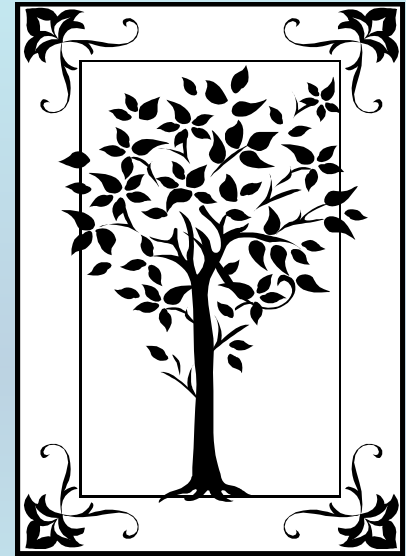


**METADATA AND NUMERICAL DATA CAPTURE:  
Activity Coefficient at Infinite Dilution  
(2 components)**

**Guided Data  
Capture (GDC)**



This tutorial describes  
**METADATA AND NUMERICAL DATA CAPTURE for :**  
**Activity Coefficient at Infinite Dilution (2 components)**  
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* 1999, 44, 1355–1359

1355

**Measurement of Activity Coefficients at Infinite Dilution Using Gas–Liquid Chromatography. 10. Results for Various Solutes with the Stationary Phases Dimethyl Sulfoxide, Propylene Carbonate, and *N*-Ethylformamide**

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Using gas–liquid chromatography (GLC), activity coefficients at infinite dilution have been measured for 37 solutes (alkanes, alkenes, cyclic hydrocarbons, aromatic hydrocarbons, alcohols, ketones, ethers, aldehydes, esters, and halocarbons) in the solvents dimethyl sulfoxide, propylene carbonate, and *N*-ethylformamide. The measurements were carried out in the temperature range between 303.15 and 333.15 K. The obtained  $\gamma^\infty$  values are compared with published data, and the observed temperature dependence of the limiting activity coefficients is confirmed using excess enthalpy data. Furthermore, the selectivities and capacities of the investigated solvents for the separation of aliphatics from aromatics are compared.

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## Activity Coefficient at Infinite Dilution for: hexane in propylene carbonate

Table 1. Experimental Activity Coefficients at Infinite Dilution  $\gamma^\infty$  for Various Solutes in the Solvent Propylene Carbonate

solute	$\gamma^\infty$			
	303.15K	313.15 K	323.15 K	333.15 K
hexane	40.6	37.6	34.6	32.0

The data considered here.

**Method:** Gas-Liquid Chromatography

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

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

- 1999 top gru 0
  - hexane
    - Sample 1 (cm:(None used);)
  - propylene carbonate
    - Sample 1 (cm:99.8m% nc:99.8m%,glc)
  - propylene carbonate + hexane**

**1. SELECT the *mixture* for which the property is to be entered.**

**2. CLICK *Property***

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

# Property & Units selection

Property and experimental method for propylene carbonate + hexane

Help

Property group: Activity; Fugacity; and Osmotic properties

Property: Activity coefficient of hexane

Units: Dimensionless

Method of measurement:

Experimental purpose:

Comment (optional)

OK Cancel

1. SELECT the **Property group:**  
*Activity; Fugacity; and Osmotic properties*

2. SELECT the **Property:**  
*Activity coefficient of hexane,*  
for the example.

3. SELECT the **Units:**  
*Dimensionless, here*

# Method selection

The image shows a software dialog box titled "Property and experimental" with the following fields and callouts:

- Property group:** Activity; Fugacity
- Property:** Activity coefficient of H
- Units:** Dimensionless
- Method of measurement:** Chromatography (highlighted with a red box and a red arrow pointing to it from the first callout)
- Experimental purpose:** Principal objective of the work (highlighted with a blue box and a blue arrow pointing to it from the second callout)
- Comment (optional):** (empty text box)
- Buttons:** OK (highlighted with a green box and a green arrow pointing to it from the third callout) and Cancel

1. SELECT the **Method of measurement** from the menu. SELECT *Other* and provide a short *Comment*, if needed.

2. SELECT the **Experimental purpose**

3. CLICK *OK*

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

Activity coefficient of hexane () (Dimensionless) as function of 1 variable(s)

Mixture: propylene carbonate + hexane

Phases in equilibrium: 2

Constraints: 1

Independent variables: 1

Phase of the Property Value(s)

Enter the # of **Phases in equilibrium**.

