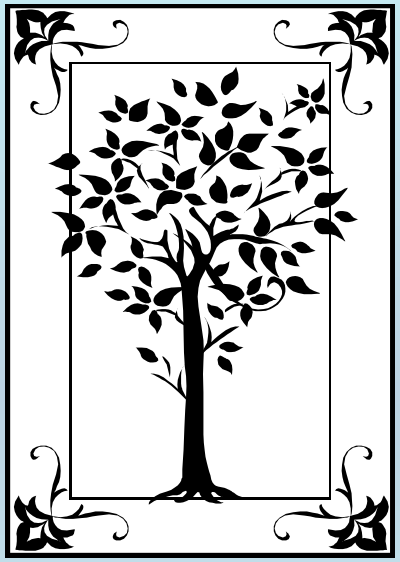
METADATA AND NUMERICAL DATA CAPTURE:
Upper Consolute Compostion
(2 – Components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components**
Upper Consolute Composition
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:

1036 *J. Chem. Eng. Data* 2000, *45,* 1036−1039

Thermodynamic Properties of *n*-Alkoxyethanols + Organic Solvent Mixtures. XIV. Liquid−Liquid Equilibria of Systems Containing 2-(2-Ethoxyethoxy)ethanol and Selected Alkanes

Rubén Martínez, Juan Antonio Gonzalez,* Isaias Garcia de la Fuente, and Jose Carlos Cobos

G.E.T.E.F. Departamento de Termodinámica y Física Aplicada, Facultad de Ciencias, Universidad de Valladolid, 47071 Valladolid, Spain

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Liquid−liquid equilibria (LLEs) data are reported for 2-(2-ethoxyethoxy)ethanol + hexane, heptane, octane, decane, dodecane, and hexadecane mixtures between 274.5 K and the upper critical solution temperatures (UCSTs). The coexistence curves were determined visually. They have a rather horizontal top, and their symmetry depends on the size of the alkane. For systems with dodecane or hexadecane, they are skewed to the region of higher mole fractions of 2-(2-ethoxyethoxy)ethanol. An opposite behavior is observed when hexane or heptane is involved. The (x_1, T) data were fitted to the equation $T = T_c + k|y - y_c|^m$, where $y = \alpha x_1/[1 + x_1(\alpha - 1)]$ and $y_c = \alpha x_{1c}/[1 + x_{1c}(\alpha - 1)]$. T_c and x_{1C} are the coordinates of the critical points fitted together with k, m, and α. Results are briefly discussed on the basis of the existence of inter- and intramolecular H-bonds as well as of dipole interactions, which occur in solutions containing hydroxyethers.

Upper Consolute Composition

(2 ñ Components)

2-(2-ethoxyethoxy)ethanol + heptane

Table 9. Coordinates of the Critical Points for Several Alkoxyethanol + Alkane Mixtures

system	T_c/K	x_{1c}
2-methoxyethanol + heptane	319.74[a]	0.556
	320.15[b]	
	321.15[c]	
2-methoxyethanol + octane	327.94[d]	0.590
2-methoxyethanol + dodecane	356.52[e]	0.717
2-methoxyethanol + methylcyclohexane	297.34[a]	0.485
	299.15[c]	
2-methoxyethanol + 2,2,4-trimethylpentane	319.25[a]	0.581
	319.55[b]	
	319.15[c]	
2-ethoxyethanol + heptane	261.15[c]	
2-ethoxyethanol + dodecane	289.62[e]	0.625
2-ethoxyethanol + 2,2,4-trimethylpentane	258.15[c]	
2-(2-methoxyethoxy)ethanol + heptane	381.15[c]	
2-(2-methoxyethoxy)ethanol + methylcyclohexane	314.04[a]	0.386
	341.14[c]	
2-(2-ethoxyethoxy)ethanol + heptane	286.98[f]	0.354
2-(2-ethoxyethoxy)ethanol + 2,2,4-trimethylpentane	290.20[a]	0.389
	301.15[c]	

[a] Carmona et al., 1999. [b] Dolch et al., 1986. [c] Francis, 1961. [d] Rubio et al., 1998a. [e] Rubio et al., 1998b. [f] This work.

This data set is considered here.

