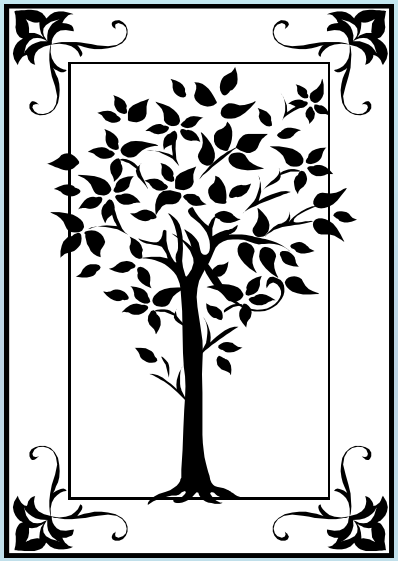
METADATA AND NUMERICAL DATA CAPTURE:
Activity Coefficient at Infinite Dilution (2 components)

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

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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Carl von Ossietzky Universität Oldenburg, Technische Chemie (FB 9), Postfach 2503, D-26111 Oldenburg, Federal Republic of Germany

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 γ^{∞} 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.

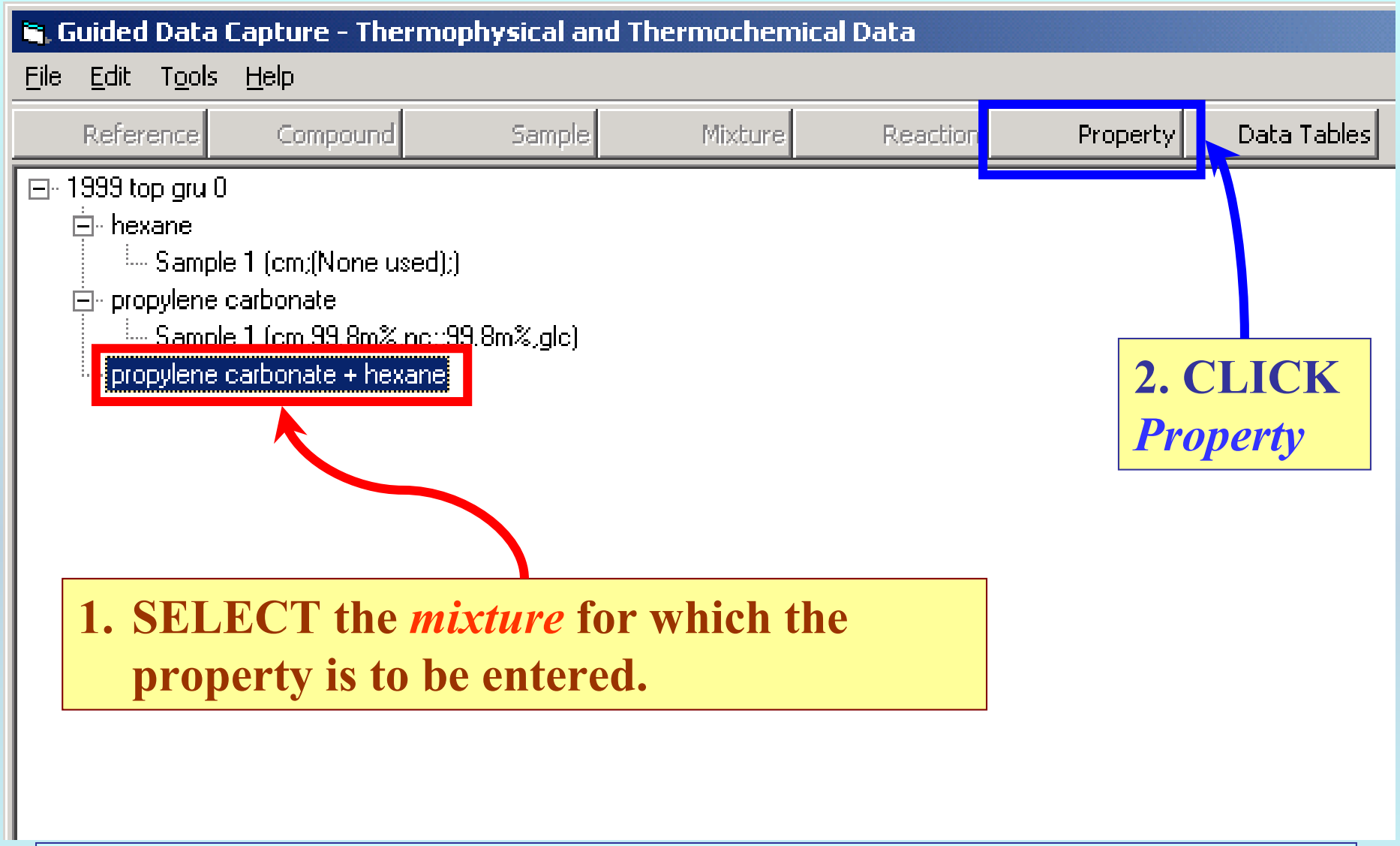
Activity Coefficient at Infinite Dilution for:
hexane in propylene carbonate

Table 1. Experimental Activity Coefficients at Infinite Dilution γ^{∞} for Various Solutes in the Solvent Propylene Carbonate