There are **2** phases here (*liquid and gas*).

Enter the # of **Constraints**.

There is **1** constraint; *composition*



Activity of hexane () (Dimensionless) as function of 1 variable(s)

Mixture: propylene carbonate + hexane

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

Sample #: 1 Sample #: 1

Phase of the Property Value(s):

Precision of the Property value(s):  Dimensionless  %

Definition of Measurement Results (Absolute vs Relative):

Data presentation: Experimental values

Comments (Optional): See also Knoop et al., J. Chem. Eng. Data, 1989, 34, 240-247.

Property and method Numerical Data Cancel

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

Activity of hexane (Liquid) as function of 1 variable(s)

Mixture: propylene carbonate + hexane

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)   Dimensionless  %

Phase 2

Constraint 1 (Fixed value of)

Independent variable 1

Definition of Measurement Results (Absolute vs Relative)

Data presentation

Experimental values

Cancel

**SELECT *Liquid* from the list provided for the **Phase of the Property Value**.**

**NOTE:** *Phase 2, Constraint and Independent Variable* field(s) appear automatically based on the Gibbs Phase Rule.

# Specification of 2<sup>nd</sup> phase, constraint and independent variable

1. SELECT **Phase 2** (*Gas* here) and the **Independent Variable** (*Mole fraction of benzene*, here) from the menus.

Phase of the Property Value(s) Liquid

Phase 2  
Gas

Constraint 1 (Fixed value of)  
Mole fraction of hexane

Independent variable 1  
Temperature

Value: 0 Units: Dimensionless Uncertainty:  %

Units: K Uncertainty:  %

2. SELECT **Units** for the *Variable* (K, here), the **Value** (0) and **Units** (*Dimensionless*) for the *Constraint*, and include estimated **Uncertainties**, if known.

**NOTE:** The constraint value (0) defines the property  $\gamma^\infty$ .

# Measurement definition and Data presentation

Activity of hexane (Liquid) as function of 1 variable(s)

Mixture: propylene carbonate + hexane

Phases in equilibrium: 2 Constraints: 1 Independent variable

Phase of the Property Value(s) Liquid

Phase 2 Gas

Constraint 1 (Fixed value of) Mole fraction of hexane of Liquid

Independent variable 1 Temperature of Liquid Units: K Uncertainty: %

Definition of Measurement Results (Absolute vs Relative) Direct value

Data presentation Experimental values

Standard state: Pure compound

Comments (Optional): [See also Knoop et al., J. Chem. Eng. Data, 1989, 34, 240-247.]

Numerical Data

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. SELECT the **Standard state**: *Pure compound*, here.

4. CLICK *Numerical Data*

Activity of hexane (Dimensionless) 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. Experimental Activity Coefficients at Infinite Dilution  $\gamma^\infty$  for Various Solutes in the Solvent Propylene Carbonate**

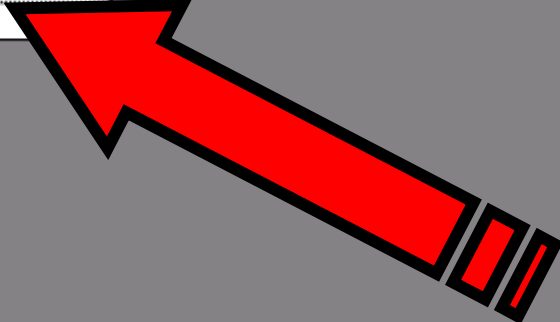
solute	$\gamma^\infty$			
	303.15K	313.15 K	323.15 K	333.15 K
hexane	40.6	37.6	34.6	32.0

Clear the Table View plot Accept Cancel

Activity of hexane (Dimensionless) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property	
1	303.15	40.6	
2	313.15	37.6	
3	323.15	34.6	
4	333.15	32.0	

