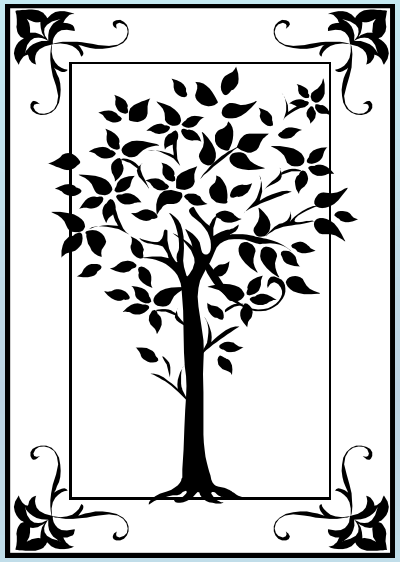
METADATA AND NUMERICAL DATA CAPTURE:
EUTECTIC TEMPERATURE
2 – Components: *Solid / Liquid*

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components: Solid/Liquid**
EUTECTIC TEMPERATURE (*T* / K)
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:

Solubility of Benzimidazoles in Alcohols

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Warsaw University of Technology, Faculty of Chemistry, Physical Chemistry Division, 00-664 Warsaw, Poland

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The solid−liquid equilibrium (SLE) has been measured from 270 K to 445 K for 10 binary mixtures of benzimidazoles (benzimidazole and 2-methylbenzimidazole) with alcohols (1-propanol, 1-butanol, 2-butanol, 2-methyl-2-propanol, 1-hexanol) using a dynamic method. The melting point, enthalpy of fusion, and heat capacity change at the melting temperature were determined by differential scanning calorimetry (DSC). The solubility of benzimidazoles in alcohols (C_3−C_6) is higher than in water and in 1-octanol and generally decreases with an increase of the alkyl chain length of the alcohol. The intermolecular solute−solvent interaction is higher for the 1-alcohol than for the secondary or tertiary alcohol. The solubility of 2-methylbenzimidazole in alcohols (C_3−C_6) is higher than that of benzimidazole. Experimental results of solubility were correlated by means of the Wilson, UNIQUAC ASM, and NRTL 1 equations utilizing parameters derived from SLE results. The existence of a solid−solid first-order phase transition in benzimidazole and 2-methylbenzimidazole has been observed in the DSC measurements and has been taken into consideration in the solubility calculation. The best correlation of the solubility data has been obtained by the NRTL 1 equation.

ASAP article: JE020228x

EUTECTIC TEMPERATURE

(2 ñ Components)

