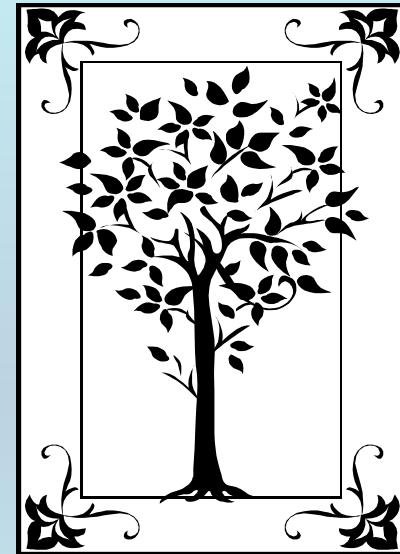


# METADATA AND NUMERICAL DATA CAPTURE: **INTERFACIAL TENSION**

## **3 – Components**

### *Guided Data* **Capture (GDC)**



This tutorial describes  
METADATA AND NUMERICAL DATA CAPTURE:  
for **3-components**  
**INTERFACIAL TENSION**  
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:

## **Interfacial Tensions of Two-Phase Ternary Systems**

**Elzo Sada,<sup>1</sup> Shigeharu Kito, and Mineo Yamashita<sup>2</sup>**

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**Interfacial tensions of two-phase aqueous ternary systems are presented. Measurements are conducted by use of the capillary rise method of Bartell and Miller for seven systems at 25°C and under the condition of equilibrium distributions of solute concentrations between the phases.**

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## INTERFACIAL TENSION (3 ñ Components) BENZENE, WATER, ETHANOL

**Table I. Interfacial Tensions of Ternary Systems at 25°C**

Aqueous phase		Organic phase			Inter- facial tension, dyn/cm	
Concn, wt %	Density, g/cc	Concn, wt %	Density, g/cc			
Benzene(1)–water(2)–ethanol(s)						
(1)	(s)		(1)	(s)		
0.2	10.8	0.9782	98.6	1.2	0.8726	17.20
0.3	21.7	0.9626	97.1	2.6	0.8711	9.37
1.6	36.2	0.9365	94.0	5.4	0.8679	3.64
3.6	43.7	0.9172	91.3	7.9	0.8656	1.99
8.6	50.1	0.8944	87.3	11.4	0.8629	1.09
21.2	52.0	0.8690	79.3	18.0	0.8588	0.04

**This data set is  
considered here.**

## **Experimental Method Info:**

**Capillary rise**

**Temperature control: 0.02 K**

## Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

Sample

Mixture

Reaction

Property

Data Tables

[-] 1975 sad kit 0  
[-] benzene  
    ... Sample 1 (cm;;98m%,est)  
[-] water  
    ... Sample 1 (cm;;99.9m%,est)  
[-] ethanol  
    ... Sample 1 (cm;;98m%,est)  
    ethanol + benzene + water

2. CLICK  
*Property*

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

**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 ethanol + benzene + water

Help

Property group: Refraction; Surface tension; and Speed of sound

Property: Interfacial tension

Units: N/m  
N/m  
ALL OTHER UNITS

Method of measurement:

Experimental purpose:

Comment (optional)

OK Cancel

1. SELECT the **Property Group**: *Refraction; Surface tension; and Speed of sound* from the menu.

2. SELECT the **Property**: *Interfacial tension*, for the example.

3. SELECT **ALL OTHER UNITS** to add a multiplier (i.e., 0.001) as in the present example.

**1. TYPE** the conversion factor to convert the values in the manuscript table to  $\hat{\text{N/m}}$ .

**Non-standard conversion factor**

Property value in the original units multiplied by a conversion factor is property value in N/m:

$(\text{Original Value}) * (\text{Conversion Factor}) = (\text{Converted Value}) \text{ in N/m}$

Enter the Conversion Factor here

0.001

OK

Cancel

**2. CLICK *OK***



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.