	γ^{∞}			
solute	303.15K	313.15 K	323.15 K	333.15 K
hexane	40.6	37.6	34.6	32.0

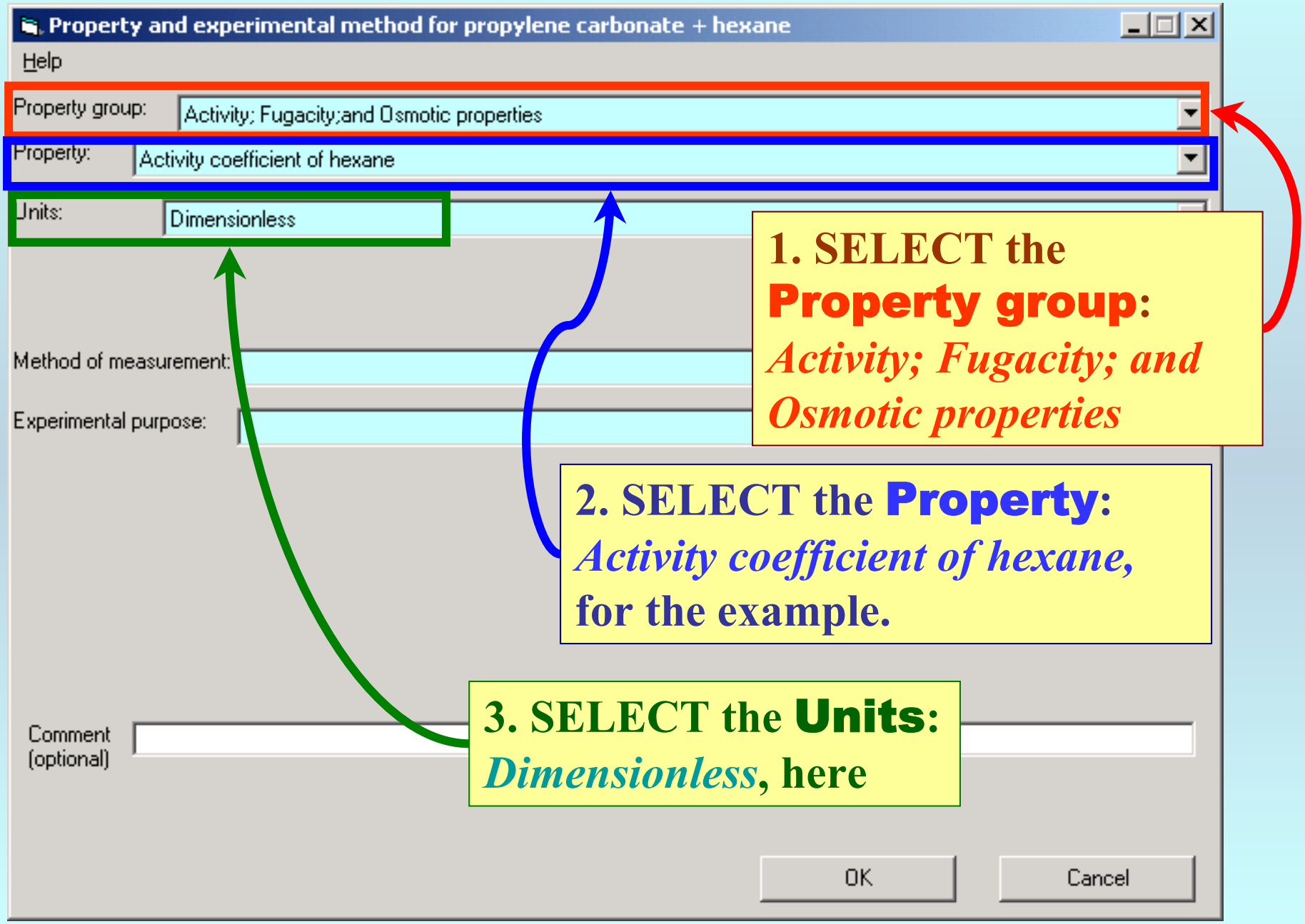
The data considered here.

Method: Gas-Liquid Chromatography

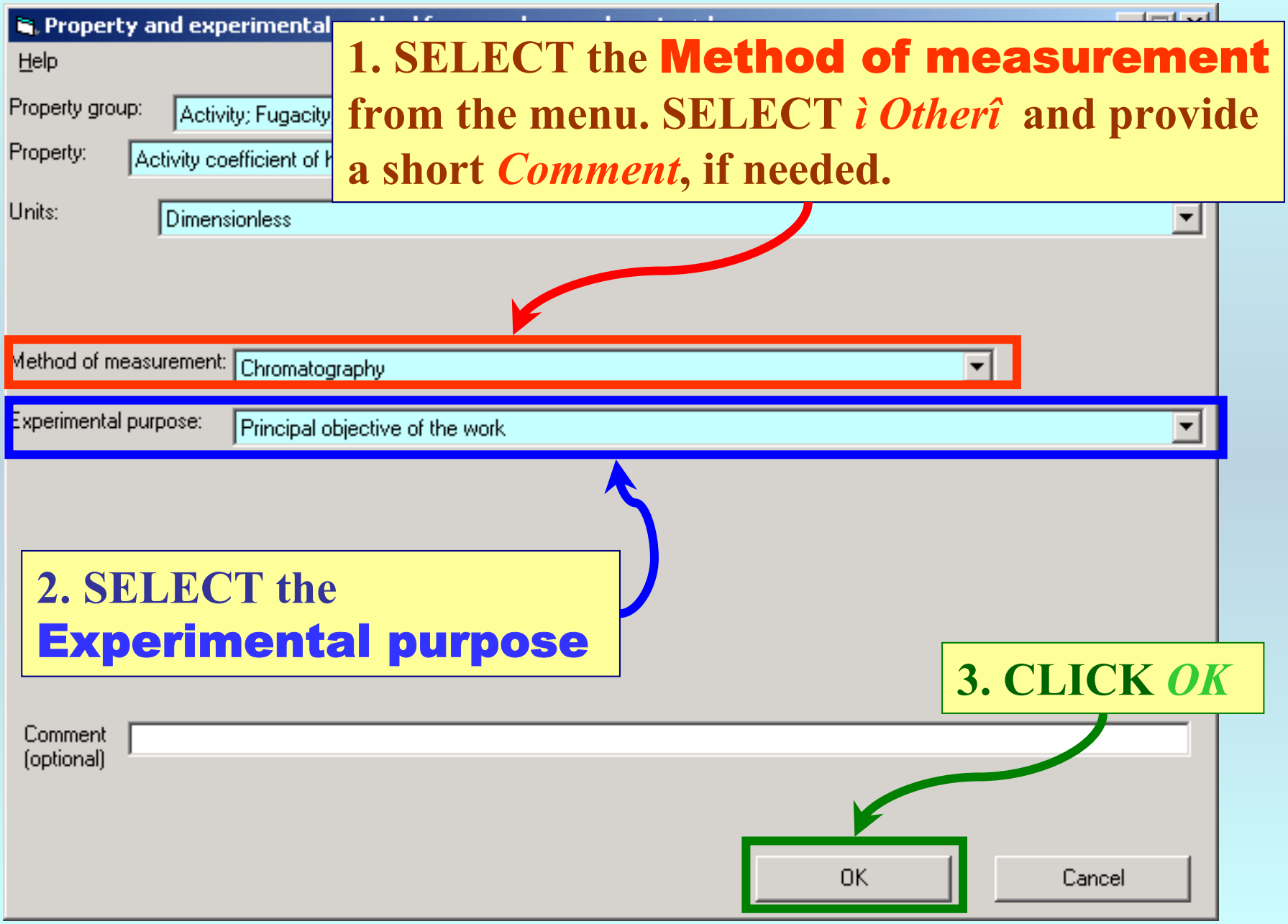


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials related to capture of this information.)

