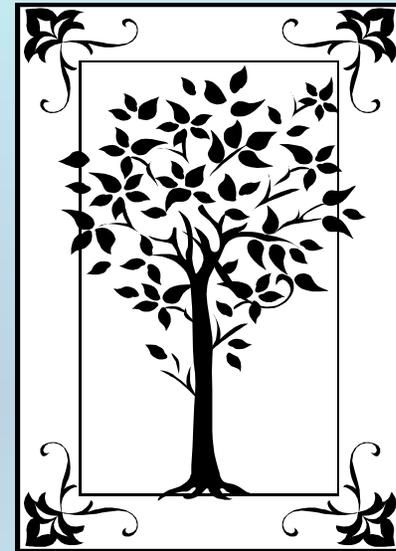


**METADATA AND NUMERICAL DATA CAPTURE:  
Viscosity  $\eta$  as  $f(T)$  with  $p = \text{const.}$   
(1 – Component)**

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



This tutorial describes  
**METADATA AND NUMERICAL DATA CAPTURE:**  
for **Viscosity  $\eta$  as  $f(T)$  with  $p = \text{const.}$**   
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* 2001, 46, 1149–1152

1149

## **Densities and Viscosities of Binary Mixtures of 1,4-Dioxane with 1-Propanol and 2-Propanol at (25, 30, 35, and 40) °C**

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Densities and viscosities for 1,4-dioxane with 1-propanol and 2-propanol mixtures have been measured as a function of mole fraction at atmospheric pressure at (25, 30, 35, and 40) °C. The calculated excess volumes ( $V^E$ ) are positive over the whole range of composition in both systems. The  $V^E$  data were fitted by means of a Redlich–Kister type equation. Furthermore, McAllister's three-body-interaction model was used to correlate the kinematic viscosities of these systems.

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## Viscosities for 1 component as $f(T)$ with $p$ constrained dioxane

Table 1. Densities and Viscosities for the Pure Liquids at Different Temperatures

liquid	$t/^{\circ}\text{C}$	$\rho /(\text{g}\cdot\text{cm}^{-3})$		$\eta /(\text{mPa}\cdot\text{s})$	
		exptl	lit.	exptl	lit.
dioxane	25	1.027882	1.02812 <sup>a</sup>	1.196	1.1944 <sup>a</sup>
	30	1.022219	1.02223 <sup>a</sup>	1.101	1.0937 <sup>a</sup>
			1.02225 <sup>b</sup>		
	35	1.016595	1.01689 <sup>a</sup>	1.014	1.0112 <sup>a</sup>
40	1.011033	1.01157 <sup>b</sup>	0.9425	—	

This data set is  
considered here.

## **Experimental Method & Uncertainty Info :**

**Method: Ubbelohde viscometers**

**Uncertainty: 0.5%**

The screenshot shows the 'Guided Data Capture - Thermophysical and Thermochemical Data' application. The menu bar includes File, Edit, Tools, and Help. The main window has several tabs: Reference, Compound, Sample, Mixture, Reaction, Property, and Data Tables. The 'Property' tab is highlighted with a blue box. A blue arrow points from this tab to a yellow callout box containing the text '2. CLICK *Property*'. In the tree view on the left, 'Sample 1 (cm,99x%,nc;dc;fd)' is selected and highlighted with a red box. A red arrow points from this box to a yellow callout box containing the text '1. SELECT the *sample* of the *compound* for which the data are to be captured.'

1. SELECT the *sample* of the *compound* for which the data are to be captured.

2. CLICK *Property*

**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 1,4-dioxane

Help

Property group: Transport properties

Property: Viscosity

Units: mPa\*s

Method of measurement:

Experimental purpose:

Comment (optional)

1-Variable data

2-Variable data

Cancel

1. SELECT the **Property Group**: *Transport properties* from the menu.

2. SELECT the **Property**: *viscosity*, for this example.

3. SELECT the **Units** from the menu: *mPa\*s*, here.

Property and experimental method for 1,4-dioxane

Help  
Property g  
Property:  
Units: mPa\*s

Method of measurement: Capillary tube (Ostwald; Ubbelohde) method

Experimental purpose: Principal objective of the work

Comment (optional)

1-Variable data

2-Variable data

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 *1-Variable Data* for the example. It is assumed that  $p$  = atmospheric pressure. (CLICK *2-Variable Data* if  $p \neq 101.3$  kPa or is not constant.)

Viscosity (mPa\*s) as function of 1 variable(s)

Substance: 1,4-dioxane Sample # 1

Independent variable: Temperature  
Temperature Units: C Uncert:   C  %

Definition of Measurement Results (Absolute vs Relative)  
Direct value

Data presentation  
Experimental values

Property set # 1 Constraint:

Phase 1:  Phase 2:

mPa\*s  %

Property and method Numerical Data Cancel

1. The **Independent variable** (*Temperature*) is autofilled. **SELECT** the **Units** from the menu. Include the approximate **Uncertainty**, if known.