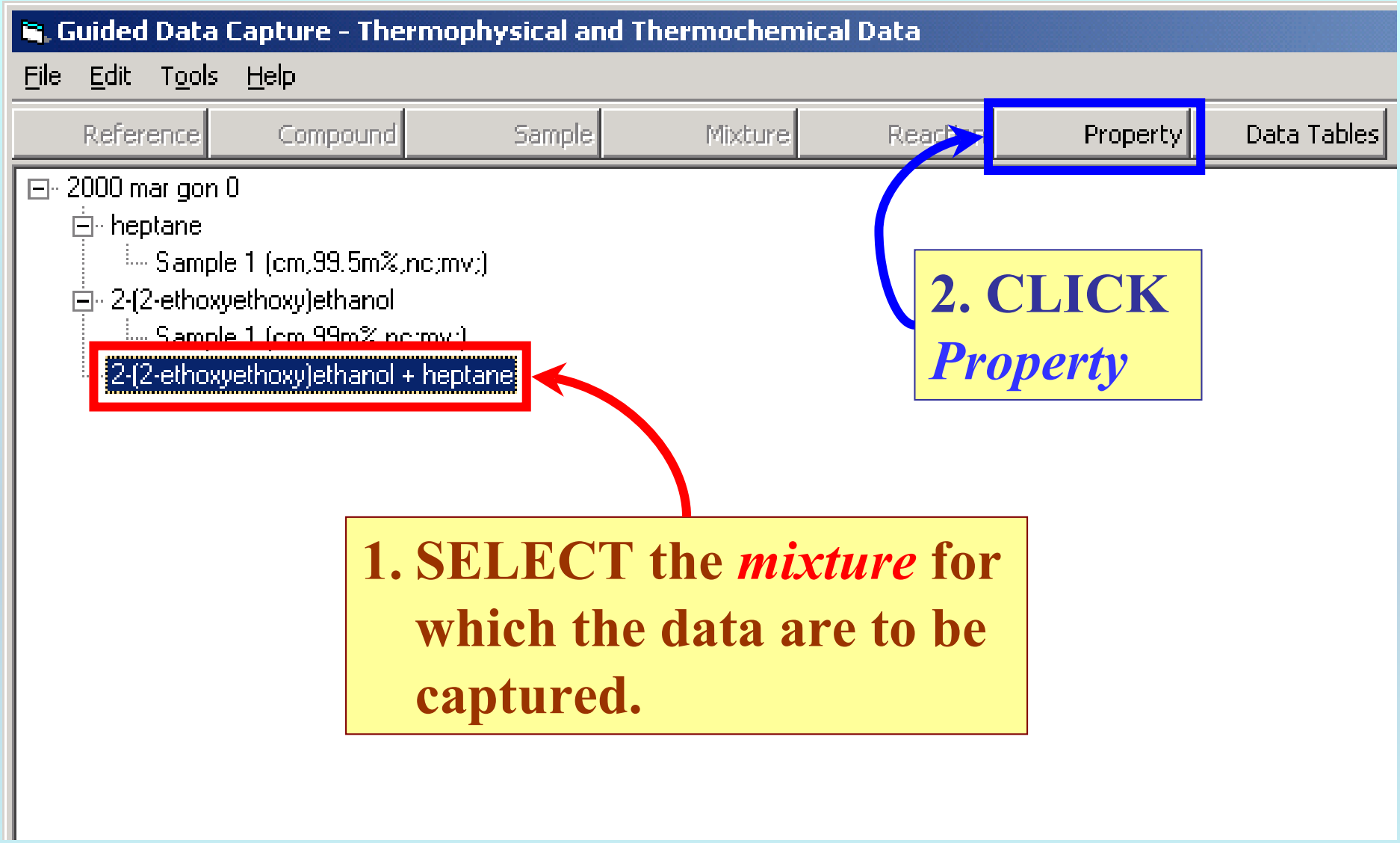
Experimental Method Info:

The coexistence curves of the binary mixtures were determined visually (Loven and Rice, 1955; Young, 1969; Snyder and Eckert; 1973).