2-methyl-2-propanol & benzimidazole

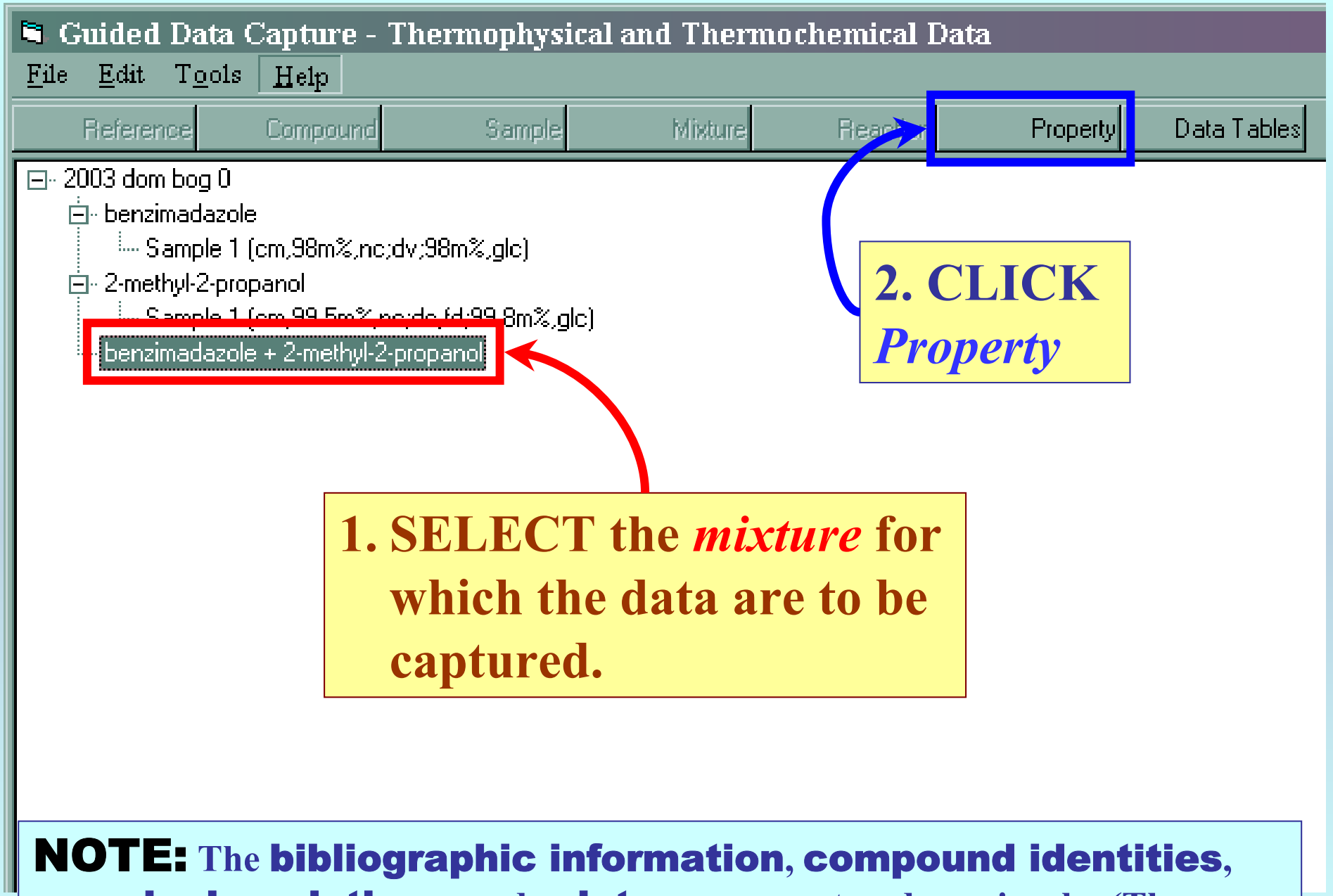
Table 4. Eutectic Temperatures, $T_{l,e}$, and Composition, $x_{l,e}$, Detected Graphically for Systems of {Benzimidazole or 2-Methylbenzimidazole (1) + 2-Methyl-2-propanol(2)}

system	$x_{l,e}$	$T_{l,e}$ /K
benzimidazole + 2-methyl-2-propanol	0.09 ± 0.01	286.60 ± 0.1
2-methylbenzimidazole + 2-methyl-2-propanol	0.10 ± 0.01	281.71 ± 0.1