Units: ALL OTHER UNITS

Method of measurement: Other experimental method (please, describe in "Comments")

Experimental purpose: Principal objective of the work

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

Comment (optional) Capillary Rise. Bartell and Miller; J. Am. Chem. Soc., 50, 1961 (1928)

3. CLICK *OK*

OK

Cancel

# SELECTION of # of Phases in Equilibrium and # of Constraints

Interfacial tension (\* 0.001 N/m) as function of 1 variable(s)

Mixture: ethanol + benzene + water

Phases in equilibrium: 2 Constraints: 2 Independent variables: 1

Phase of the Property Value(s)

Definition of Measurement Results (Absolute vs Relative)

SELECT the # of **Phases in equilibrium**. There are **2** phases; *liquid mixture 1* and *liquid mixture 2*.

SELECT the # of **Constraints** (*temperature* and *pressure*, here).

**Interfacial tension (\* 0.001 N/m) as function of 1 variable(s)**

Mixture: ethanol + benzene + water

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

Sample # 1 Sample # 1 Sample # 1

Phase of the Property Value(s):

Units: \* 0.001 N/m

Uncertainty: %

Definition of Measurement Results (Absolute vs Relative):

Data presentation: Experimental values

Comments (Optional): Capillary Rise. Bartell and Miller; J. Am. Chem. Soc., 50, 1961 (1928)

Property and method Numerical Data Cancel

**Multiple *samples* for a given component can be accommodated, but this is rarely needed.**

Interfacial tension (\* 0.001 N/m) as function of 1 variable(s)

Mixture: ethanol + benzene + water

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

Phase of the Property Value(s) Liquid mixture 1 Precision of the Property Value(s) \* 0.001 N/m

Phase 2  
Constraint 1 (Fixed value of)  
Constraint 2 (Fixed value of)  
Independent variable 1

Definition of Measurement Result (Absolute vs Relative)

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

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

**1. SELECT Phase 2 (Liquid mixture 2), Constraint(s) (Temperature & Pressure) and the Independent Variable(s) (Temperature) from the menus.**

Mixture: ethanol + benzene + water

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

Phase of the Property Value(s): Liquid mixture 1 Precision of the Property Value(s): \* 0.001 N/m %

Phase 2: Liquid mixture 2

Constraint 1 (Fixed value of): Temperature of Liquid mixture 1 Value: 25 Units: C Uncertainty: 0.02 %

Constraint 2 (Fixed value of): Pressure of Liquid mixture 1 Value: 101.3 Units: kPa Uncertainty: %

Independent variable 1: Weight fraction of benzene of Liquid mixture 1 Units: Dimensionless Uncertainty: %

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

Data presentation: Experimental

Comments (

**2. TYPE the Constraint Values and SELECT Units for the Variable(s) and Constraint(s). Include approximate Uncertainties, if known.**

Interfacial tension (\* 0.001 N/m) as function of 1 variable(s)

Mixture: ethanol + benzene + water

Phases in equilibrium: 2 Constraints: 2 Independent variable: 1

Phase of the Property Value(s) Liquid mixture 1

Phase 2 Liquid mixture 2

Constraint 1 (Fixed value of) Temperature of Liquid mixture 1

Constraint 2 (Fixed value of) Pressure of Liquid mixture 1 Value: 101.3 Units: kPa Uncertainty: %

Independent variable 1 Weight fraction of benzene of Liquid mixture 1 Units: Dimensionless Uncertainty: %

Definition of Measurement Results (Absolute vs Relative) Direct value

Data presentation Experimental values

Comments (Optional): Capillary Rise. Bartell and Miller; J. Am. Chem. Soc., 50, 1961 (1928)

Property and method Numerical Data Cancel

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*

Interfacial tension (\* 0.001 N/m) as function of 1 variable(s)