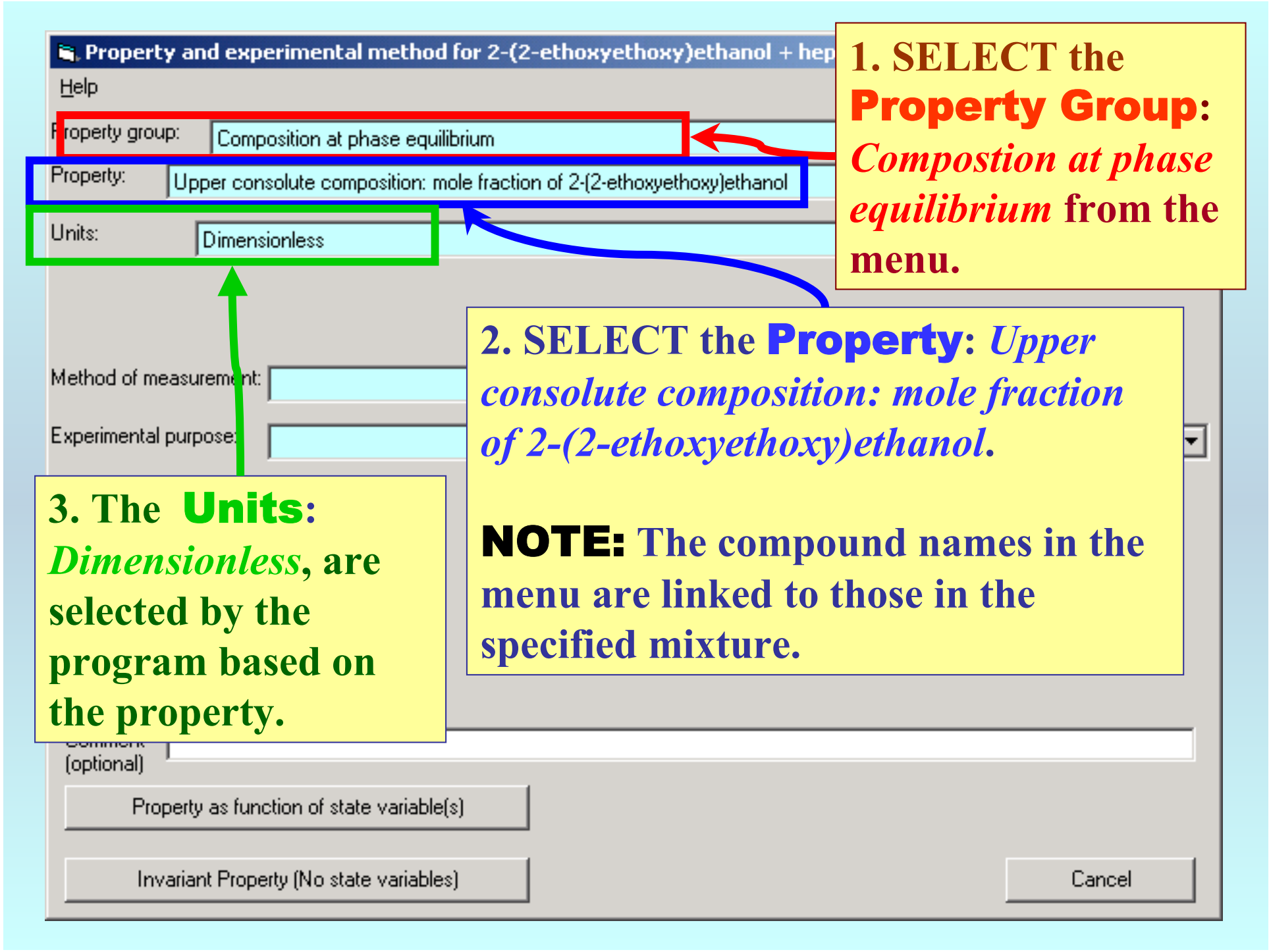
Uncertainties:

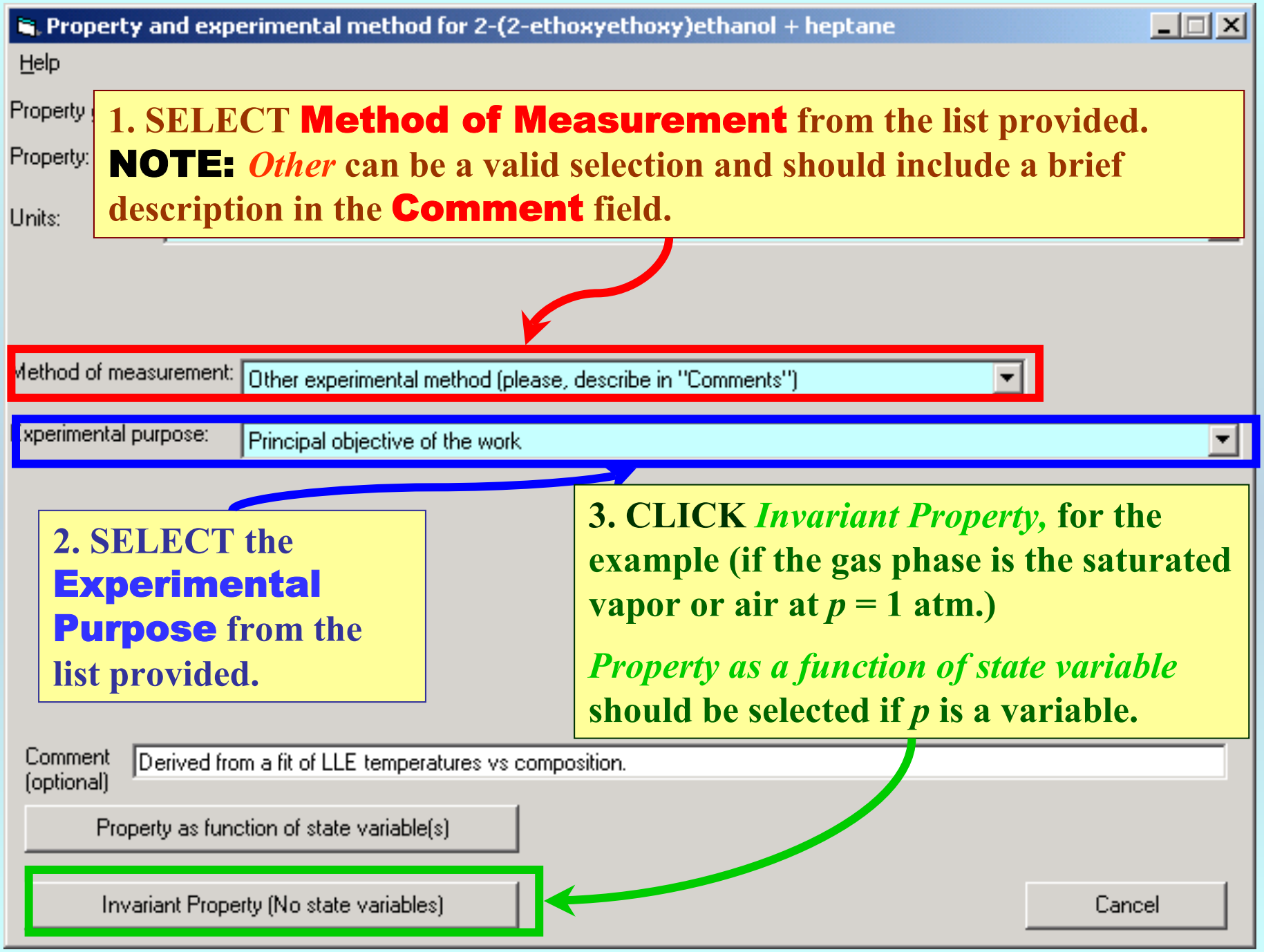
The precision of the equilibrum composition is expected to be better than 0.0005 mole fraction. The weighing technique gives a precision better than 0.0001 in mole fraction, but this is reduced slightly due to partial evaporation of the more volatile component to the free volume of the ampule ($\simeq$1.17 cm^3).

The temperature was measured with a precision of $\pm$0.01 K and an estimated accuracy of $\pm$0.1 K

