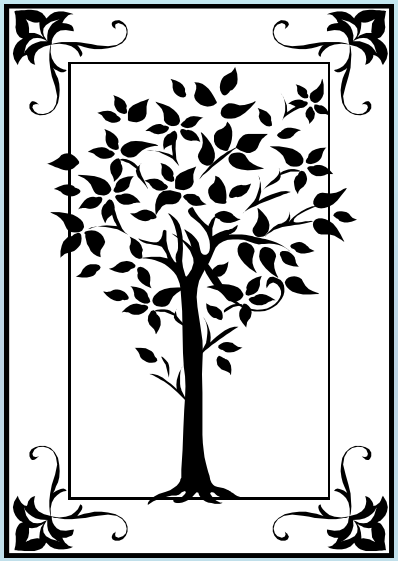
METADATA AND NUMERICAL DATA CAPTURE:
Common pure-component properties
density *d* at 1 temperature and pressure

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Common pure-component properties 1: density *d* at 1 temperature and pressure**
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*, 203−208

Azeotropic Behavior in the System Methanol + Methyl 1,1-Dimethylethyl Ether

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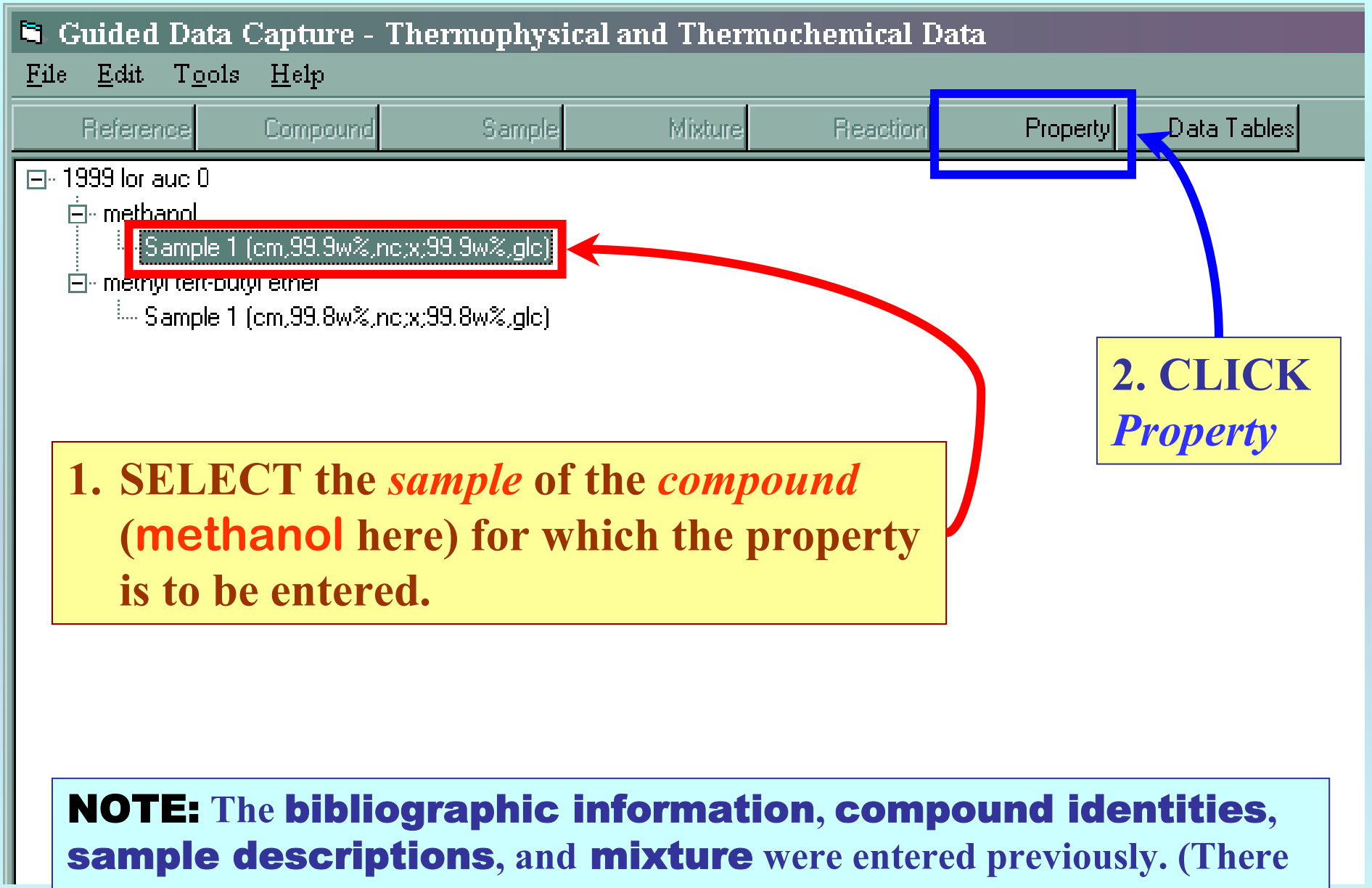
Vapor−liquid equilibrium for the binary system methanol + methyl 1,1-dimethylethyl ether has been measured at 50, 78.4, and 94 kPa. The system presents a minimum boiling point azeotrope that is enriched in the ether when the pressure decreases. The activity coefficients and boiling points of the solutions were correlated with its composition by the Wohl, Wilson, UNIQUAC, NRTL, and Wisniak−Tamir equations.