File Edit Action Help

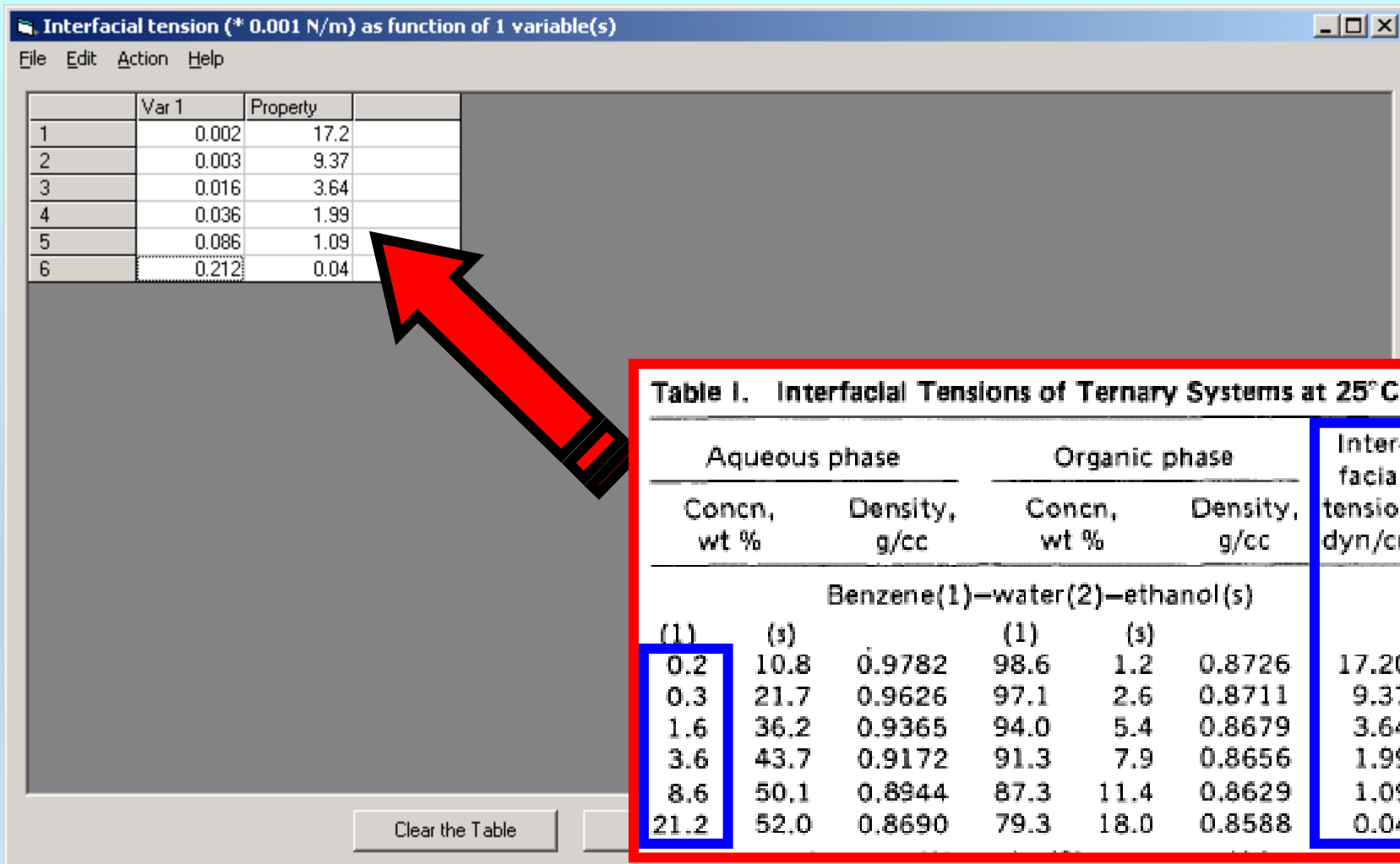
	Var 1	Property	
1			

**TYPE, or much preferably, PASTE the variable and property values into the table. See next page...**

**Table I. Interfacial Tensions of Ternary Systems at 25°C**

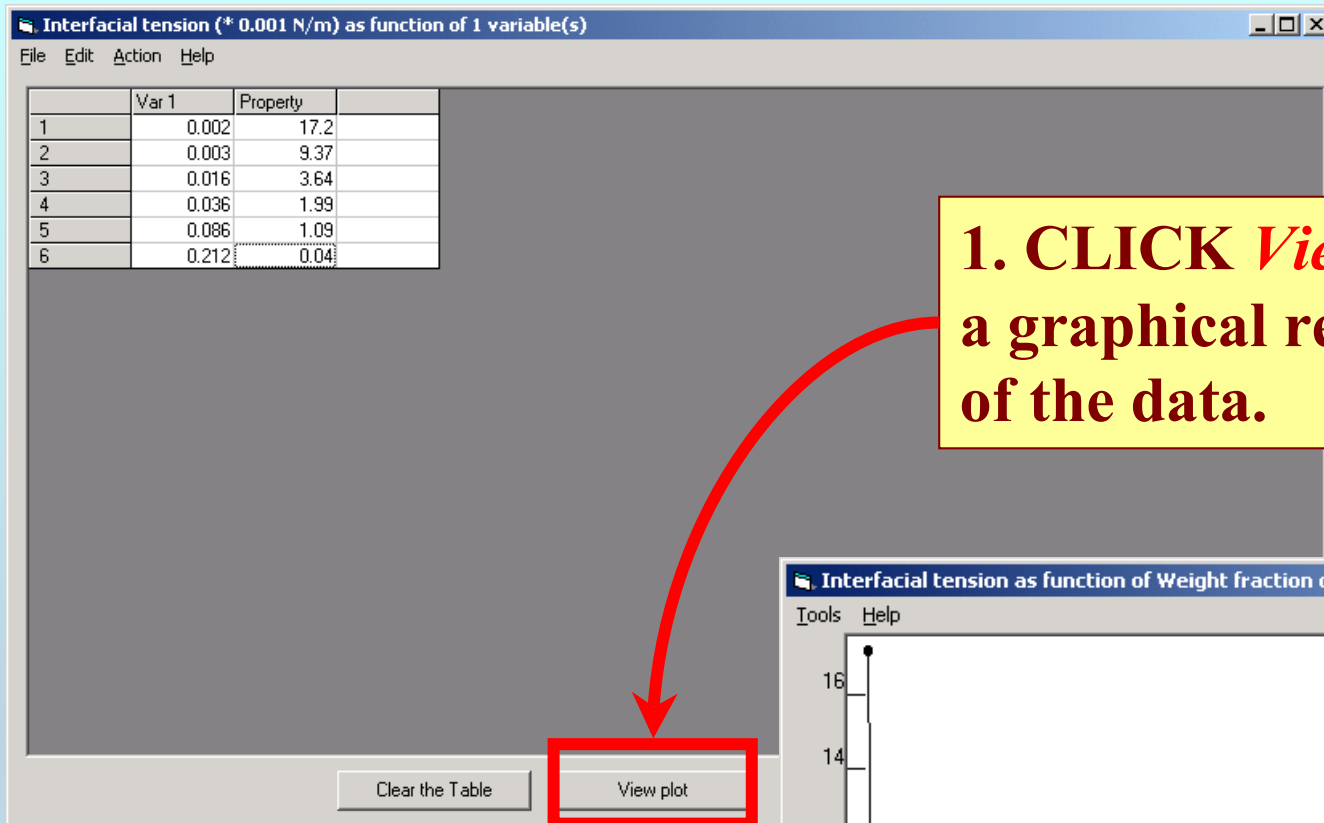
Aqueous phase		Organic phase		Interfacial tension, dyn/cm
Concn, wt %	Density, g/cc	Concn, wt %	Density, g/cc	
Benzene(1)–water(2)–ethanol(3)				
(1)	(3)	(1)	(3)	
0.2	10.8	98.6	1.2	17.20
0.3	21.7	97.1	2.6	9.37
1.6	36.2	94.0	5.4	3.64
3.6	43.7	91.3	7.9	1.99
8.6	50.1	87.3	11.4	1.09
21.2	52.0	79.3	18.0	0.04

