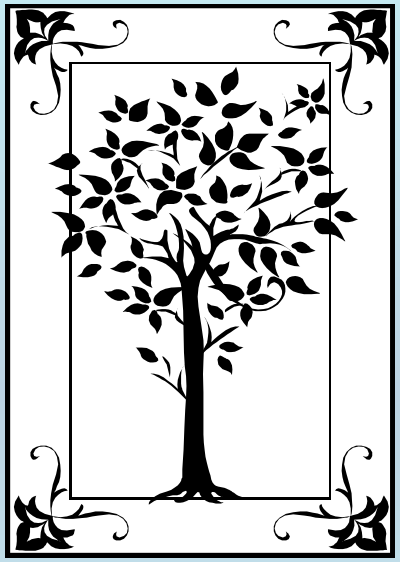
METADATA AND NUMERICAL DATA CAPTURE:
Upper Consolute Temperature, K
(2 – Components)

Guided Data Capture (GDC)



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

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

---

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 Critical Solution Temperature, K

(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.

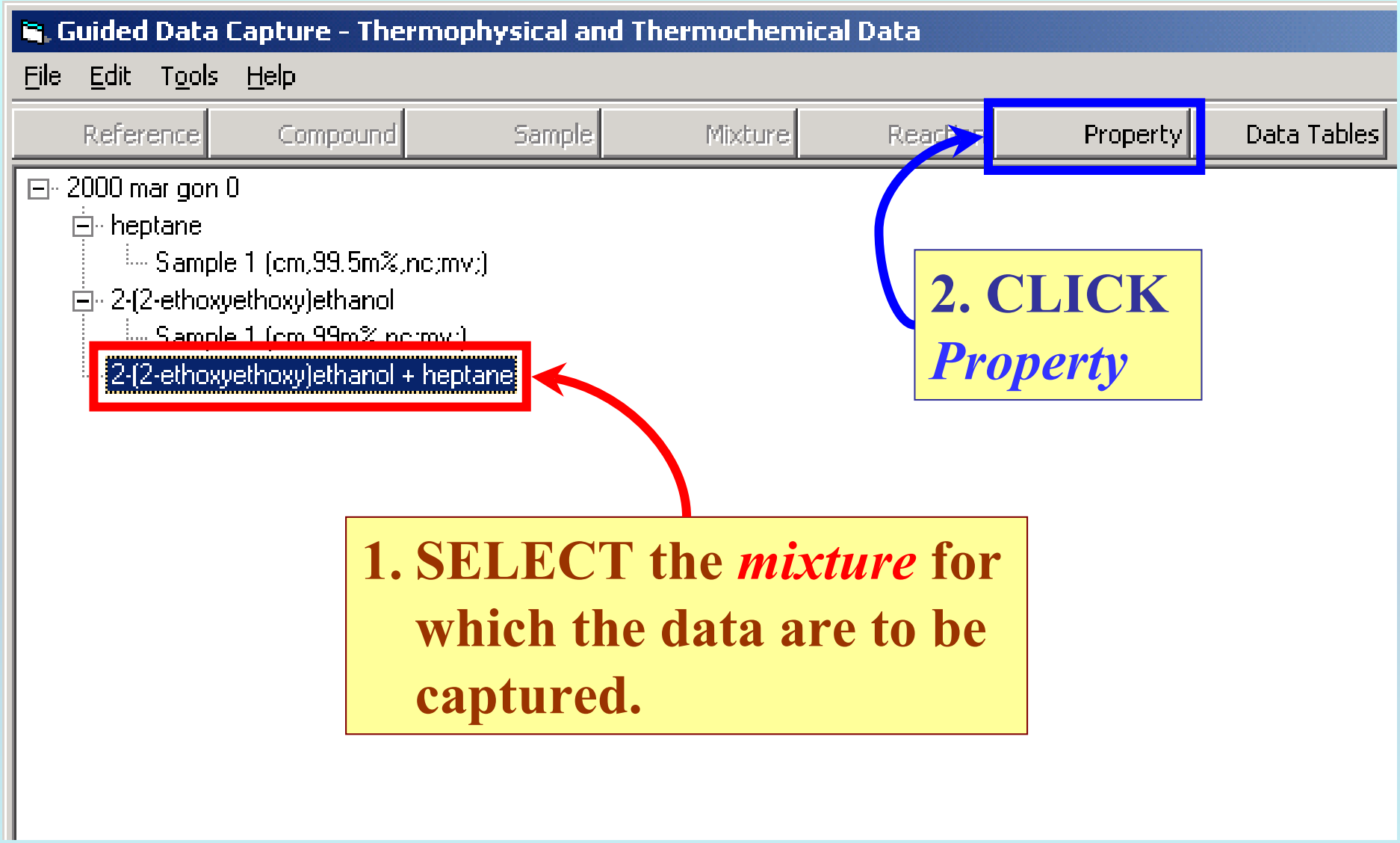
Experimental Method Info:

