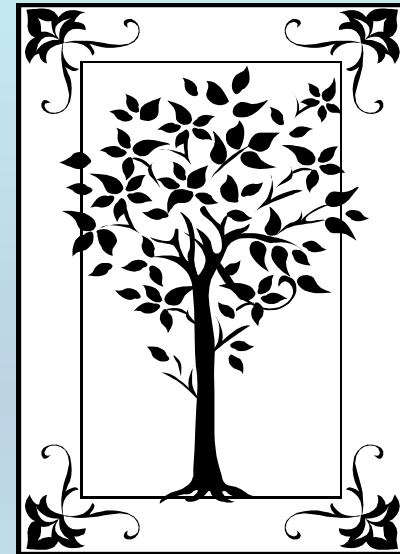


METADATA AND NUMERICAL DATA CAPTURE:
Surface Tension
(for 1 – Component)

Guided Data
Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Surface Tension (1 component)**
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:

1442

J. Chem. Eng. Data 2002, 47, 1442–1445

Surface Tension of Heptane, Decane, Hexadecane, Eicosane, and Some of Their Binary Mixtures

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Surface tension measurements were performed by the Wilhelmy plate method. Measured systems included pure heptane, decane, hexadecane, eicosane, and some of their binary mixtures at temperatures from 293.15 K to 343.15 K with an average absolute deviation of 1.6%. The results were compared with a new corresponding states model. The average absolute deviation was found to be 1.0%.

Surface Tension for 1 component n-heptane

Table 1. Pure Component Data and Comparison with Literature

<i>n</i> -alkane	<i>T</i> /K	this work	$\gamma/\text{mN}\cdot\text{m}^{-1} \pm 0.02 \text{ mN}\cdot\text{m}^{-1}$			
			Jasper ³	McLure ⁴	Jasper ⁵	Koefoed ⁶
<i>n</i> -C ₇ H ₁₆	293.15	20.53	20.28	20.21	20.14	20.30
	303.15	19.49	19.27	19.17	19.17	19.31
	313.15	18.50	18.25	18.19	18.18	
	323.15	17.44	17.24	17.18	17.20	
	333.15	16.50	16.22	16.19	16.22	

These data are
considered here.



Experimental Method Info :

**NIMA DST 9005 tensiometer from NIMA Technology:
Wilhelmy plate method**

Author's uncertainty estimates:

***Surface tension:*
0.02 mN/m**

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction **Property** Data Tables

2002 rol cac 0
heptane
Sample 1 [cm,99x%,no,mv:]

2. CLICK *Property*

1. SELECT the *sample* of the *compound* 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 heptane

Help

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

Property: Surface tension liquid-gas

Units: N/m
ALL OTHER UNITS

Method of measurement:

Experimental purpose:

Comment (optional)

Cancel

The image shows a software dialog box titled "Property and experimental method for heptane". It contains several input fields: "Property group" (set to "Refraction; Surface tension; and Speed of sound"), "Property" (set to "Surface tension liquid-gas"), "Units" (with a dropdown menu showing "N/m" and "ALL OTHER UNITS"), "Method of measurement", "Experimental purpose", and "Comment (optional)". A "Cancel" button is at the bottom right. Three callout boxes with arrows point to specific elements: a red box points to the "Property group" field, a blue box points to the "Property" field, and a green box points to the "Units" dropdown menu.

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

2. SELECT the **Property:** *Surface tension liquid-gas.*

3. SELECT the **Units** from the menu.
NOTE: Choose *ALL OTHER UNITS* for the example because the units in the table are *mN/m* and not *N/m*.

1. TYPE the appropriate **Conversion Factor** in the field; *0.001*, here.

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

OK
Cancel

2. CLICK *OK*

Property and experimental method for heptane

Help

Property group

Property:

Units:

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.

Method of measurement: Ring tensiometer

Experimental purpose: Principal objective of the work

2. SELECT the Experimental Purpose from the list provided.

Comment (optional)

NIMA DST 9005 tensiometer from NIMA Technology with Wilhelmy Plate or DuNuoy ring.

1-Variable data

3. CLICK
1-Variable data.

Cancel

1. SELECT the **Units** for the temperature, and enter the **Uncertainty**, if known.

Surface tension software interface showing Substance: heptane, Sample #: 1, Independent variable: Temperature, Units: K, and Uncertainty input field.

2. SELECT the **Data Presentation**; *Experimental Values*

Data presentation dropdown menu set to Experimental values.

3. SELECT **Phase 1** and **Phase 2**, as shown. TYPE the **Precision of the Property Value**, if known.

Phase 1: Liquid, Phase 2: Air at 1 atmosphere, Precision of the Property Value(s): 0.02, * 0.001 N/m.

4. CLICK *Numerical Data*

Numerical Data button and Cancel button.