Density for $T = 298.15$ K and $p = 101.3$ kPa for **methanol**

Table 1. Purities (mass %), Densities d, Refractive Index n_D, and Normal Boiling Points T_b of Pure Components

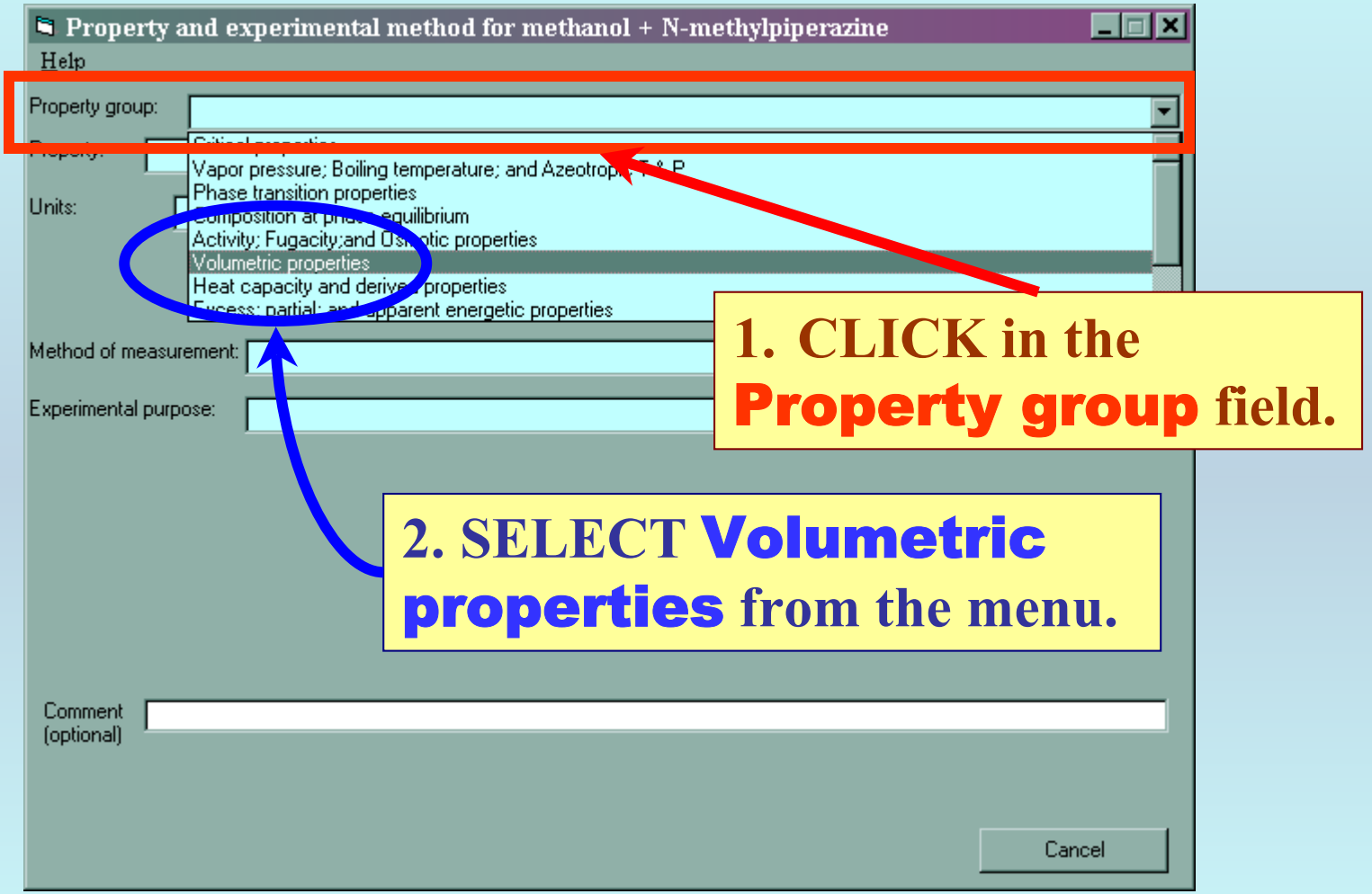
component (purity/mass %)	d(298.15 K)/(g·cm^{-3})		n_D (298.15 K)		T_b (101.3 kPa)/K	
	exptl[a]	lit.	exptl[a]	lit.	exptl[a]	lit.
methanol (99.9+)	0.787 32	0.787 30[b]	1.3270	1.3267[b]	337.84	337.65[b]
MTBE (99.8)	0.735 26	0.735 28[c]	1.3664	1.3663[d]	327.83	327.83[e]