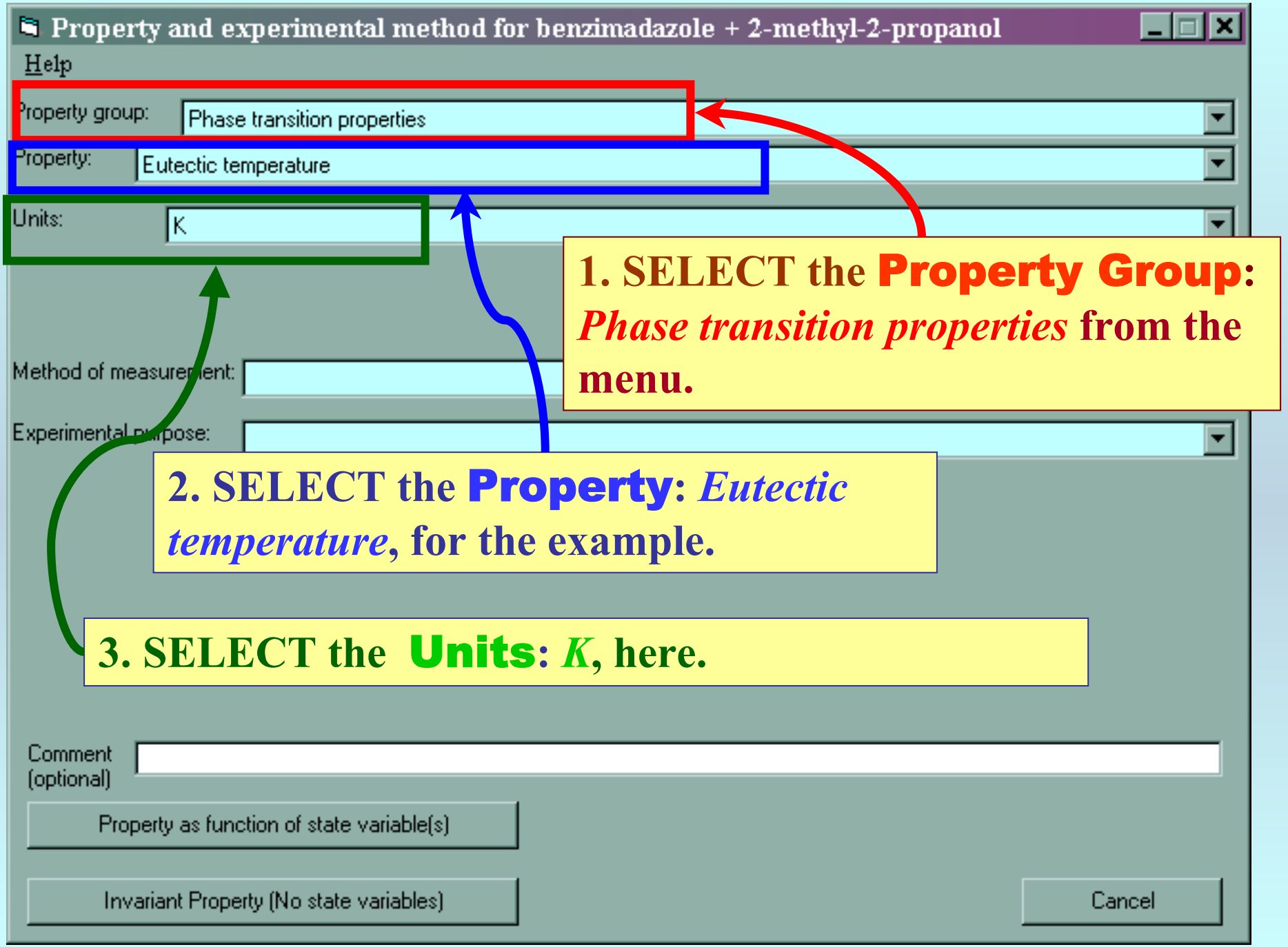
This data set is considered here.