Surface tension liquid-gas (* 0.001 N/m) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property	
1	293.15	20.53	
2	303.15	19.49	
3	313.15	18.50	
4	323.15	17.44	
5	333.15	16.50	

1. TYPE, or much preferably, PASTE the variable and property values into the table.

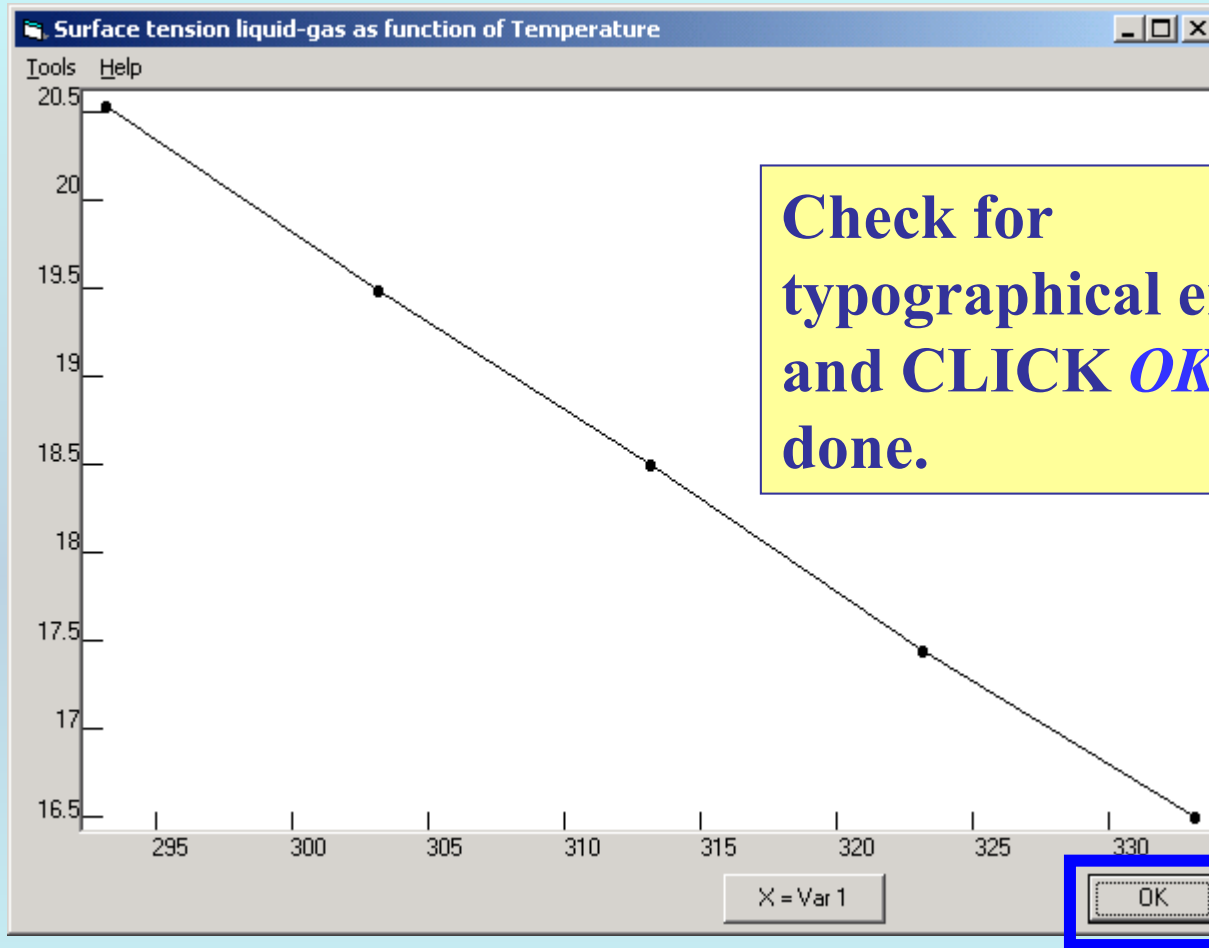
Table 1. Pure Component Data and Comparison with Literature

$\gamma/\text{mN}\cdot\text{m}^{-1} \pm 0.02 \text{ mN}\cdot\text{m}^{-1}$

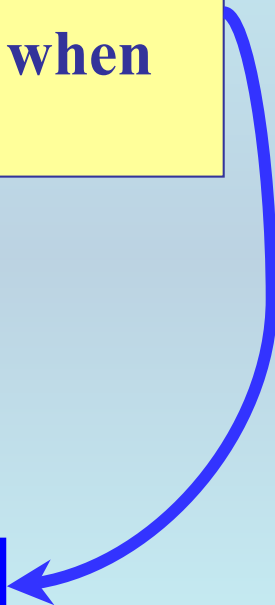
<i>n</i> -alkane	<i>T</i> /K	this work	Jasper ³	McLure ⁴	Jasper ⁵	Koefoed ⁶
<i>n</i> -C ₇ H ₁₆	293.15	20.53	20.28	20.21	20.14	20.30
	303.15	19.49	19.27	19.17	19.17	19.31
	313.15	18.50	18.25	18.19	18.18	
	323.15	17.44	17.24	17.18	17.20	
	333.15	16.50	16.22	16.19	16.22	