Clear the Table



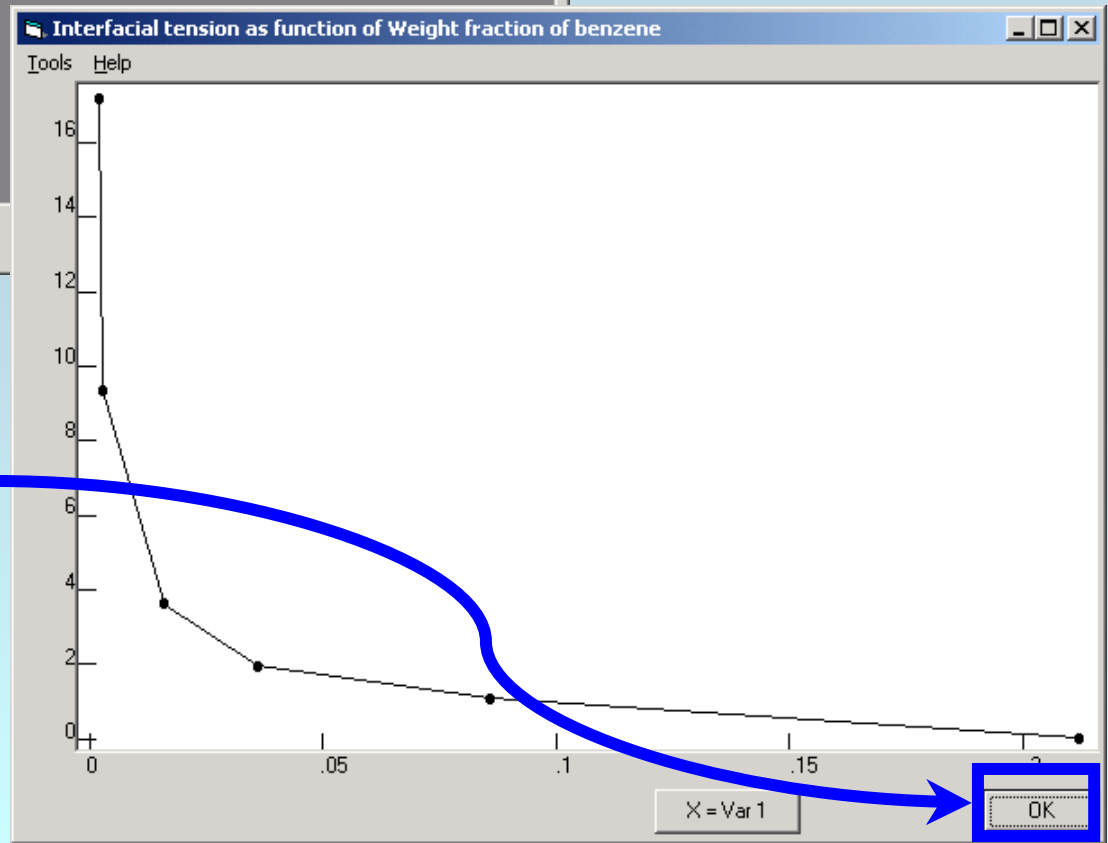
**NOTE:** Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)