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

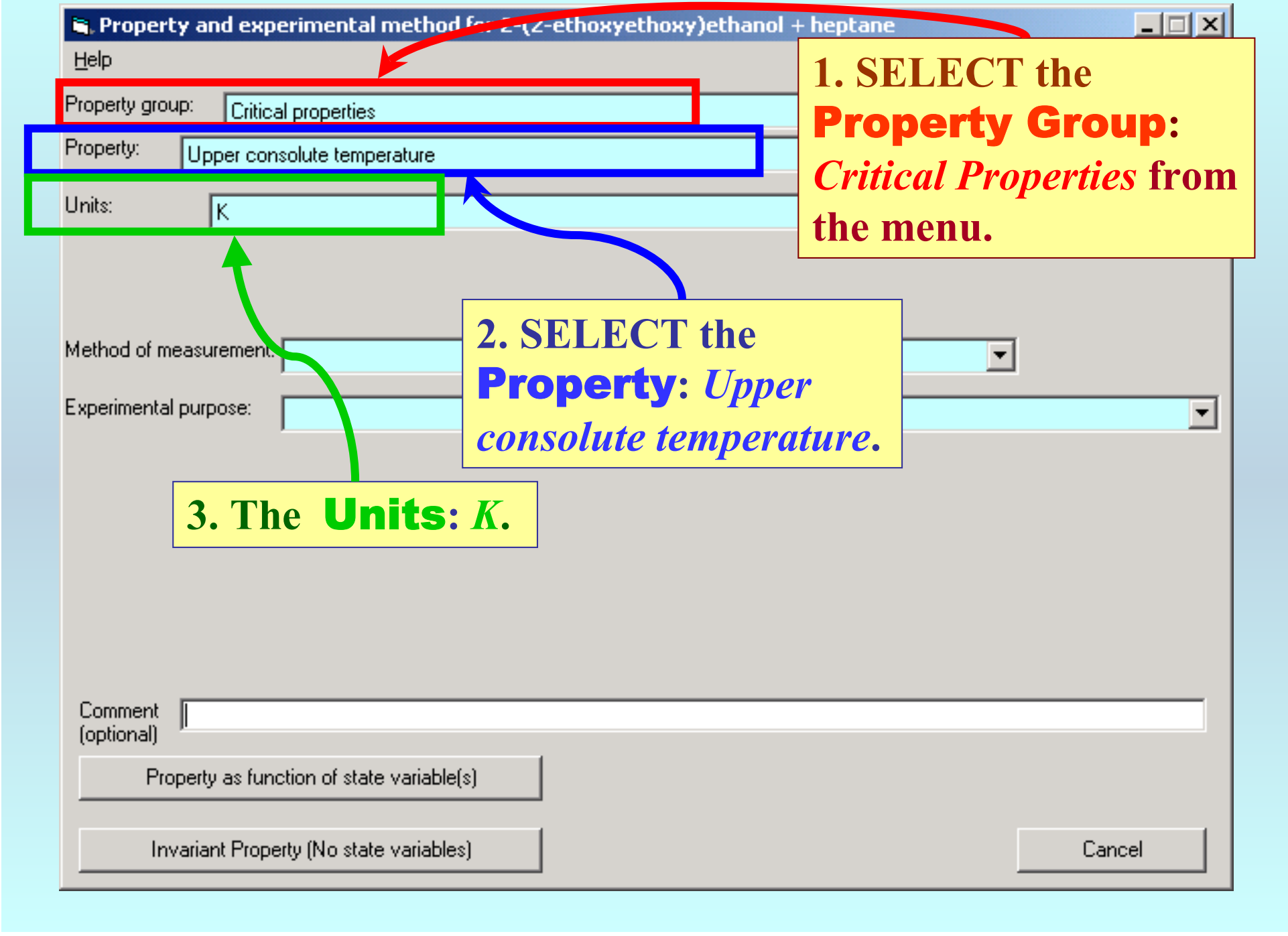
Uncertainties:

