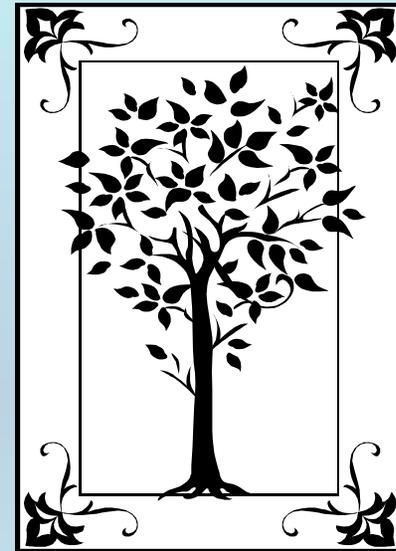


METADATA AND NUMERICAL DATA CAPTURE:

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:

1098

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*

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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

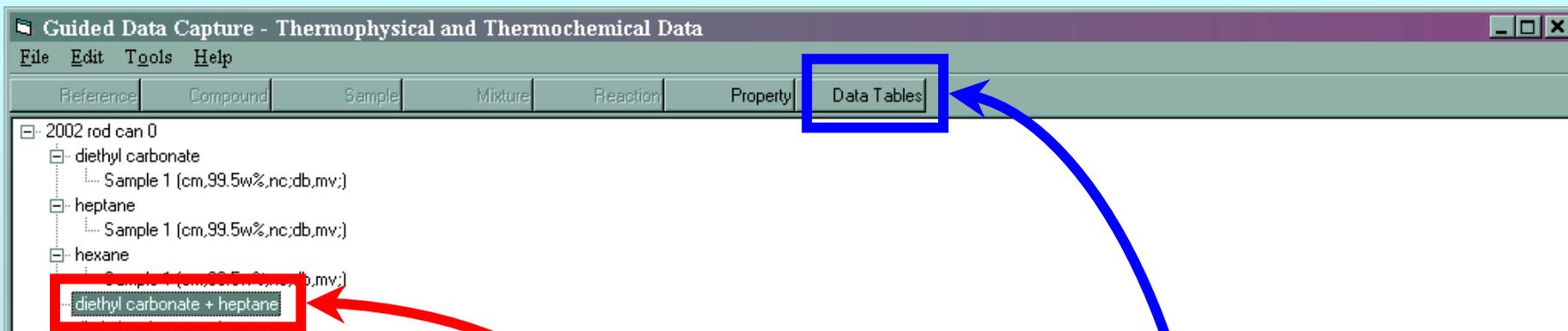
T/K	x	y	γ_1	γ_2
398.17	0.0133	0.0614	2.366	0.975
397.09	0.0213	0.0935	2.309	0.978
394.61	0.0438	0.1677	2.133	0.985
392.20	0.0695	0.2326	1.974	0.999
390.80	0.0858	0.2746	1.951	1.001
389.21	0.1064	0.3160	1.881	1.011
387.08	0.1381	0.3711	1.794	1.027
384.73	0.1782	0.4324	1.718	1.043
383.04	0.2175	0.4775	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	1.278	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	1.267
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

Experimental Method:

Apparatus and Procedure. A glass Fischer LABOD-EST 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.

This data set is considered here.



1. SELECT the *mixture* for which the data are to be captured.

2. CLICK *Data Tables*

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:



Data Table Processing

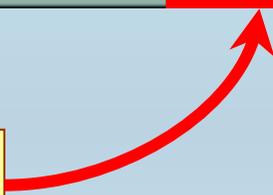
Select type of table: VLE and LLE in binary and ternary mixtures

diethyl carbonate + heptane

Composition as independent variable

OK Cancel

CLICK *OK*



VLE and LLE in diethyl carbonate + heptane

File Edit Help

Property			
Units			
Phase			
1			

Clear the Table View plot ... Process

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) + DMC (2) System at 101.3 kPa