2. **SELECT** *Direct value* for the **Definition of Measurement Results** and *Experimental values* for **Data Presentation**, here.

**Viscosity (mPa\*s) as function of 1 variable(s)**

Substance: 1,4-dioxane Sample # 1

Independent variable: Temperature  
Temperature Units: %

Definition of Measurement Results (Absolute vs Relative)

1. **SELECT** the phase for the property value **Phase 1: Liquid, here.**

2. Type the **Precision of the Property Value**, if known.

3. **SELECT** the **Constraint**; *Single phase at fixed pressure.  $p = 101.3$  kPa is assumed.*

Experimental values

Property set # 1 Constraint: Single phase at fixed pressure

Phase 1: Liquid

Precision of the Property Value(s)  
0.5 mPa\*s %

Comment to this record:

4. **CLICK Numerical Data**

method Numerical Data Cancel

Viscosity (mPa\*s) 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 1. Densities and Viscosities for the Pure Liquids at Different Temperatures**

liquid	t/°C	$\rho / (\text{g}\cdot\text{cm}^{-3})$		$\eta / (\text{mPa}\cdot\text{s})$	
		exptl	lit.	exptl	lit.
dioxane	25	1.027882	1.02812 <sup>a</sup>	1.196	1.1944 <sup>a</sup>
	30	1.022219	1.02223 <sup>a</sup>	1.101	1.0937 <sup>a</sup>
				1.02225 <sup>b</sup>	
	35	1.016595	1.01689 <sup>a</sup>	1.014	1.0112 <sup>a</sup>
40	1.011033	1.01157 <sup>b</sup>	0.9425	—	

Clear the Table View plot Accept Cancel

Viscosity (mPa\*s) as function of 1 variable(s)