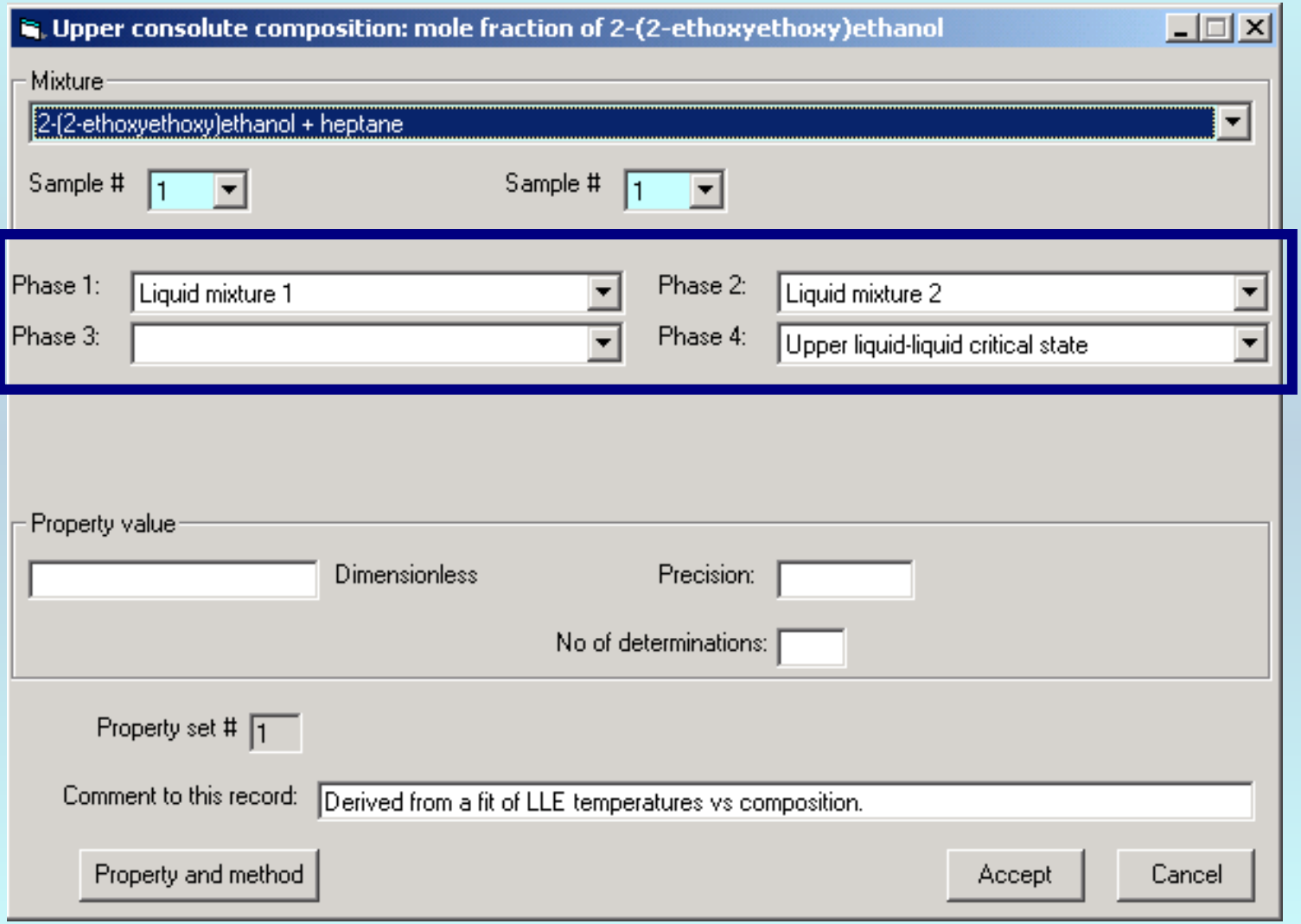


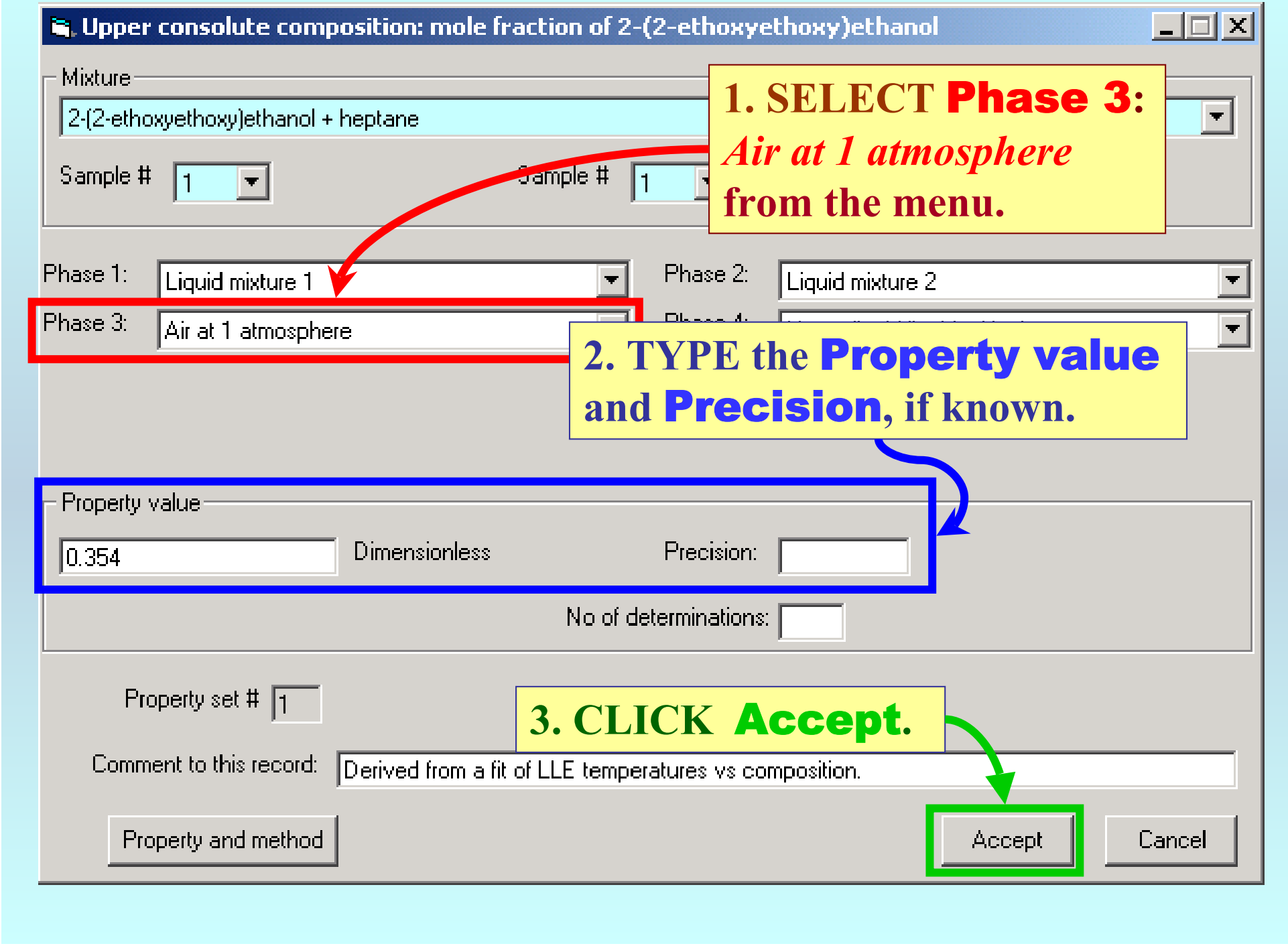
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