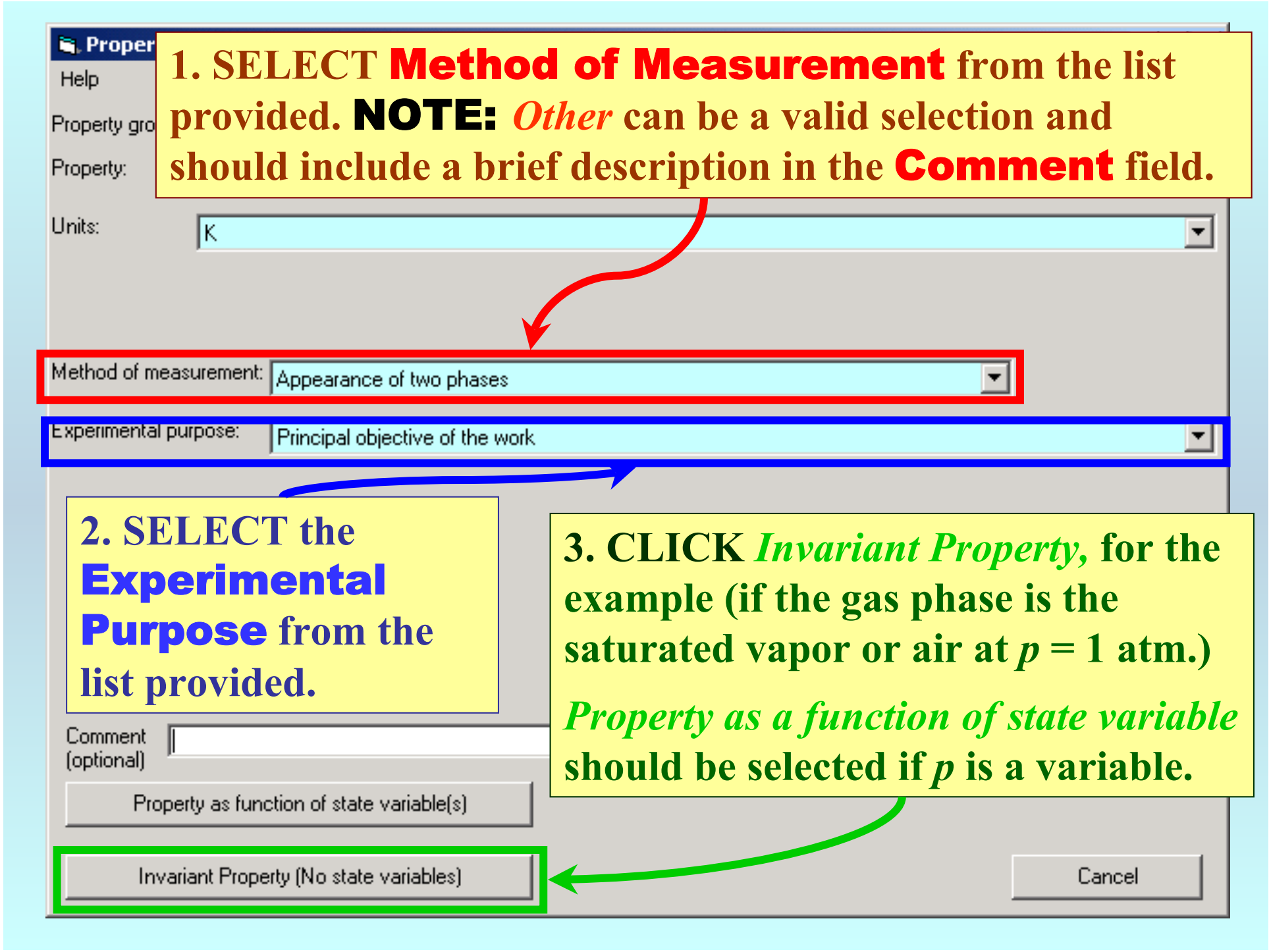
The precision of the equilibrum composition is expected to be better than 0.0005 mole fraction. The weighing technique gives a precision better than 0.0001 in mole fraction, but this is reduced slightly due to partial evaporation of the more volatile component to the free volume of the ampule ($\simeq$1.17 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
Help
Property group:
Critical properties
Property:
Upper consolute temperature
Units:
K
Method of measurement:
Experimental purpose:
Comment (optional)
Property as function of state variable(s)
Invariant Property (No state variables)
Cancel
1. SELECT the Property Group: Critical Properties from the menu.
2. SELECT the Property: Upper consolute temperature.
3. The Units: K.