File Edit Action Help

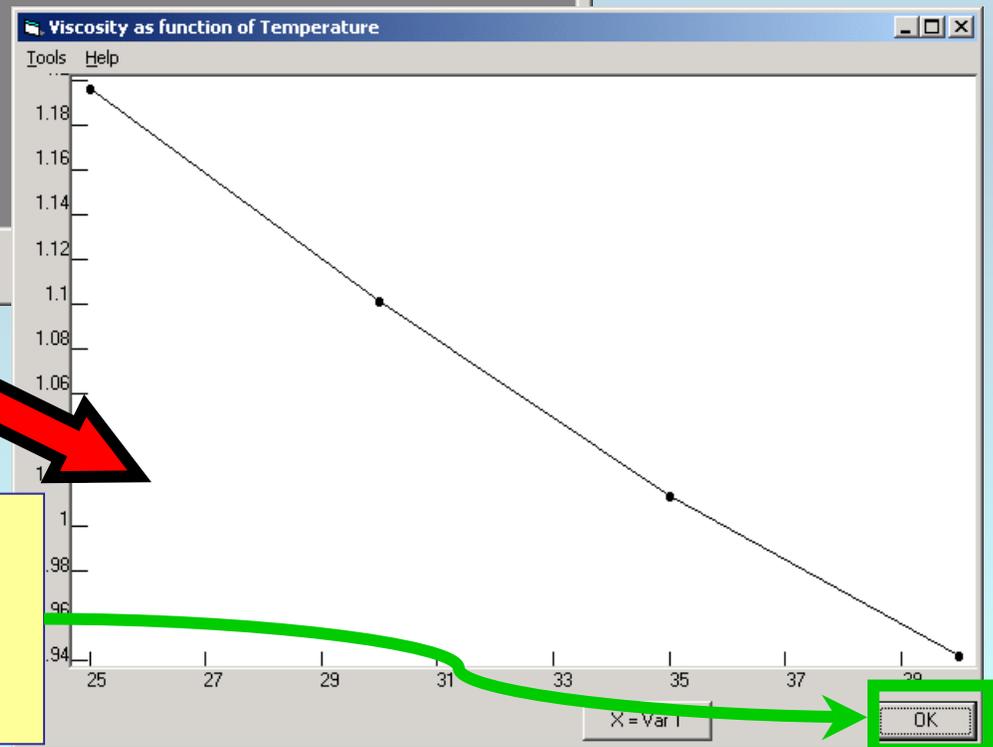
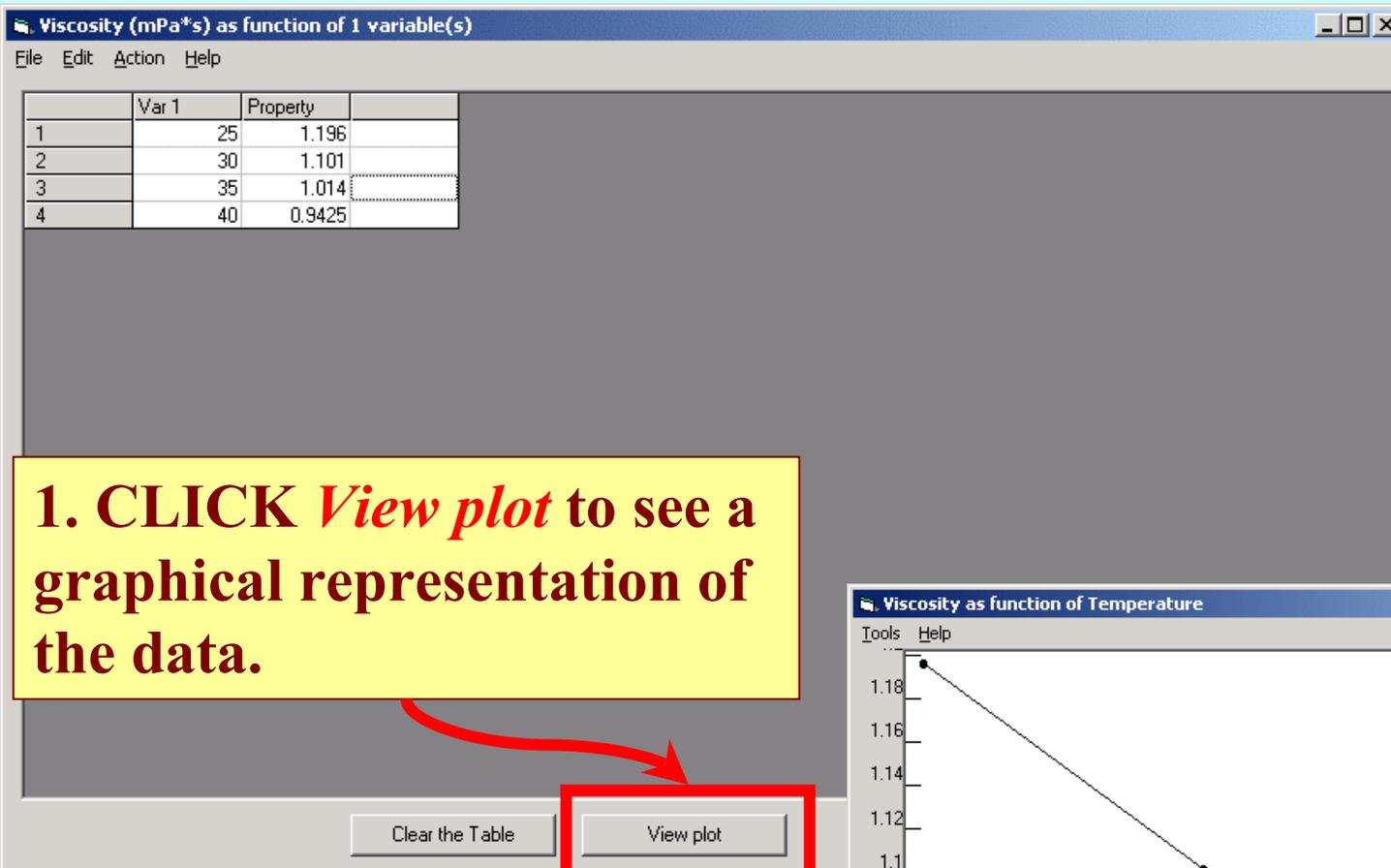
	Var 1	Property	
1	25	1.196	
2	30	1.101	
3	35	1.014	
4	40	0.9425	

**Table 1. Densities and Viscosities for the Pure Liquids at Different Temperatures**

liquid	$t/^{\circ}\text{C}$	$\rho /(\text{g}\cdot\text{cm}^{-3})$		$\eta /(\text{mPa}\cdot\text{s})$	
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	30	1.022219	1.02223 <sup>a</sup> 1.02225 <sup>b</sup>	1.101	1.0937 <sup>a</sup>
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	40	1.011033	1.01157 <sup>b</sup>	0.9425	—

Clear the Table View plot Accept Cancel

**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.)



Viscosity (mPa\*s) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property	
1	25	1.196	
2	30	1.101	
3	35	1.014	
4	40	0.9425	

**CLICK *Accept***

Clear the Table View plot **Accept** Cancel

## Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

[-] 2001 con & 0

[-] 1,4-dioxane

[-] Sample 1 (cm,99x%,nc;dc,fd;)

... ^1: VDN (L), Set 1, B Method:VIBTUB dVDN=0.000005 dT=0.01

... ^1: NVC (L), Set 1, B Method:CAPTUB dNVC=0.5%

**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.***