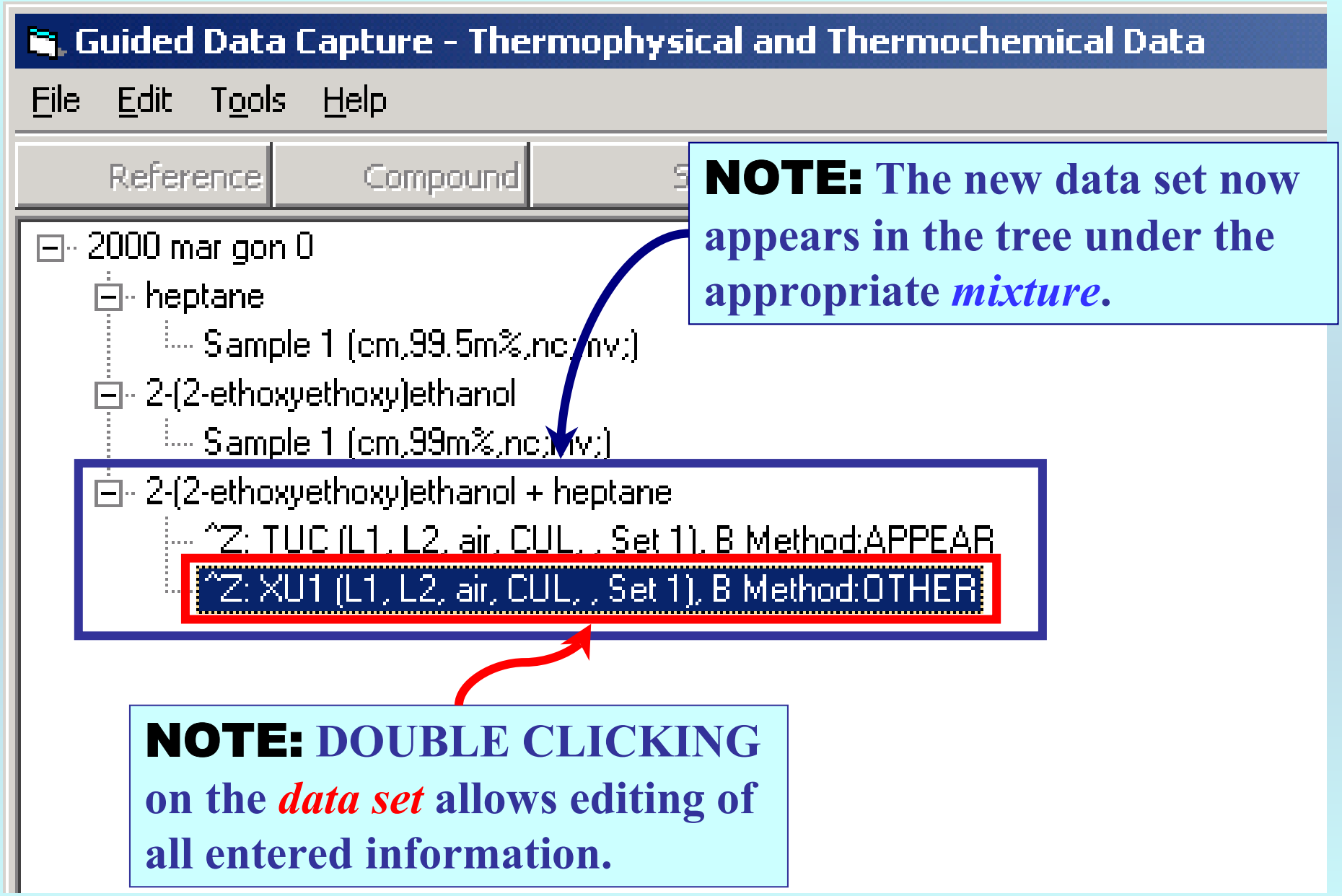

Property and experimental method for 2-(2-ethoxyethoxy)ethanol + hep
Help
Property group:
Composition at phase equilibrium
Property:
Upper consolute composition: mole fraction of 2-(2-ethoxyethoxy)ethanol
Units:
Dimensionless
Method of measurement:
Experimental purpose:
(optional)
Property as function of state variable(s)
Invariant Property (No state variables)
Cancel
1. SELECT the Property Group: Compostion at phase equilibrium from the menu.
2. SELECT the Property: Upper consolute composition: mole fraction of 2-(2-ethoxyethoxy)ethanol.
NOTE: The compound names in the menu are linked to those in the specified mixture.
3. The Units: Dimensionless, are selected by the program based on the property.


Property and experimental method for 2-(2-ethoxyethoxy)ethanol + heptane
Help
Property
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:
Other experimental method (please, describe in "Comments")
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
3. CLICK Invariant Property, for the example (if the gas phase is the saturated vapor or air at p = 1 atm.)
Property as a function of state variable should be selected if p is a variable.
Comment (optional)
Derived from a fit of LLE temperatures vs composition.
Property as function of state variable(s)
Invariant Property (No state variables)
Cancel

NOTE: Most phases filled automatically by the GDC program.




Upper consolute composition: mole fraction of 2-(2-ethoxyethoxy)ethanol
Mixture
2-(2-ethoxyethoxy)ethanol + heptane
Sample #
1
Sample #
1
1. SELECT Phase 3:
Air at 1 atmosphere
from the menu.
Phase 1:
Liquid mixture 1
Phase 2:
Liquid mixture 2
Phase 3:
Air at 1 atmosphere
2. TYPE the Property value
and Precision, if known.
Property value
0.354
Dimensionless
Precision:
No of determinations:
Property set #
1
3. CLICK Accept.
Comment to this record:
Derived from a fit of LLE temperatures vs composition.
Property and method
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
2000 mar gon 0
heptane
Sample 1 (cm,99.5m%,nc;nv;)
2-(2-ethoxyethoxy)ethanol
Sample 1 (cm,99m%,nc;nv;)
2-(2-ethoxyethoxy)ethanol + heptane
^Z: TUC (L1, L2, air, CUL, , Set 1), B Method:APPEAR
^Z: XU1 (L1, L2, air, CUL, , Set 1), B Method:OTHER
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.**