The data considered here.

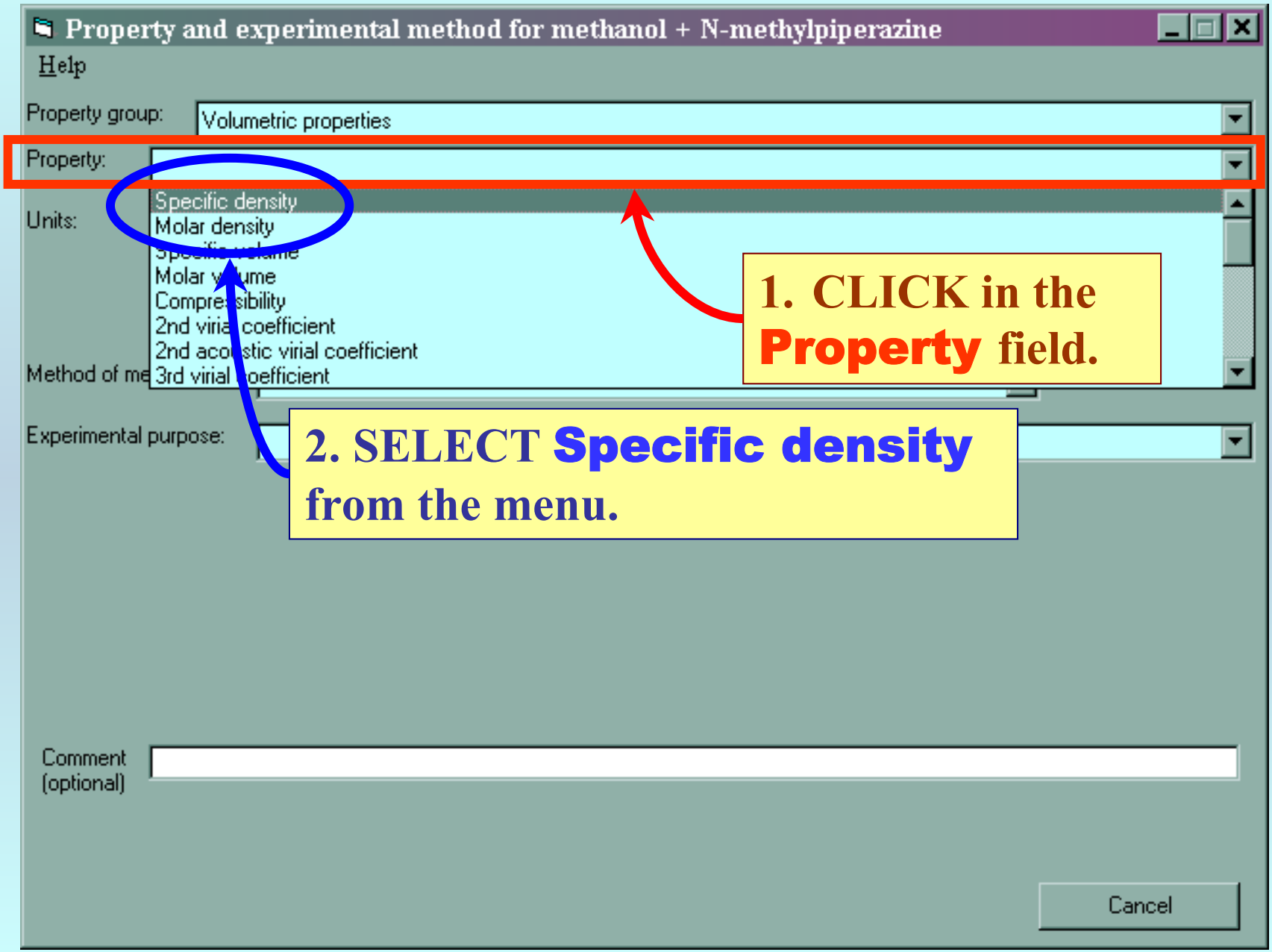


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials related to capture of this information.)