**1. CLICK *View plot* to see a graphical representation of the data.**

**2. Check for typographical errors, and CLICK *OK*, when done.**



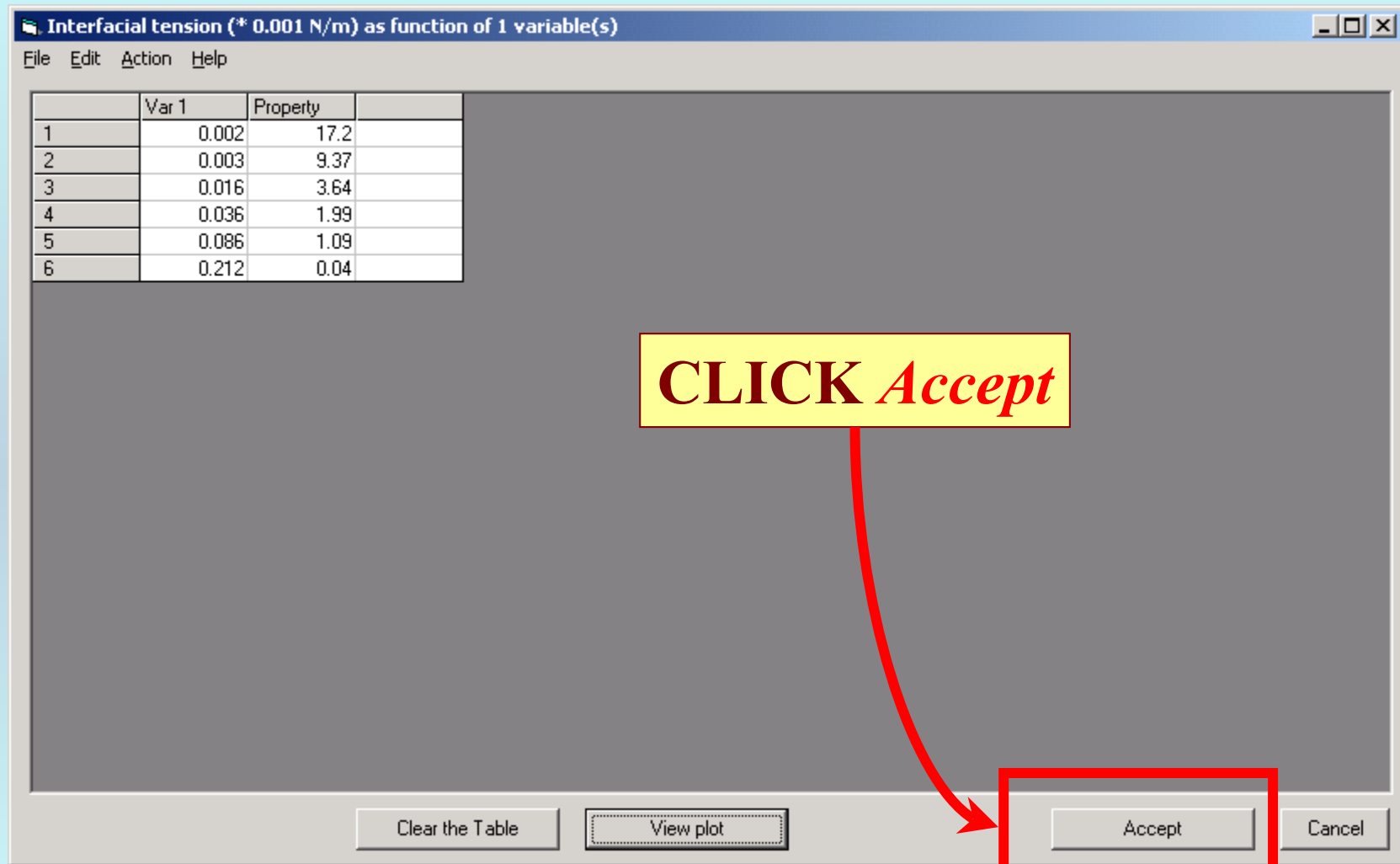
Interfacial tension (\* 0.001 N/m) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	0.002	17.2
2	0.003	9.37
3	0.016	3.64
4	0.036	1.99
5	0.086	1.09
6	0.212	0.04

**CLICK *Accept***

Clear the Table View plot **Accept** Cancel

A screenshot of a software dialog box titled "Interfacial tension (\* 0.001 N/m) as function of 1 variable(s)". The dialog has a menu bar with "File", "Edit", "Action", and "Help". On the left, there is a table with two columns: "Var 1" and "Property". The table contains six rows of data. In the center of the dialog, there is a yellow box with the text "CLICK *Accept*" in red, bold, italicized font. A red arrow points from this box to the "Accept" button at the bottom right of the dialog. The "Accept" button is also highlighted with a red rectangular border. Other buttons at the bottom include "Clear the Table", "View plot", and "Cancel".

## Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

Sample

- [-] 1975 sad kit 0
  - [-] benzene
    - ... Sample 1 (cm;98m%,est)
  - [-] water
    - ... Sample 1 (cm;99.9m%,est)
  - [-] ethanol
    - ... Sample 1 (cm;98m%,est)
  - [-] ethanol + benzene + water

^1: IIT (Set 1), B Method:OTHER dT=0.02

**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.***