T/K	y	y ₁	y ₂
398.17	0.0133	0.0614	2.366
397.09	0.0213	0.0935	2.309
394.61	0.0438	0.1677	2.133
392.20	0.0695	0.2326	1.974
390.80	0.0858	0.2746	1.951
389.21	0.1064	0.3160	1.881
387.08	0.1381	0.3711	1.794
384.73	0.1782	0.4324	1.718
383.04	0.2175	0.4775	1.621
381.48	0.2595	0.5204	1.541
379.95	0.3083	0.5643	1.463
379.31	0.3390	0.5833	1.399
378.21	0.3805	0.6173	1.357
377.72	0.4039	0.6330	1.328
376.97	0.4448	0.6580	1.279
375.97	0.4930	0.6933	1.248
375.40	0.5322	0.7149	1.211
374.87	0.5660	0.7336	1.185
374.48	0.5934	0.7502	1.168
373.79	0.6514	0.7766	1.122
373.33	0.6882	0.7980	1.105
373.05	0.7235	0.8172	1.085
372.65	0.7658	0.8380	1.063
372.32	0.8175	0.8649	1.037
372.14	0.8526	0.8872	1.025
371.96	0.8833	0.9042	1.013
371.77	0.9262	0.9352	1.004
371.62	0.9580	0.9605	1.001
371.49	0.9774	0.9786	1.004

VLE and LLE in diethyl carbonate + heptane

File Edit Help

Property				
Units				
Phase				
1	398.17	0.0133	0.0614	
2	397.09	0.0213	0.0935	
3	394.61	0.0438	0.1677	
4	392.20	0.0695	0.2326	
5	390.80	0.0858	0.2746	
6	389.21	0.1064	0.3160	
7	387.08	0.1381	0.3711	
8	384.73	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	
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

Table 5. Vapor-Liquid Equilibrium Data for the Heptane (1) + D₂C (2) System at 101.3 kPa

T/K	y	y ₁	y ₂
398.17	0.0133	0.0614	2.366
397.09	0.0213	0.0935	2.309
394.61	0.0438	0.1677	2.133
392.20	0.0695	0.2326	1.974
390.80	0.0858	0.2746	1.951
389.21	0.1064	0.3160	1.881
387.08	0.1381	0.3711	1.794
384.73	0.1782	0.4324	1.718
383.04	0.2175	0.4775	1.621
381.48	0.2595	0.5204	1.541
379.95	0.3083	0.5643	1.463
379.31	0.3390	0.5833	1.399
378.21	0.3805	0.6173	1.357
377.72	0.4039	0.6330	1.328
376.97	0.4448	0.6580	1.279
375.97	0.4930	0.6933	1.248
375.40	0.5322	0.7149	1.211
374.87	0.5660	0.7336	1.185
374.48	0.5934	0.7502	1.168
373.79	0.6514	0.7766	1.122
373.33	0.6882	0.7980	1.105
373.05	0.7235	0.8172	1.085
372.65	0.7658	0.8380	1.063
372.32	0.8175	0.8649	1.037
372.14	0.8526	0.8872	1.025
371.96	0.8833	0.9042	1.013
371.77	0.9262	0.9352	1.004
371.62	0.9580	0.9605	1.001
371.49	0.9774	0.9786	1.004

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

Property, Units, and Phase Definitions:

DOUBLE CLICK in each zone to define the **Property** (blue here), **Units** (red here), and **Phase** (green here) for each column from menus. *(See next page...)*

Property	Units	Phase		
1	398.17	0.0133	0.0614	
2	397.09	0.0213	0.0935	
3	394.61	0.0438	0.1677	
4	392.20	0.0695	0.2326	
5	390.80	0.0858	0.2746	
6	389.21	0.1064	0.3160	
7	387.08	0.1381	0.3711	
8	384.73	0.1782	0.4324	
9	383.04	0.2175	0.4775	
10	381.49	0.2595	0.5204	
11				
12				
13				
14				
15				
16				
17				
18				
19				
20				
21	373.33	0.6882	0.7980	
22	373.05	0.7235	0.8172	

VLE and LLE in diethyl carbonate + heptane

File Edit Help

Property			
Units	Nothing		
Phase	Temperature		
1	Pressure	0.0133	0.0614
2	Mole fraction of diethyl carbonate	0.0213	0.0935
3	Mole fraction of heptane	0.0438	0.1677
4	Weight fraction of diethyl carbonate	0.0695	0.2326
5	Weight fraction of heptane		0.746
6	Molarity of diethyl carbonate		160
7			711
8			824
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

Define the **Property**:
(here, it is *Temperature*)