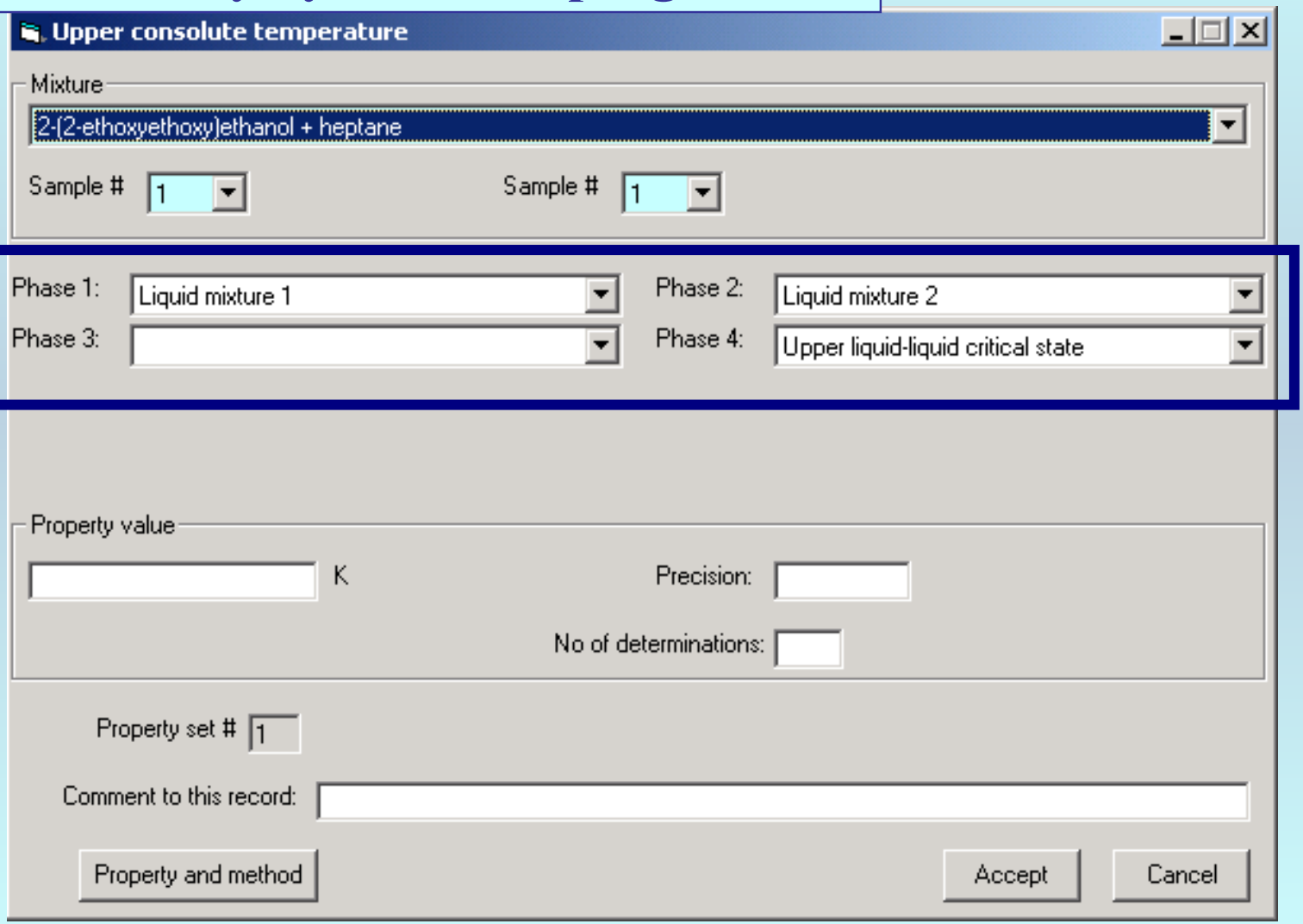
1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