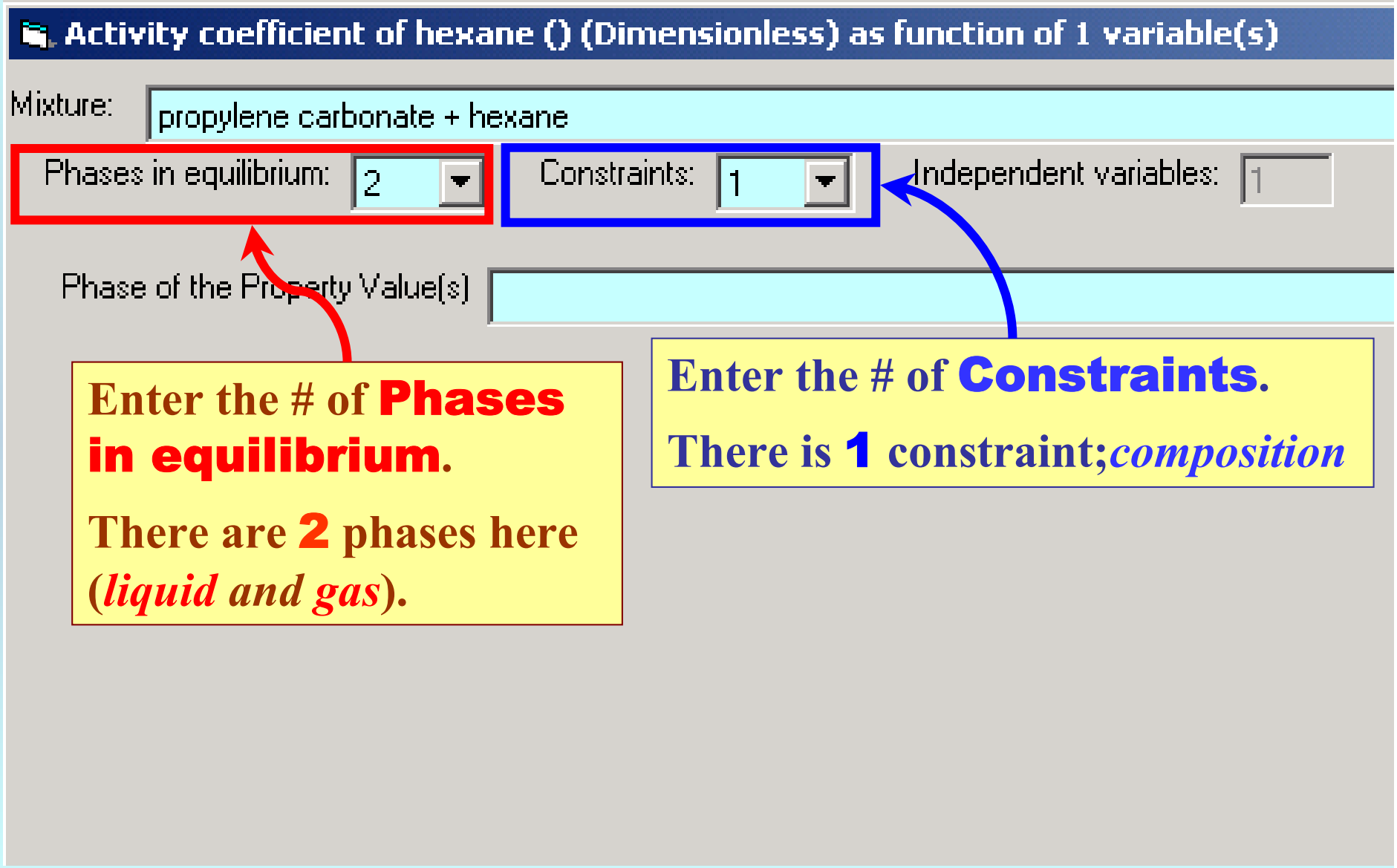
Property & Units selection

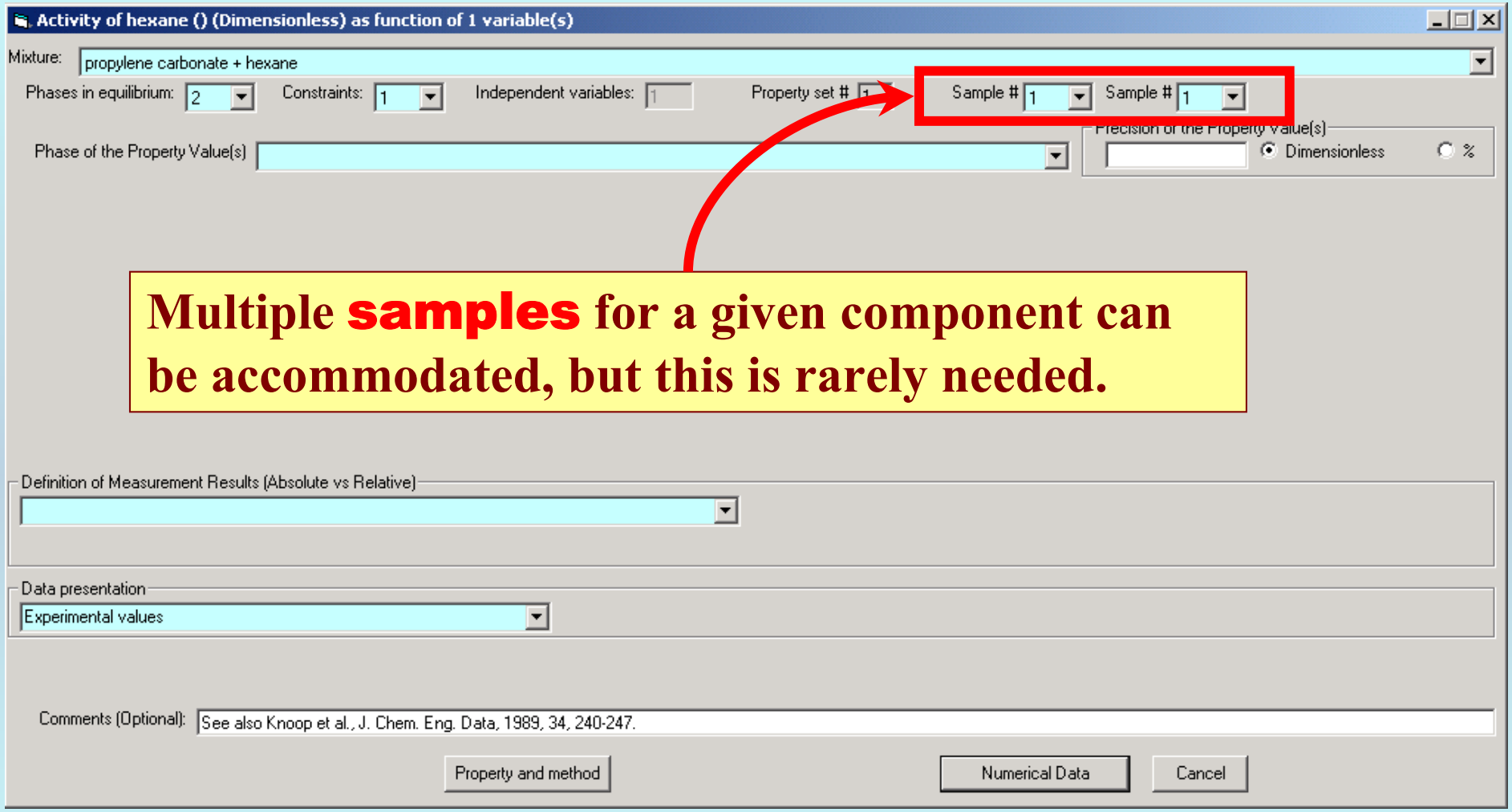


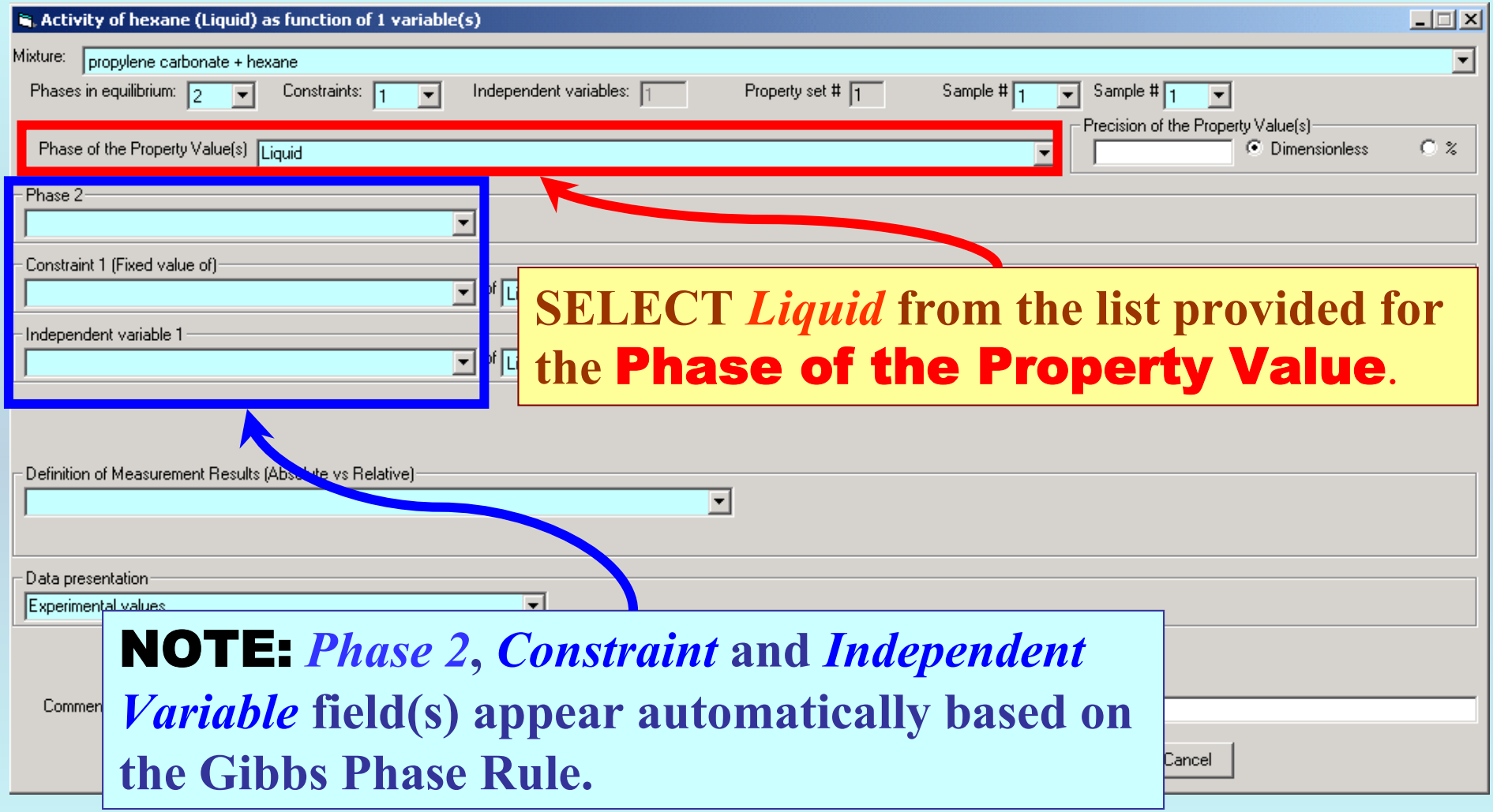
Method selection



SELECTION of # of Phases in Equilibrium and # of Constraints

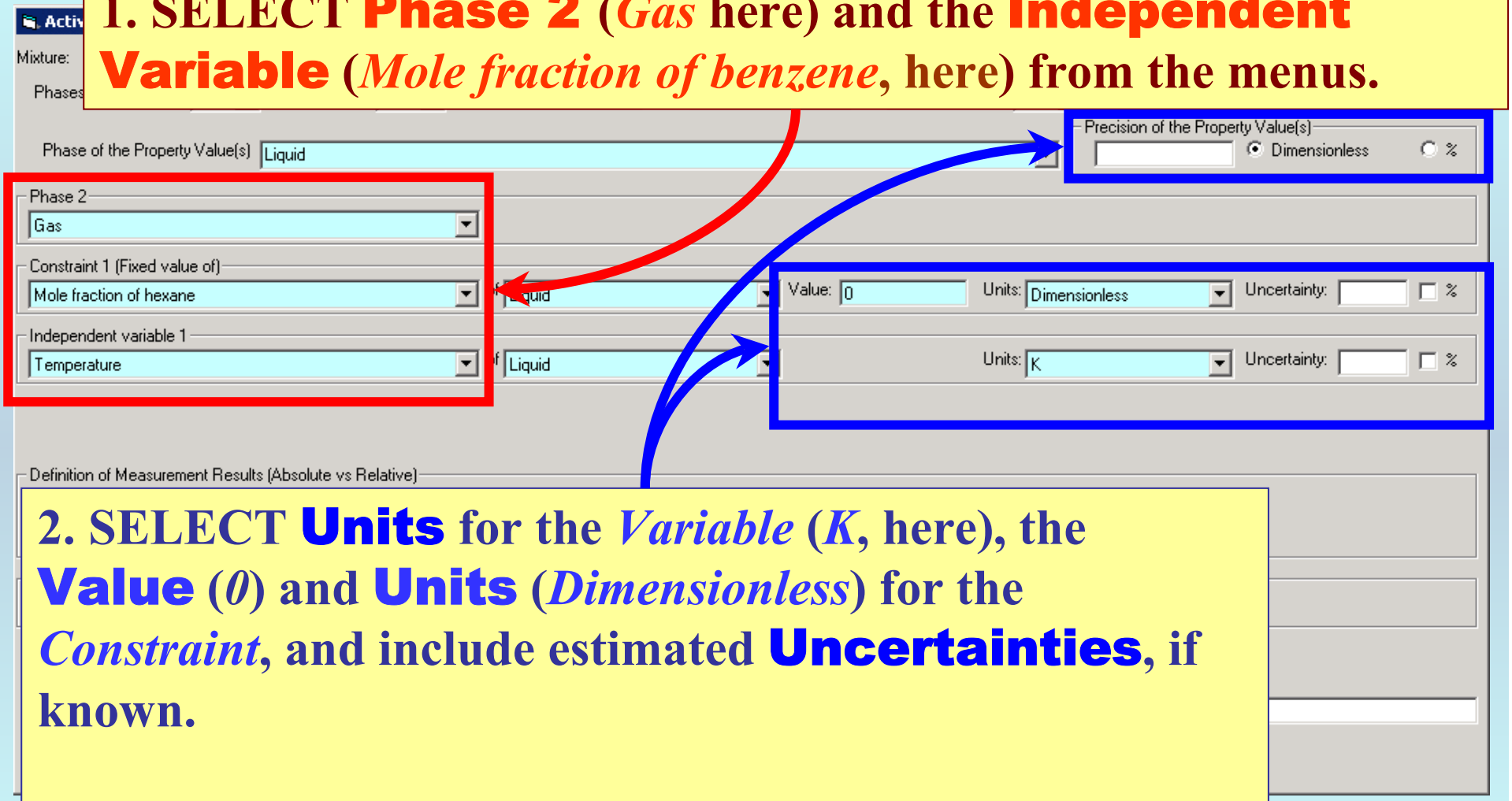