Clear the Table View plot ... Process Cancel

VLE and LLE in diethyl carbonate + heptane

File Edit Help

Property	Temperature		
Units			
Phase			
1		0.0133	0.0614
2		0.0213	0.0935
3		0.0438	0.1677
4		0.0695	0.2326
5	392.20	0.0858	0.2746
6	390.80	0.1054	0.3160
7	389.21	0.1311	0.3711
8	387.08		0.4324
9	384.73		0.4775
10	383.04		0.5204
11	381.48		0.5643
12	379.95	0.3390	0.5833
13	379.31	0.3805	0.6173
14	378.21	0.4039	0.6330
15	377.72	0.4448	0.6580
16	376.97	0.4930	0.6933
17	375.97	0.5322	0.7149
18	375.40	0.5660	0.7336
19	374.87	0.5934	0.7502
20	374.48	0.6514	0.7766
21	373.79	0.6882	0.7980
22	373.33	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			
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	0.1081	0.3160
7	387.08		0.3711
8	384.73		0.4324
9	383.04		0.4775
10	381.48		0.5204
11	379.95		0.5643
12	379.31		0.5833
13	378.21		0.6173
14	377.72		0.6330
15	376.97		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 ...

Define the **Phase**:
 (here, any selection will
 suffice, because
Temperature is extensive)

Continue for the
 remaining columns...

VLE and LLE in diethyl carbonate + heptane

File Edit Help

Property	Temperature		
Units	K		
Phase	Liquid		
1	398.1		
2	397.0		
3	394.6		
4	392.2		
5	390.8		
6	389.2	0.1084	0.3160
7	387.08	0.1381	0.3711
8	384.73	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
			0.6330
			0.6580
			0.6933
			0.7149
			0.7336
			0.7502
			0.7766
			0.7980
			0.8172

- Temperature
- Temperature
- Pressure
- Mole fraction of diethyl carbonate
- Mole fraction of heptane
- Weight fraction of diethyl carbonate
- Weight fraction of heptane
- Molarity of diethyl carbonate
- Molarity of heptane

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

Please make selections with care...

Clear the Table View plot ... Process Cancel

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

Property	Temperature	Mole fraction of heptane	
Units	K	Dimensionless	
Phase	Liquid		
1	398.17		0.0614
2	397.09		0.0935
3	394.61		0.1677
4	392.20		0.2326
5	390.80	0.0858	0.2746
6	389.21	0.1064	0.3160
7	387.08	0.1381	0.3711
8	384.73	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			
13			
14			
15			
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