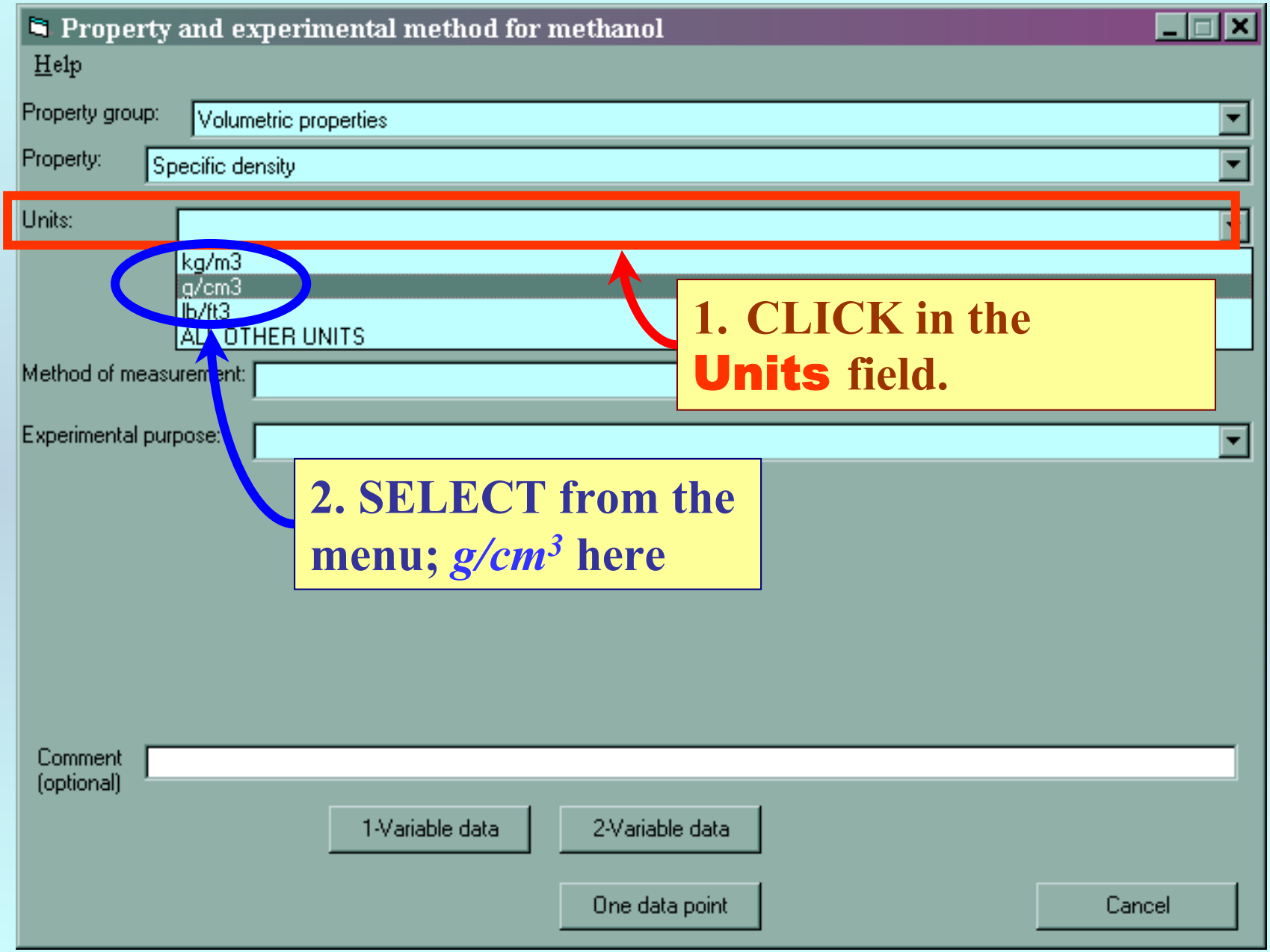
Property Group selection



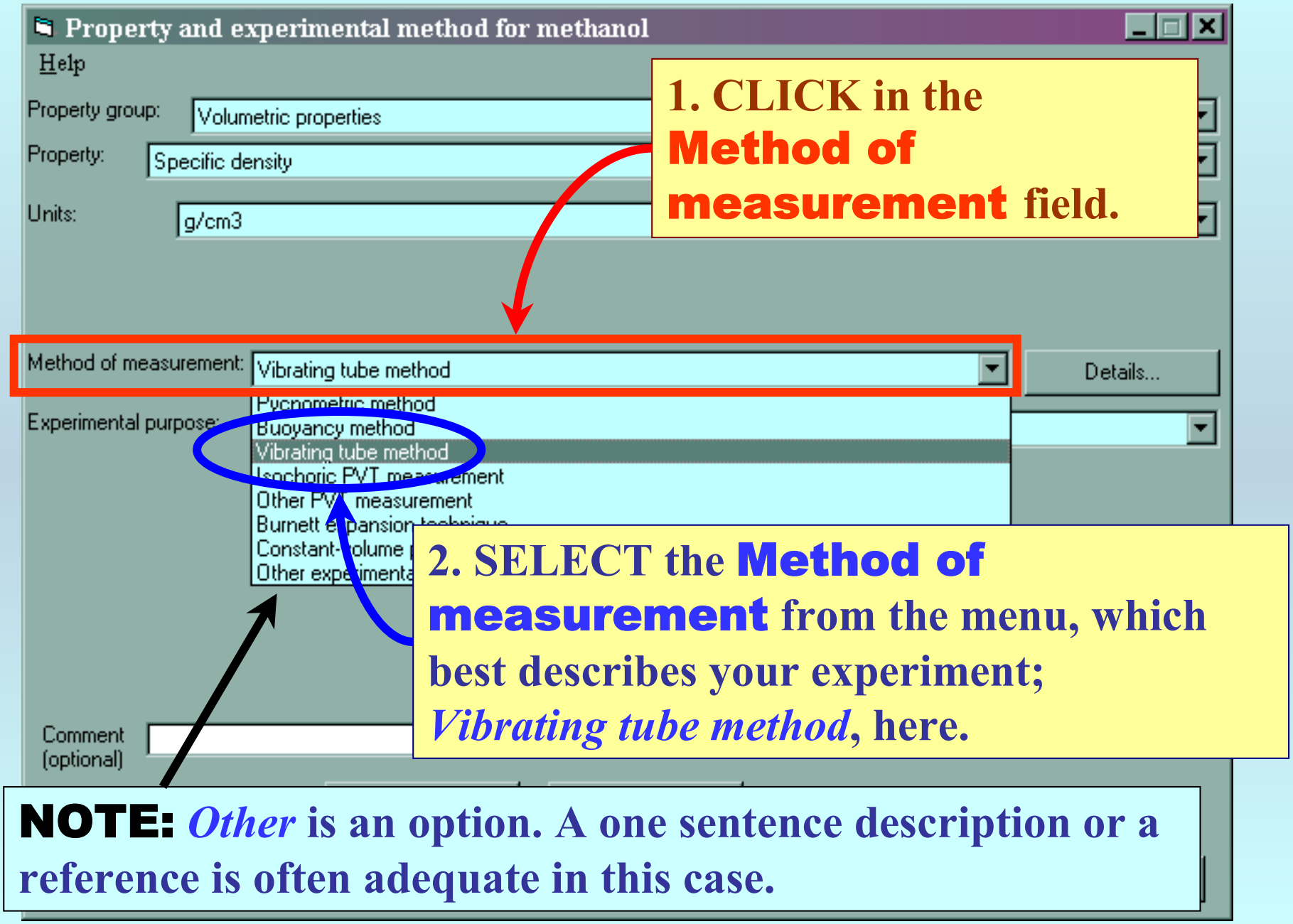
