083 0.5643
12 0.3390 0.5833
13 0.3805 0.6173
14 0.4039 0.6330
15 0.4448 0.6580
16 0.4930 0.6933
17 0.5322 0.7149
18 0.5660 0.7336
19 0.5934 0.7502
20 0.6514 0.7766
21 0.6882 0.7980
22 0.7235 0.8172
23 0.7658 0.8380
24 0.8175 0.8649
25 0.8526 0.8872
Clear the Table
View plot
Accept
Cancel
View a plot, if desired.
CLICK Accept



NOTE: Two new datasets now are shown in the tree under the appropriate mixture.

NOTE: DOUBLE CLICKING on either dataset allows editing of all entered information.

END

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

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