Activity of hexane () (Dimensionless) as function of 1 variable(s)
Mixture:
propylene carbonate + hexane
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Precision of the Property Value(s)
Dimensionless
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
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


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 2nd phase, constraint and independent variable

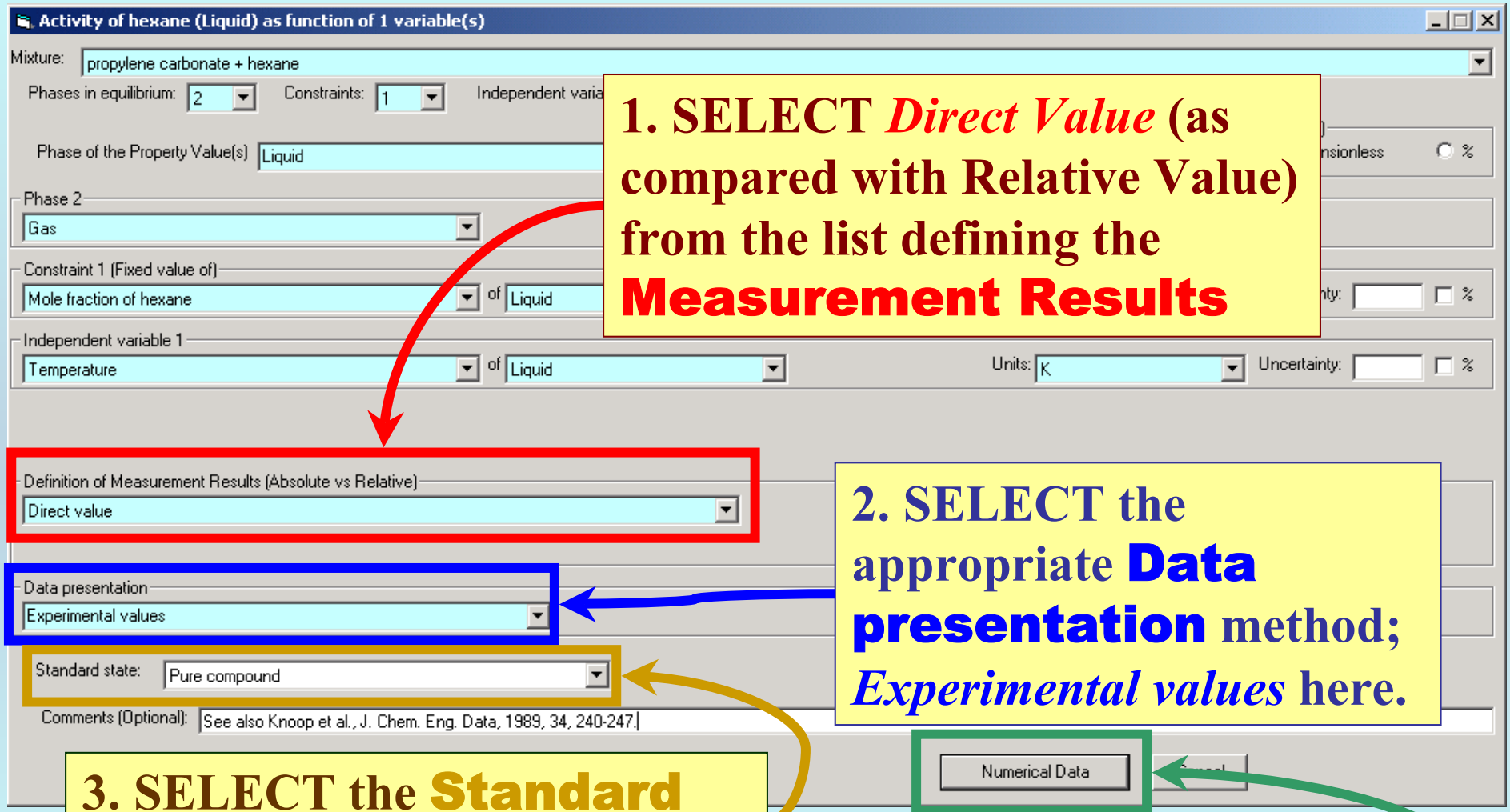
1. SELECT Phase 2 (*Gas* here) and the Independent Variable (*Mole fraction of benzene*, here) from the menus.