Property selection



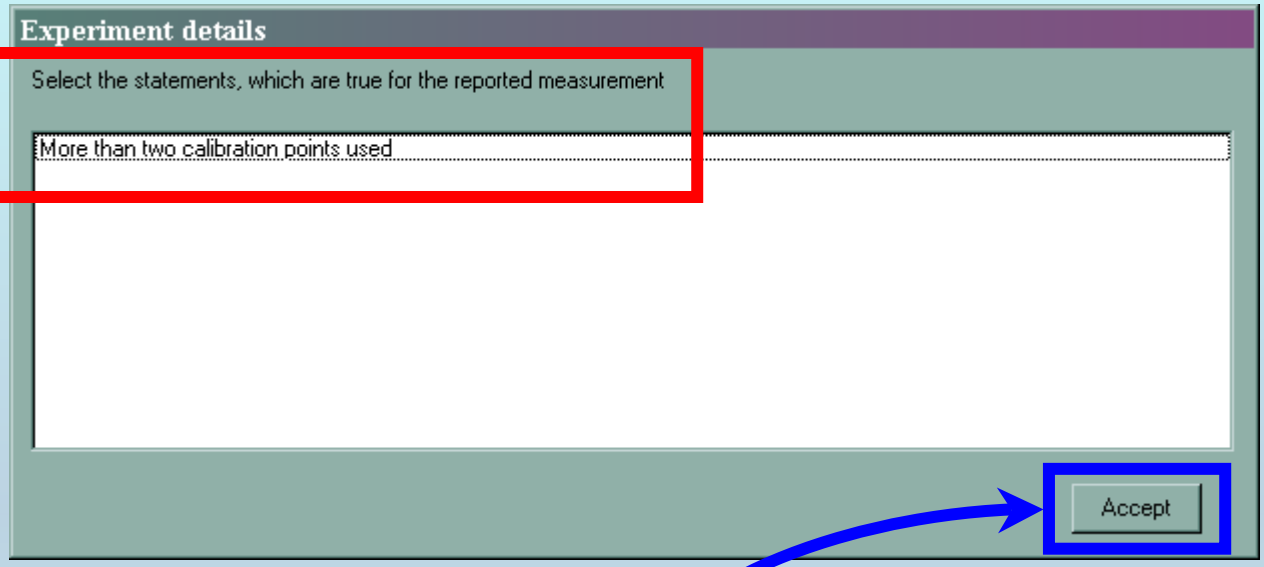
Units selection



Method selection