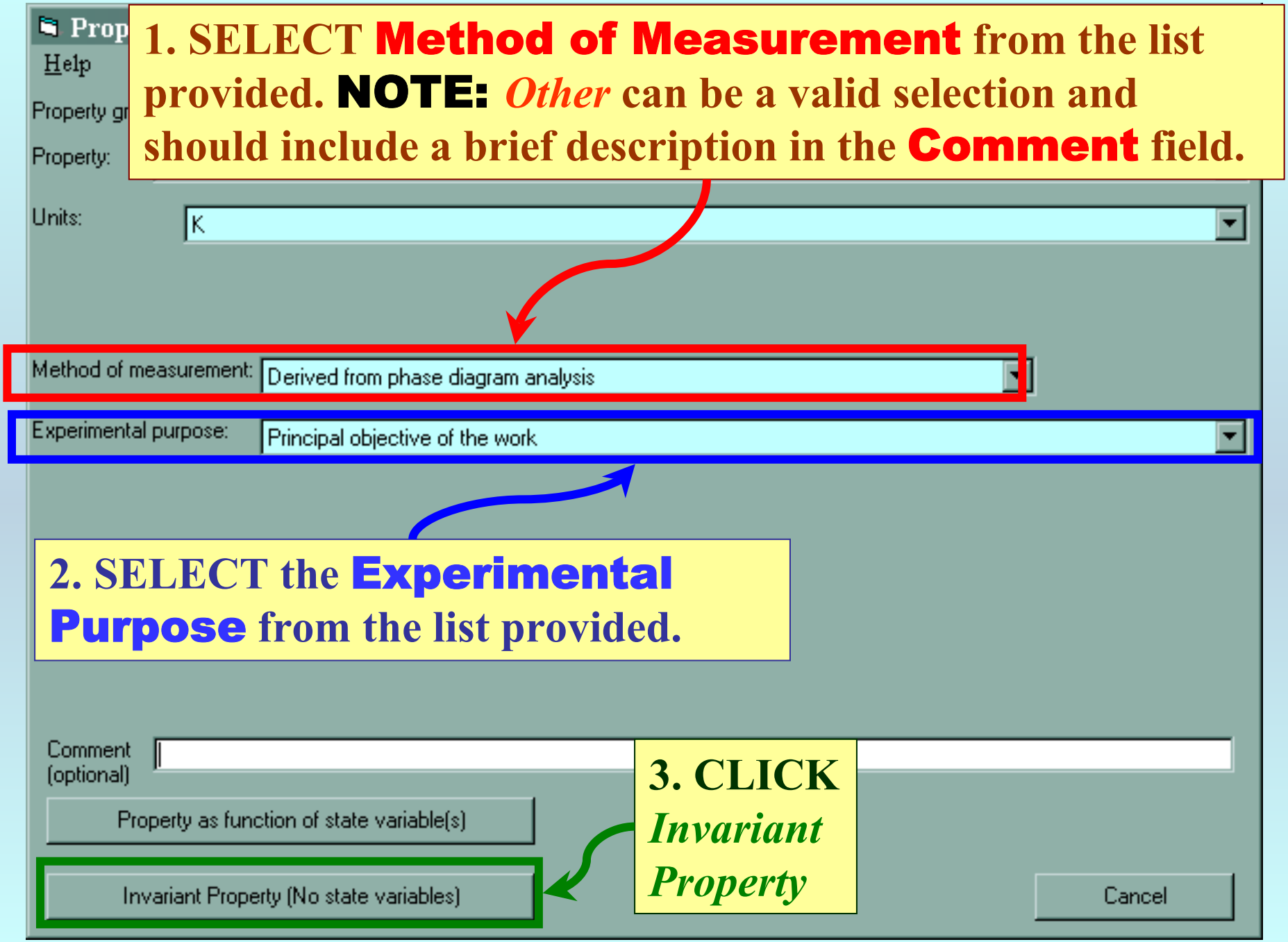
Experimental Method Info:

Graphical analysis of SLE results

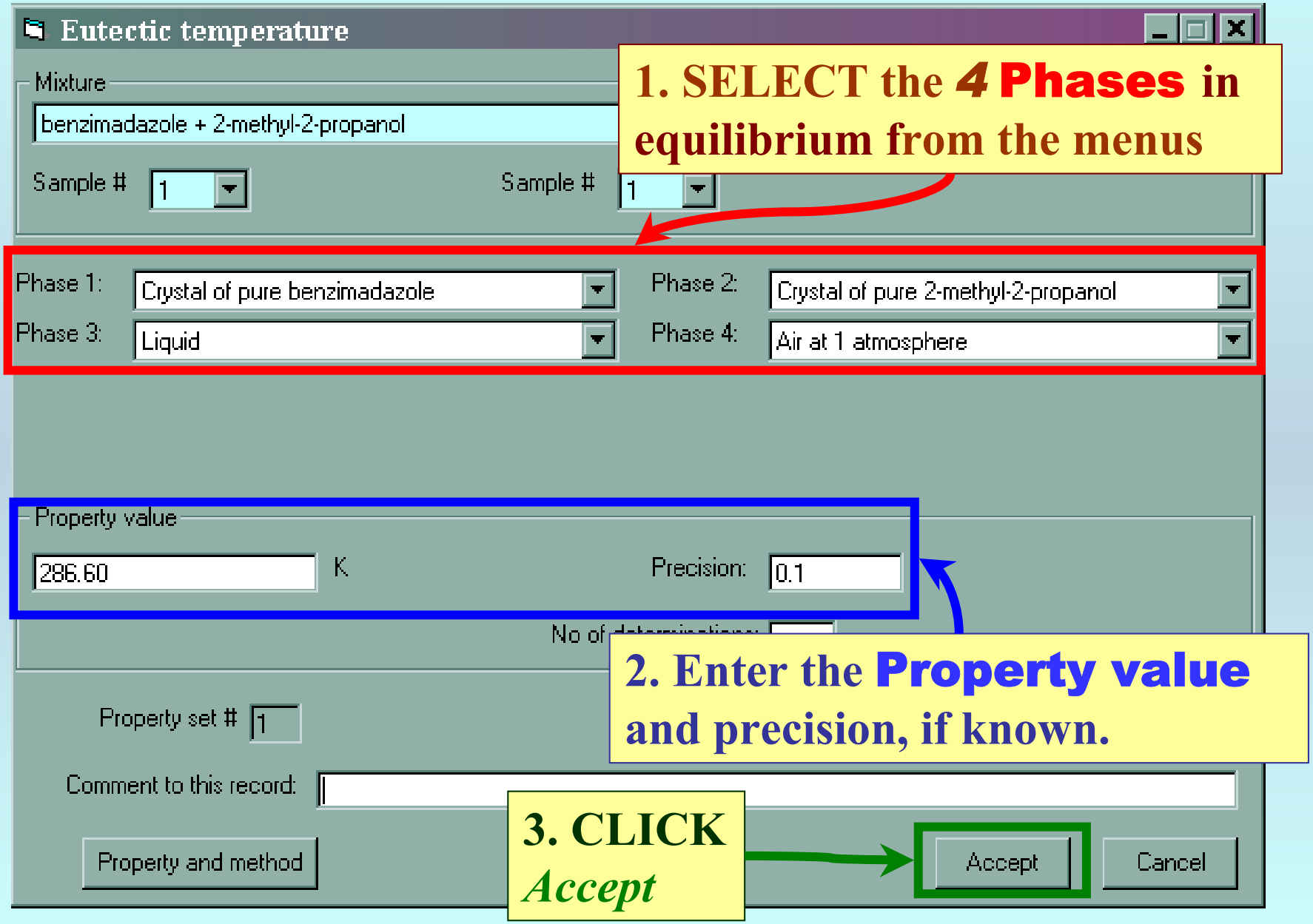


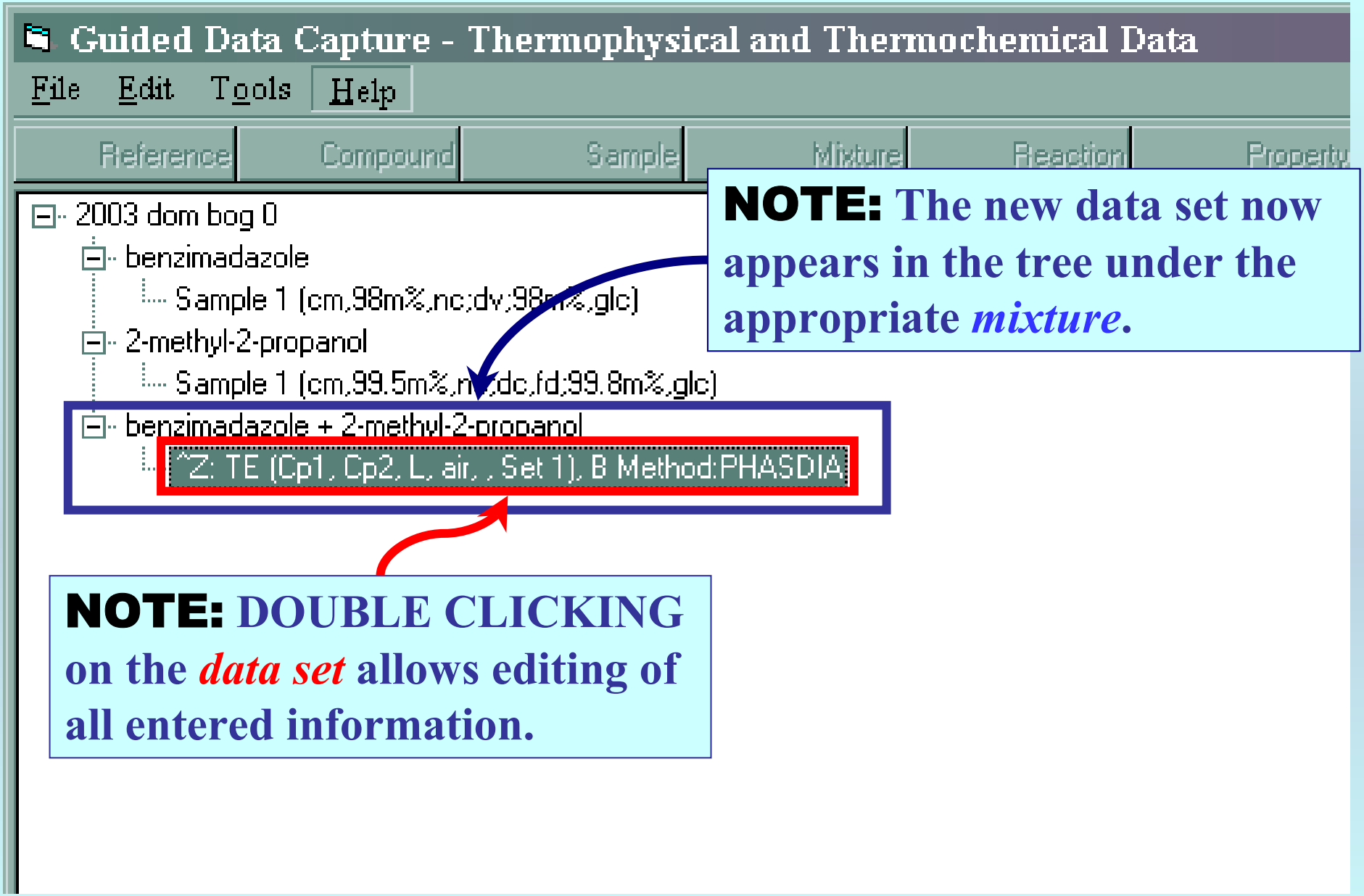
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for benzimadazole + 2-methyl-2-propanol
Help
Property group:
Phase transition properties
Property:
Eutectic temperature
Units:
K
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Phase transition properties from the menu.
2. SELECT the Property: Eutectic temperature, for the example.
3. SELECT the Units: K, here.
Comment (optional)
Property as function of state variable(s)
Invariant Property (No state variables)
Cancel


Prop
Help
Property gr
Property:
Units:
K
Method of measurement:
Derived from phase diagram analysis
Experimental purpose:
Principal objective of the work
Comment (optional)
Property as function of state variable(s)
Invariant Property (No state variables)
Cancel
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 Invariant Property

SELECTION of Phases & ENTRY of Property Value




Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
Sample
Mixture
Reaction
Property
2003 dom bog 0
benzimadazole
Sample 1 (cm,98m%,nc;dv;98m%,glc)
2-methyl-2-propanol
Sample 1 (cm,99.5m%,nc;dc,fd;99.8m%,glc)
benzimadazole + 2-methyl-2-propanol
^Z: TE (Cp1, Cp2, L, air, , Set 1), B Method:PHASDIA
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.**