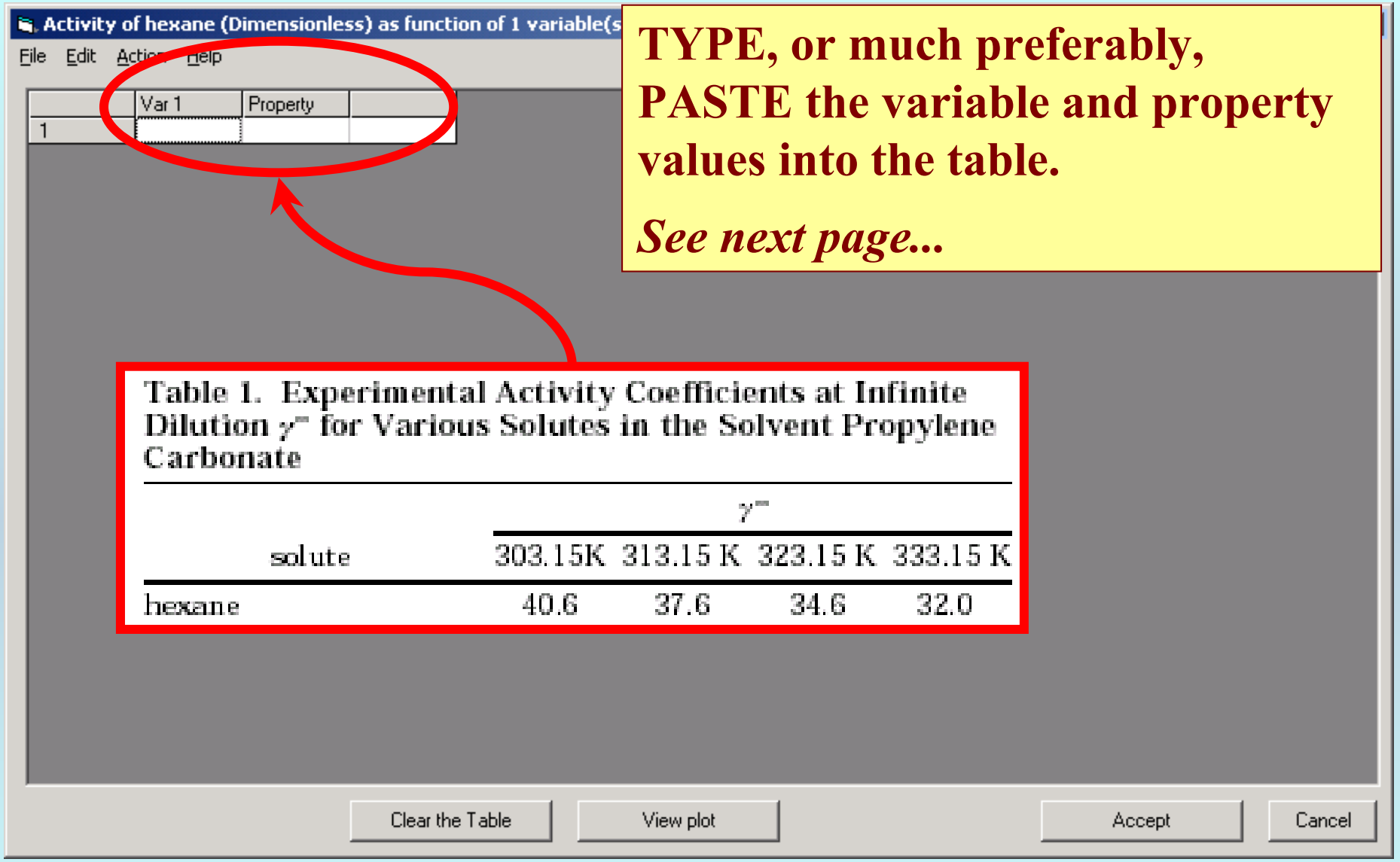


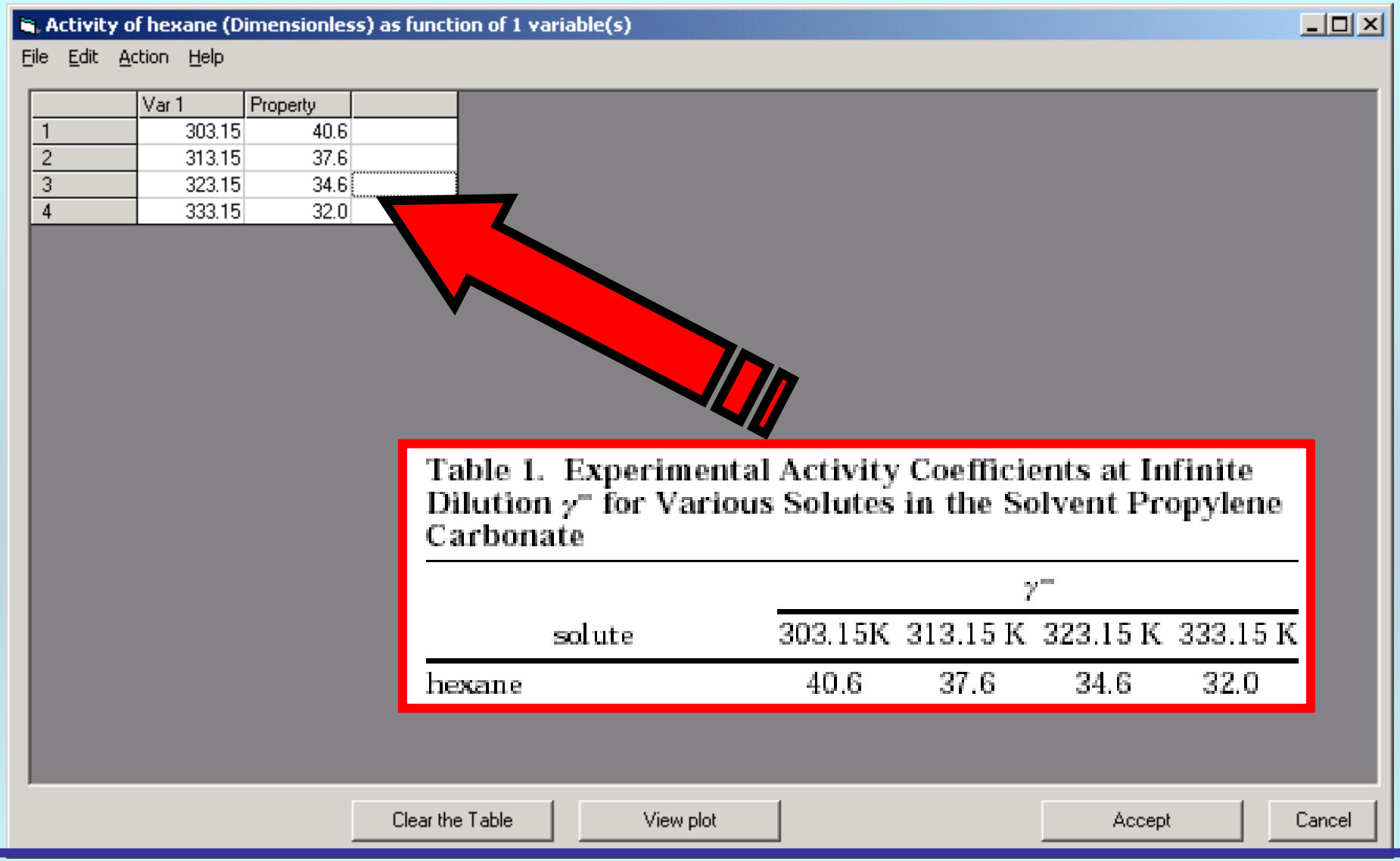
2. SELECT Units for the *Variable* (*K*, here), the Value (*0*) and Units (*Dimensionless*) for the *Constraint*, and include estimated Uncertainties, if known.