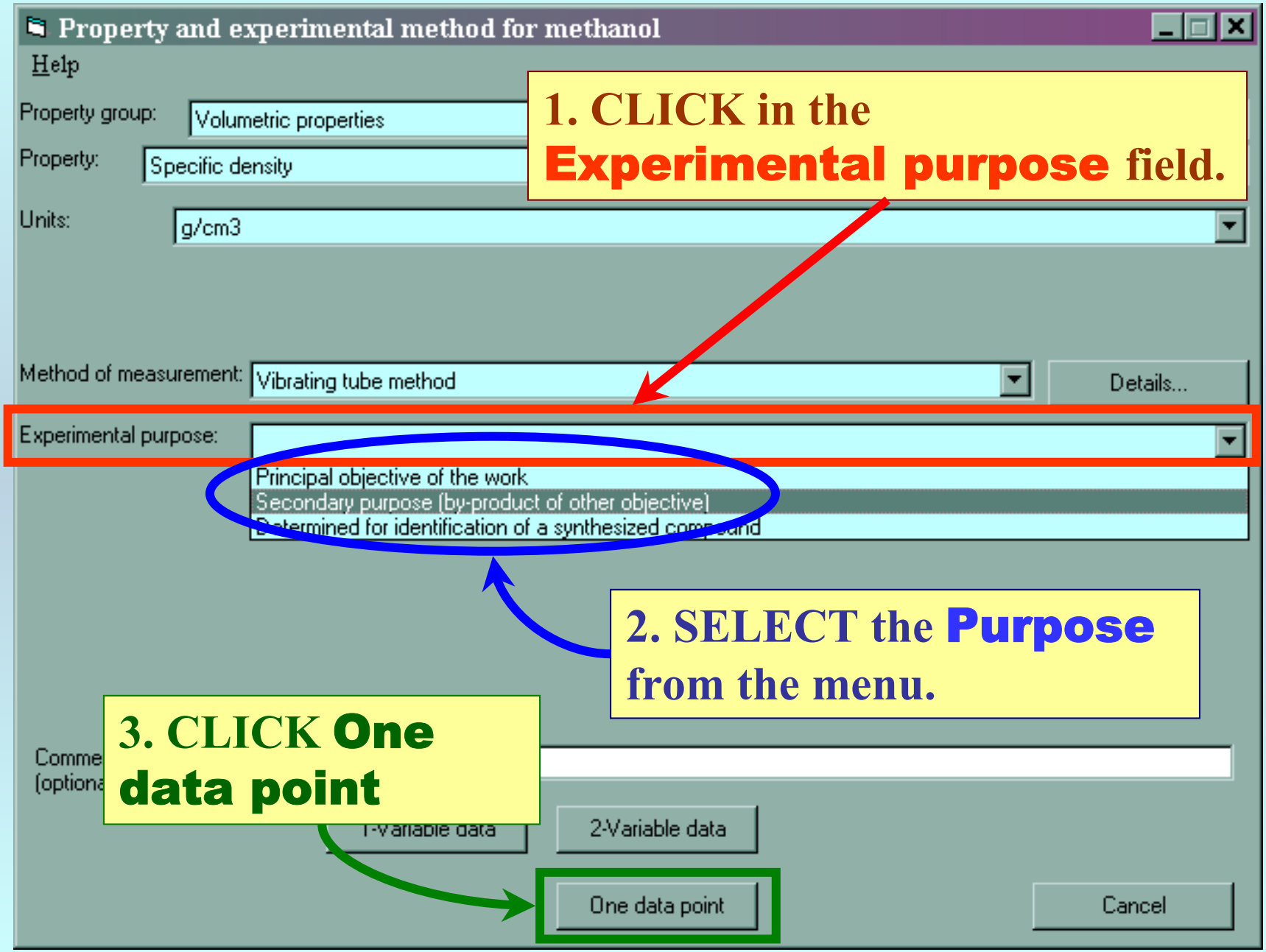


Method detail selection

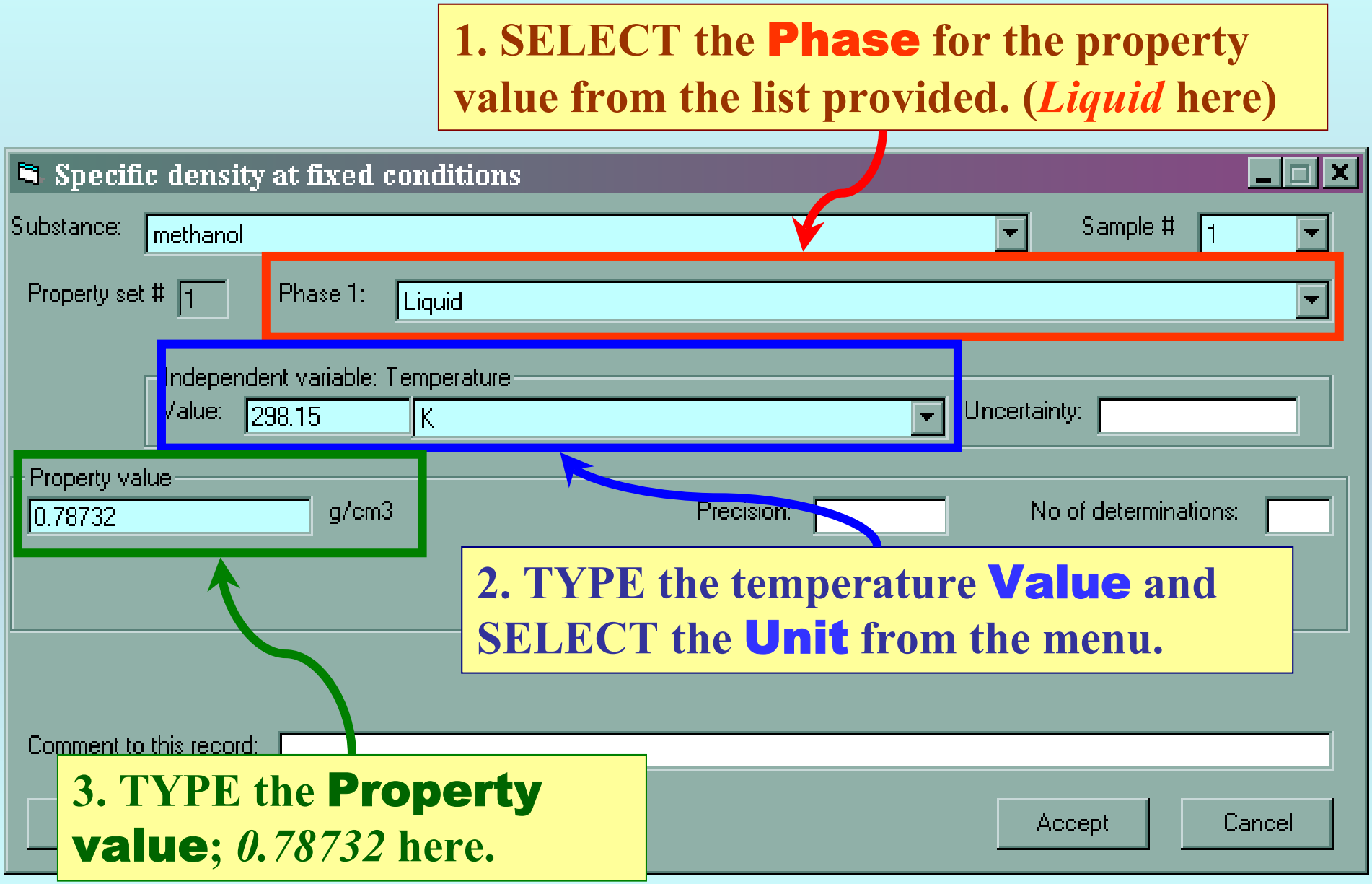


Note: For some methods, additional details are requested. SELECT those statements that apply, and CLICK *Accept*.