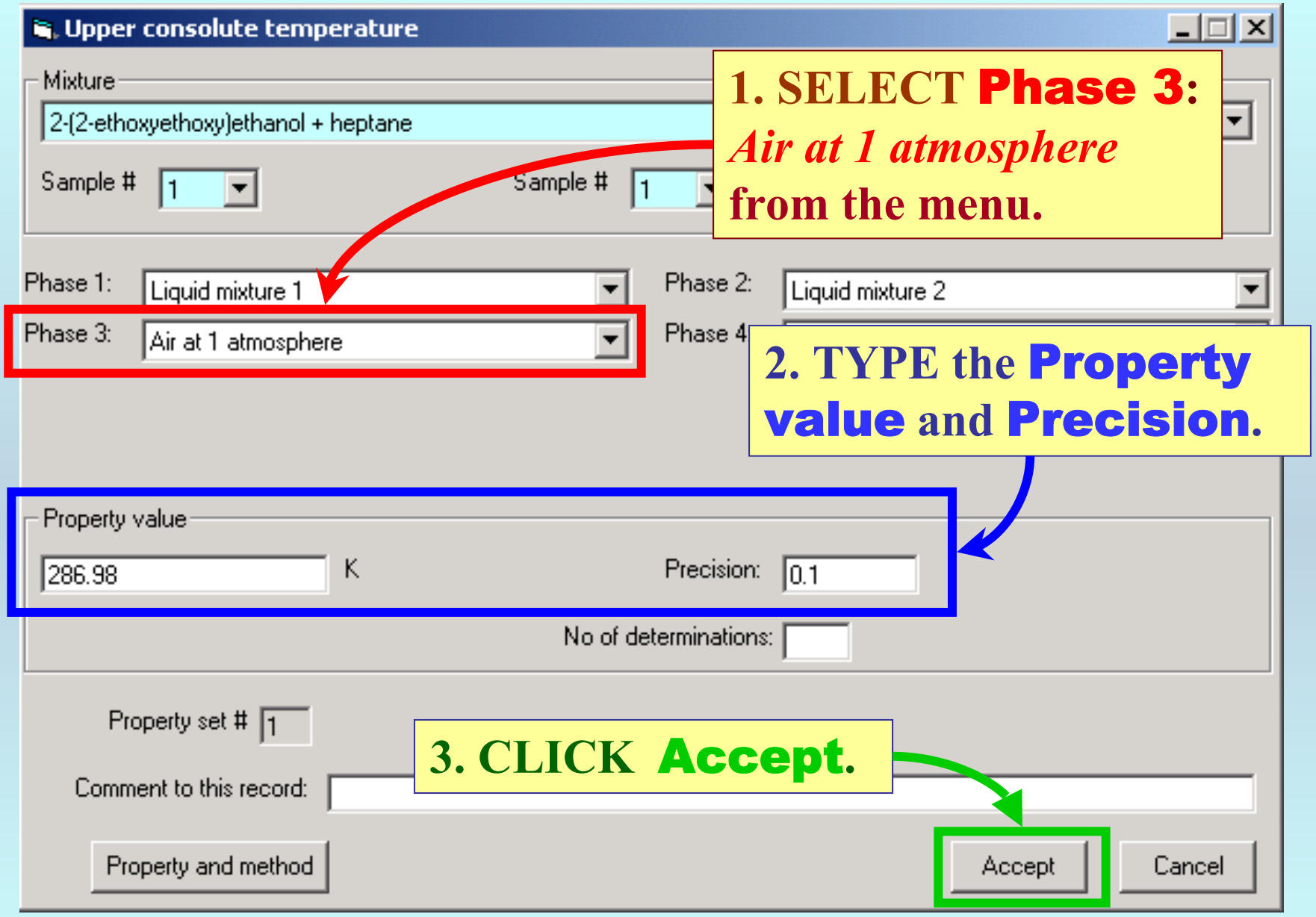
2. SELECT the **Experimental Purpose** from the list provided.