Clear the Table View plot Accept Cancel

2. CLICK
View Plot



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



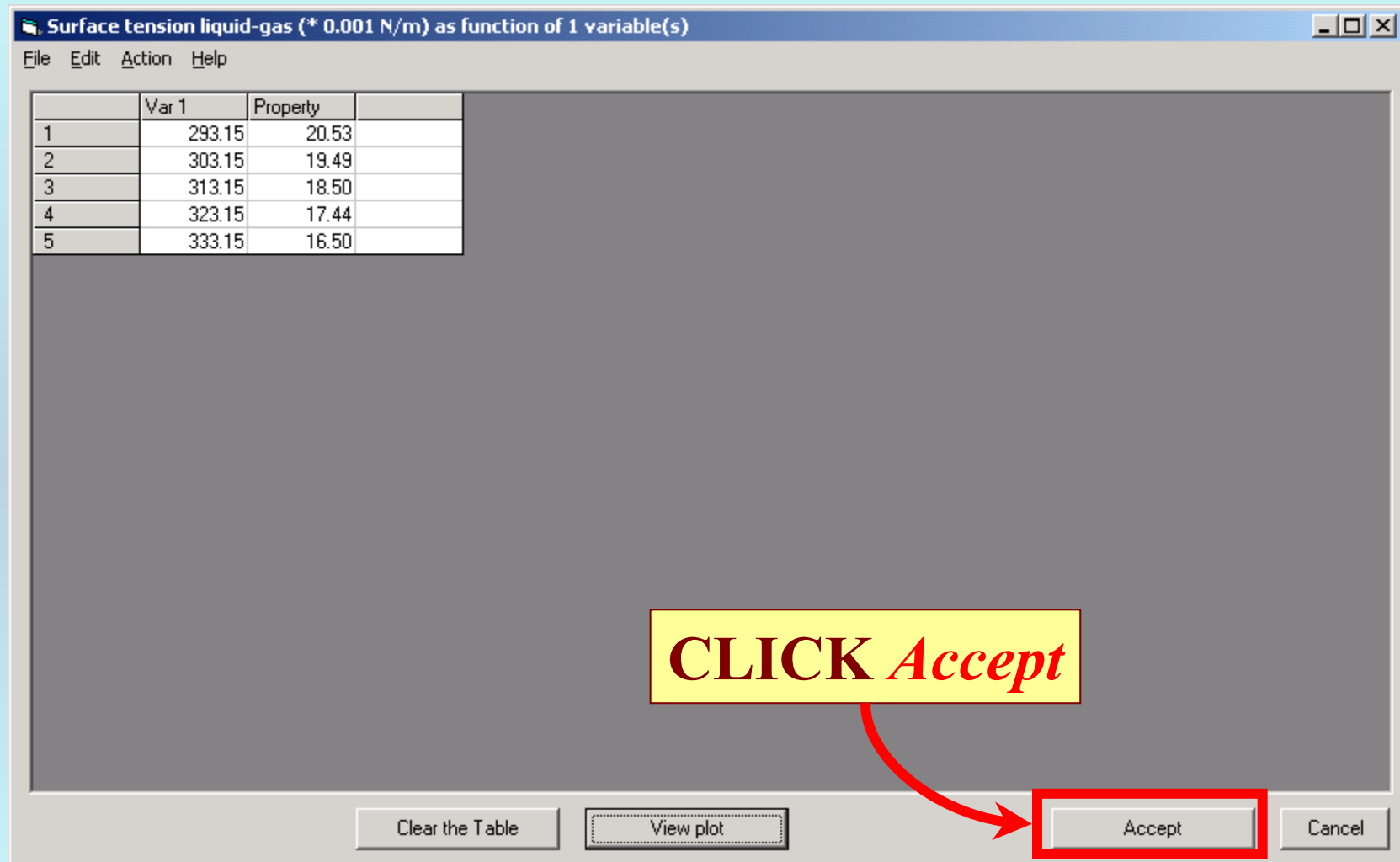
Surface tension liquid-gas (* 0.001 N/m) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	293.15	20.53
2	303.15	19.49
3	313.15	18.50
4	323.15	17.44
5	333.15	16.50

CLICK *Accept*

Clear the Table View plot **Accept** Cancel

The image shows a software window titled "Surface tension liquid-gas (* 0.001 N/m) as function of 1 variable(s)". The window has a menu bar with "File", "Edit", "Action", and "Help". Below the menu bar is a table with three columns: an empty column, "Var 1", and "Property". The table contains five rows of data. Below the table is a large grey area. At the bottom of the window are four buttons: "Clear the Table", "View plot", "Accept", and "Cancel". A yellow box with the text "CLICK *Accept*" and a red arrow points to the "Accept" button, which is also highlighted with a red rectangle.

Guided Data Capture - Thermophysical and Thermochemical

File Edit Tools Help

Reference

Compound

2002 rol cac 0

hexane

Sample 1 [cm,99x%,nc;mv;]

^1: IST (L), Set 1, B Method:RINGTE dIST=0.02

NOTE: The new data set appears in the tree under the appropriate *Sample*.

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.