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

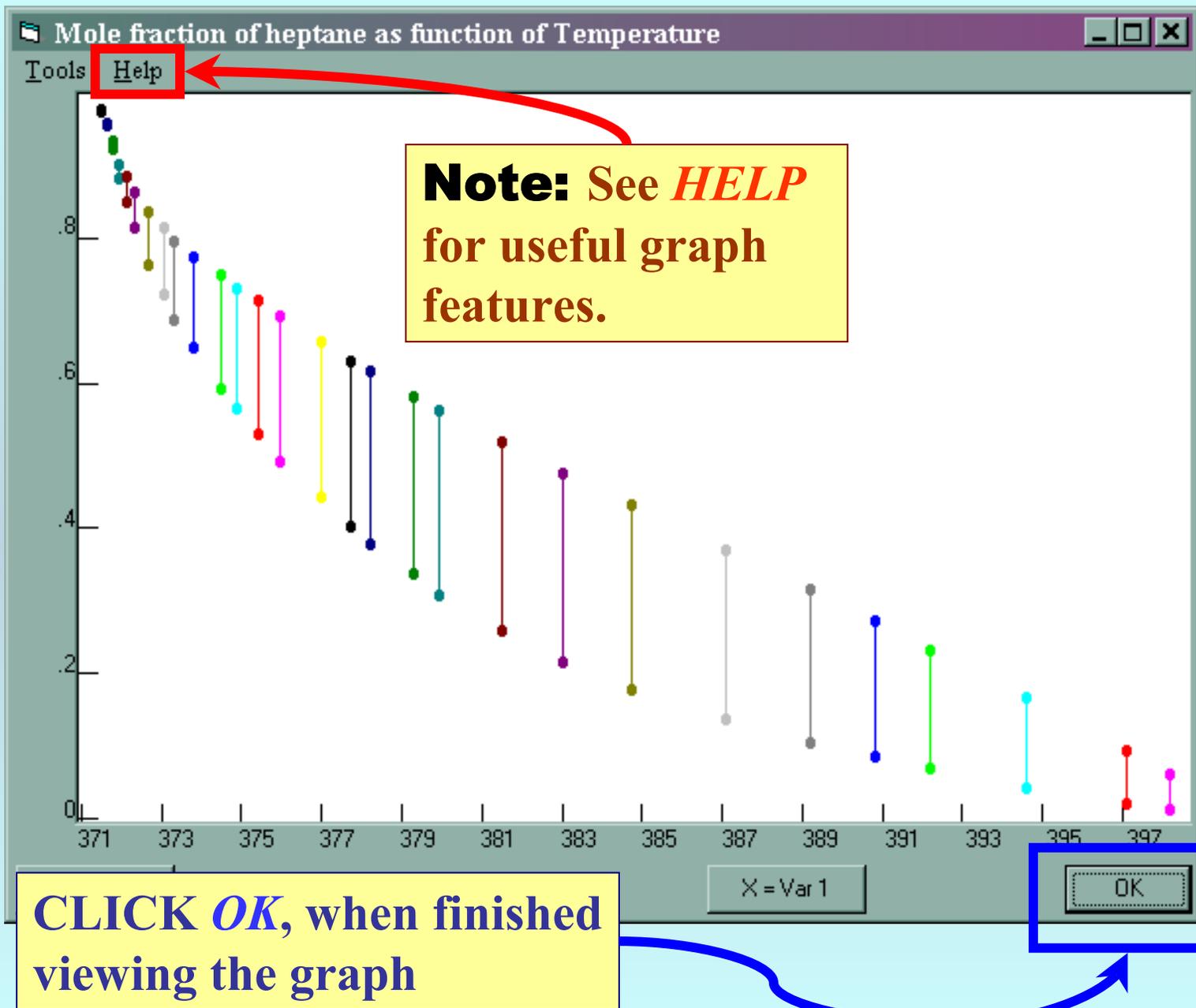
File Edit Help

Property	Temperature	Mole fraction of heptane	Mole fraction of heptane
Units	K	Dimensionless	Dimensionless
Phase	Liquid	Liquid	Gas
1	399.17	0.0133	0.0614
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
8	384.73	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
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

The completed column headings look like this.

CLICK *View Plot* to graph the data and check for typographical errors.



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
1	398.17	0.0133	0.0614
2	397.09	0.0213	0.0935
3	394.61	0.0438	0.1677
4	392.20	0.0695	0.2326
5	390.80	0.0858	0.2746
6	389.21	0.1064	0.3160
7	387.08	0.1381	0.3711
8	384.73	0.1782	0.4324
9	383.04	0.2175	0.4775
10	381.49	0.2595	0.5204
		0.3083	0.5643
		0.3390	0.5833
		0.3805	0.6173
		0.4039	0.6330
		0.4448	0.6580
		0.4930	0.6933
		0.5322	0.7149
		0.5660	0.7336
		0.5934	0.7502
20	373.79	0.6314	0.7766
21	373.33	0.6882	0.7980
22	373.05	0.7235	0.8172

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

Clear the Table View plot ... **Process** Cancel

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) In system units (preferred)

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 LABOD-EST 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 ensured that both liquid and

The screenshot shows a software dialog box titled "Property and experimental method for diethyl...". It contains several fields and controls:

- Property:** A dropdown menu with "Boiling temperature at pressure P" selected.
- Units:** A dropdown menu with "K" selected.
- You are entering the data:** Two radio buttons: "In original units (as in the source)" (selected) and "In system units (converted)".
- Method of measurement:** A dropdown menu with "Ebulliometric method (Recirculating still)" selected.
- Experimental purpose:** A dropdown menu with "Principal objective of the work" selected.
- Comment (optional):** A large empty text input field.
- Buttons:** "OK" and "Cancel" buttons at the bottom right.

A red circle highlights the "dynamic recirculating still" text in the text above, with a red arrow pointing to the "Method of measurement" dropdown. A blue arrow points from a yellow box at the bottom to the "OK" button.

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.

Edit: Boiling temperature at pressure P (K) as function of 1 variable(s)

Mixture: diethyl carbonate + heptane

Phases in equilibrium: 2 Constraints: 1 dependent variables: 1 Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s) Liquid Precision of the Property Value(s) K %

Phase 2 Gas

Constraint 1 (Fixed value of) Pressure Liquid Value: Units: kPa Uncertainty: %

Independent variable 1 Mole fraction of heptane of Liquid Units: Dimensionless Uncertainty: %

Definition of Measurement Results (Absolute vs Relative) Direct value

Data presentation Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

Continue with tutorial...