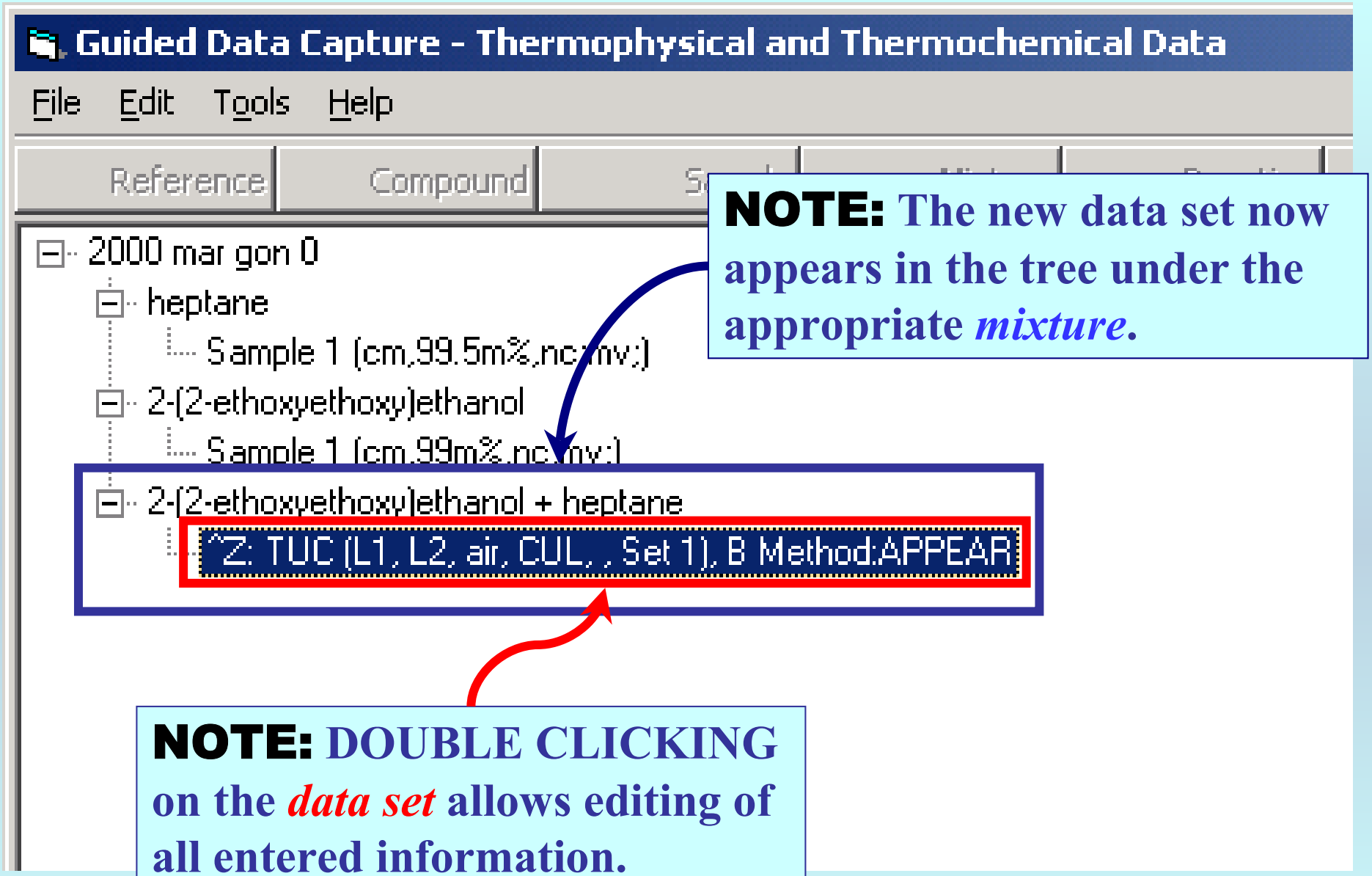
3. CLICK *Invariant Property*, for the example (if the gas phase is the saturated vapor or air at $p = 1$ atm.)

Property as a function of state variable should be selected if p is a variable.

NOTE: Most phases filled automatically by the GDC program.




Upper consolute temperature
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
Phase 4
2. TYPE the Property value and Precision.
Property value
286.98
K
Precision: 0.1
No of determinations:
Property set # 1
3. CLICK Accept.
Comment to this record:
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;mv;)
2-(2-ethoxyethoxy)ethanol
Sample 1 (cm,99m%,nc;mv;)
2-(2-ethoxyethoxy)ethanol + heptane
^Z: TUC (L1, L2, air, CUL, , Set 1), B Method:APPEAR
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.**