NOTE: The constraint value (*0*) defines the property γ^{∞}.

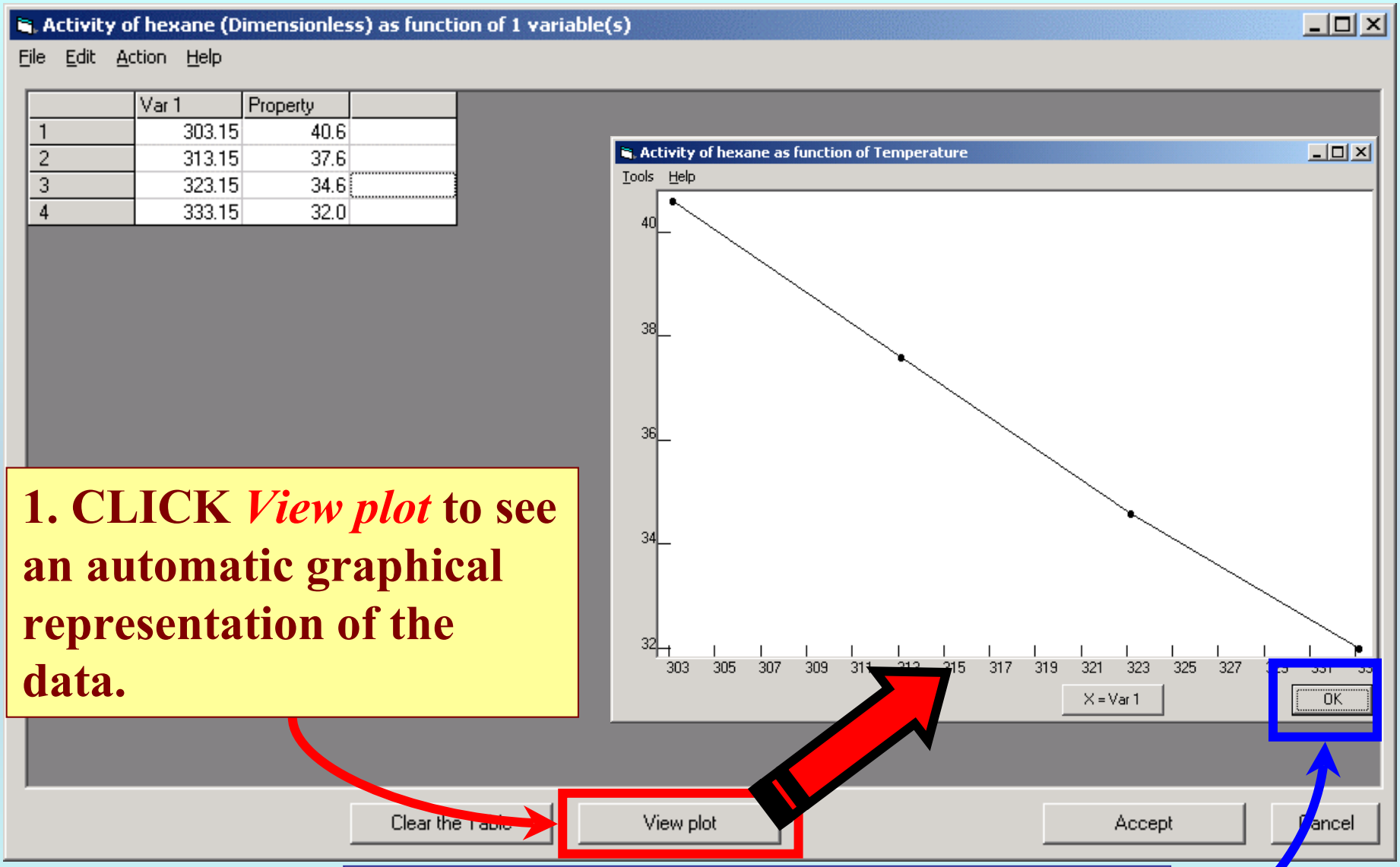
Measurement definition and Data presentation




Activity of hexane (Dimensionless) as function of 1 variable(s
File
Edit
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 γ^{∞} for Various Solutes in the Solvent Propylene Carbonate
γ^{∞}
solute
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