Edit: Boiling temperature at pressure P (K) as function of 1 variable(s)

Mixture: diethyl carbonate + heptane

Phases in equilibrium: 2 Constraints: 1 Independent variables: 1 Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s) Liquid Precision of the Property Value(s) K %

Phase 2 Gas

Constraint 1 (Fixed value of) Pressure of Liquid Value: Units: kPa Uncertainty: %

Independent variable 1 Mole fraction of heptane of Liquid Units: Dimensionless Uncertainty: %

Definition of Measurement Results (Absolute vs Relative)

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.

Phases in equilibrium: 2 Constraints: 1 Independent variables: 1 Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s) Liquid Precision of the Property Value(s) 0.01 K %

Phase 2 Gas

Constraint 1 (Fixed value of) Pressure of Liquid Value: 101.3 Units: kPa Uncertainty: %

Independent variable 1 Mole fraction of heptane of Liquid Units: Dimensionless Uncertainty: 0.001 %

Definition of Measurement Results (Absolute vs Relative) Direct value

Data presentation Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

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

The screenshot shows a software window titled "Boiling temperature at pressure P (K) as function of 1 variable(s)". It contains a table with 25 rows of data. The table has three columns: an index, "Var 1", and "Property". The "Property" column shows a decreasing trend from 398.17 to 372.14. Below the table are four buttons: "Clear the Table", "View plot", "Accept", and "Cancel". The "View plot" button is highlighted with a blue rectangular box. A blue callout box with the text "View a plot, if desired." has a curved arrow pointing to the "View plot" button.

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.

Mole fraction of heptane (Gas) as function of 1 variable(s)

Mixture: diethyl carbonate + heptane

Phases in equilibrium: 2 Constraints: 1 Independent variables: 1 Property set #: 1 Sample #: 1 Sample #: 1

Phase of the Property Value(s): Gas Precision of the Property Value(s): 0.001 Dimensionless %

Phase 2: Liquid

Constraint 1 (Fixed value of): Pressure of Liquid Value: 101.3 Units: kPa Uncertainty: %

Independent variable 1: Mole fraction of heptane of Liquid Units: Dimensionless Uncertainty: %

Definition of Measurement Results (Absolute vs Relative): Direct value

Data presentation: Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

1. TYPE *precisions*, if known. (optional)

2. CLICK *Property and method*

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

Comment (optional)

OK Cancel

SELECT the *method of measurement* used to determine the listed *property*.

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.

Method for diethyl carbonate + heptane

Units: Dimensionless

You are entering the data:

In original units (as in the source) In system units (converted)

Method of measurement:

- Chromatography
- Calculated by Gibbs-Duhem equation
- Titration method
- Static method
- Dynamic method
- Calculated by Gibbs-Duhem equation
- Phase equilibration
- Other experimental method (please, describe in "Comments")

Experimental purpose:

Comment (optional)

OK Cancel

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...**

Edit: Mole fraction of heptane (Gas) (Dimensionless) as function of 1 variable(s)

Mixture: diethyl carbonate + heptane

Phases in equilibrium: 2 Constraints: 1 Independent variables: 1 Property set #: 1 Sample #: 1 Sample #: 1

Phase of the Property Value(s): Gas Precision of the Property Value(s): 0.001 Dimensionless %

Phase 2: Liquid

Constraint 1 (Fixed value of): Pressure of Liquid Value: 101.3 Units: kPa Uncertainty: %

Independent variable 1: Mole fraction of heptane of Liquid Units: Dimensionless Uncertainty: 0.001 %

Definition of Measurement Results (Absolute vs Relative): Direct value

Data presentation: Experimental values

Comments (Optional): Vibrating tube densimetry using mixtures of known composition.

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*

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables

- 2002 rod can 0
 - diethyl carbonate
 - Sample 1 (cm,99.5w%,nc;db,mv;)
 - heptane
 - Sample 1 (cm,99.5w%,nc;db,mv;)
 - hexane
 - Sample 1 (cm,99.5w%,nc;db,mv;)
 - diethyl carbonate + heptane**
 - ^1: vle, T (Set 1), B Method:EBULLIO dT=0.01 dX2=0.001
 - ^1: vle, X2 (G, Set 1), B Method:OTHER dX2=0.001 dX2=0.001

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.