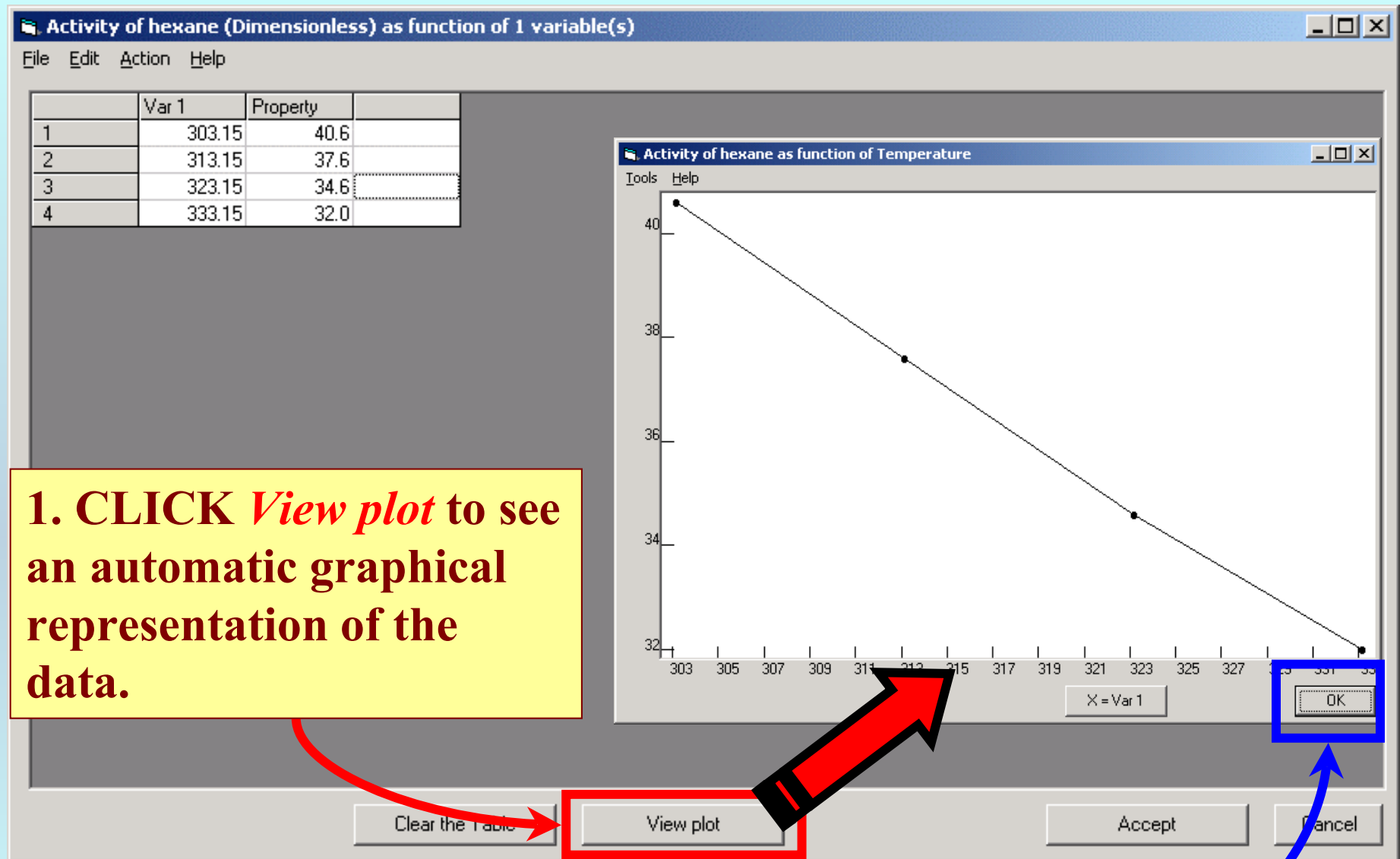


**Table 1. Experimental Activity Coefficients at Infinite Dilution  $\gamma^{\infty}$  for Various Solutes in the Solvent Propylene Carbonate**

solute	$\gamma^{\infty}$			
	303.15K	313.15 K	323.15 K	333.15 K
hexane	40.6	37.6	34.6	32.0

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.)



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

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

**You are returned to the previous screen...**

Activity of hexane (Dimensionless) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property	
1	303.15	40.6	
2	313.15	37.6	
3	323.15	34.6	
4	333.15	32.0	

**CLICK *Accept***

Clear the Table View plot **Accept** Cancel



## Guided Data Capture - Thermophysical and Thermochemical

File Edit Tools Help

Reference

Compound

Sample

Mixture

[-] 1999 top gru 0

[-] hexane

... Sample

[-] propylene c

... Sample 1 (cm,99.8m%,nc;99.8m%,glc)

[-] propylene carbonate + hexane

^1: AC2 (Set 1), B Method:CHROM

**NOTE:** The new *Property* appears below the *Mixture* in the navigation tree.

**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.***