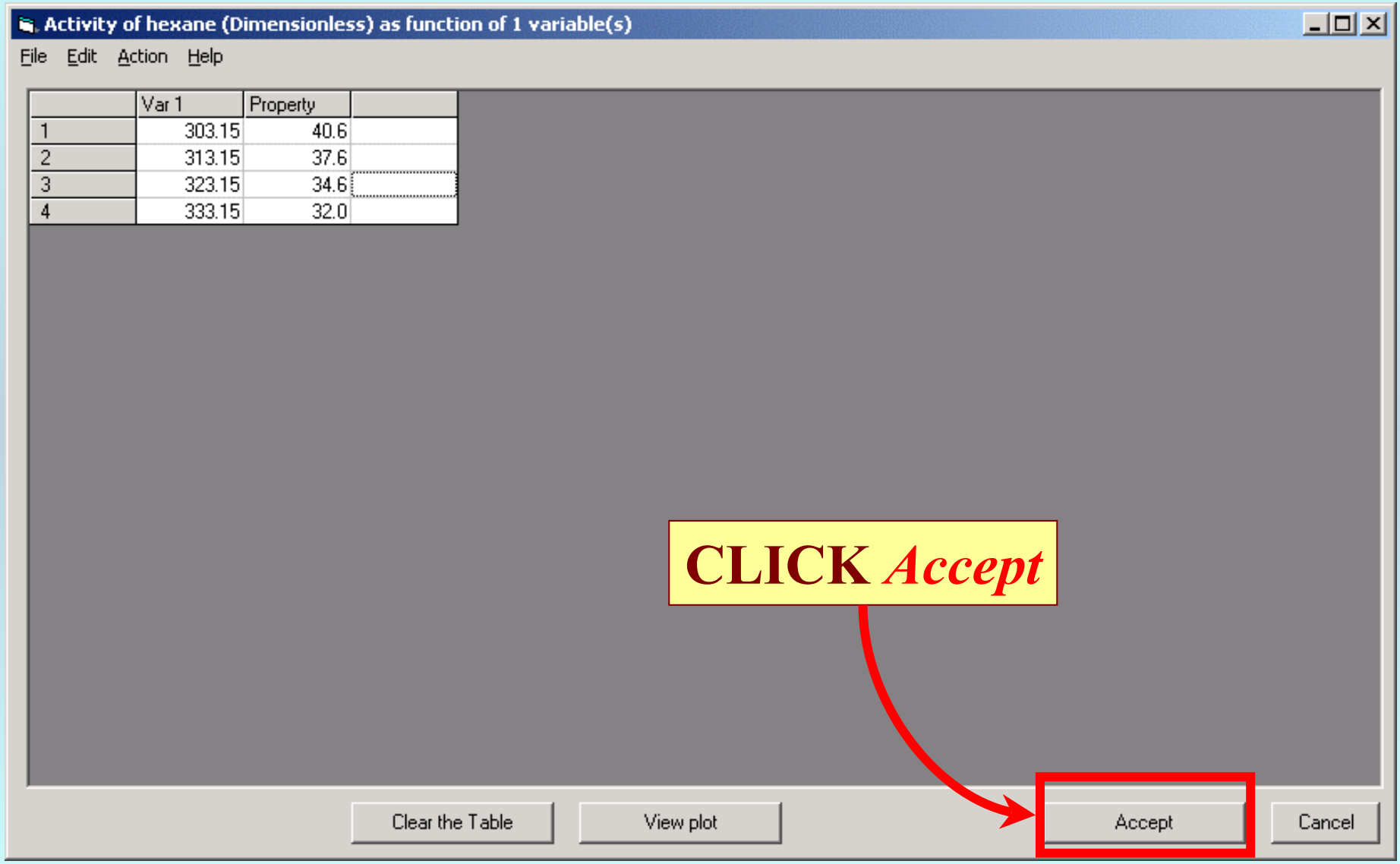
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software; e.g., EXCEL.)

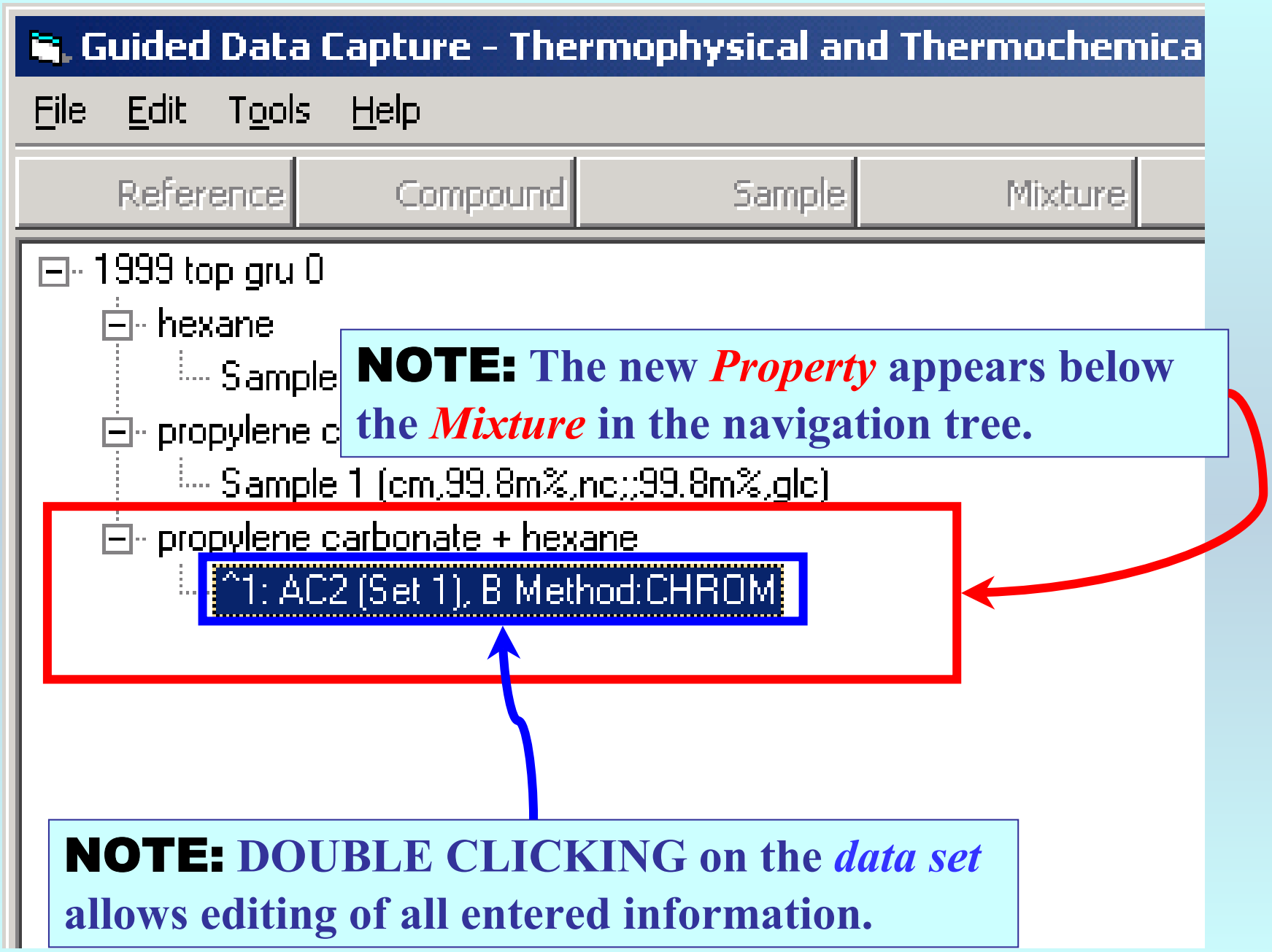


1. CLICK *View plot* to see an automatic graphical representation of the data.

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

You are returned to the previous screen...




Guided Data Capture - Thermophysical and Thermochemica
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.**