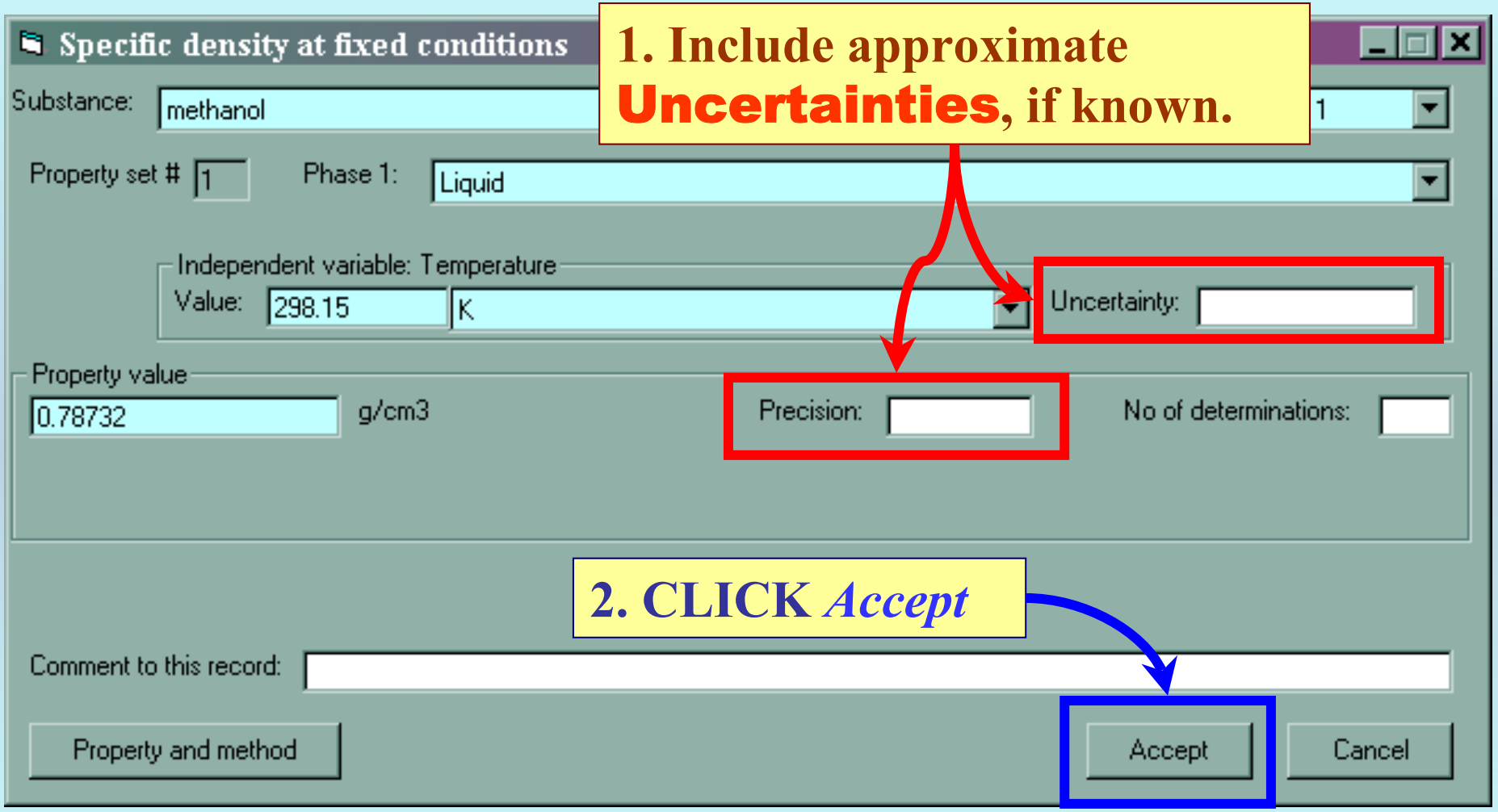
Experimental purpose selection



Specification of phase, temperature, and value



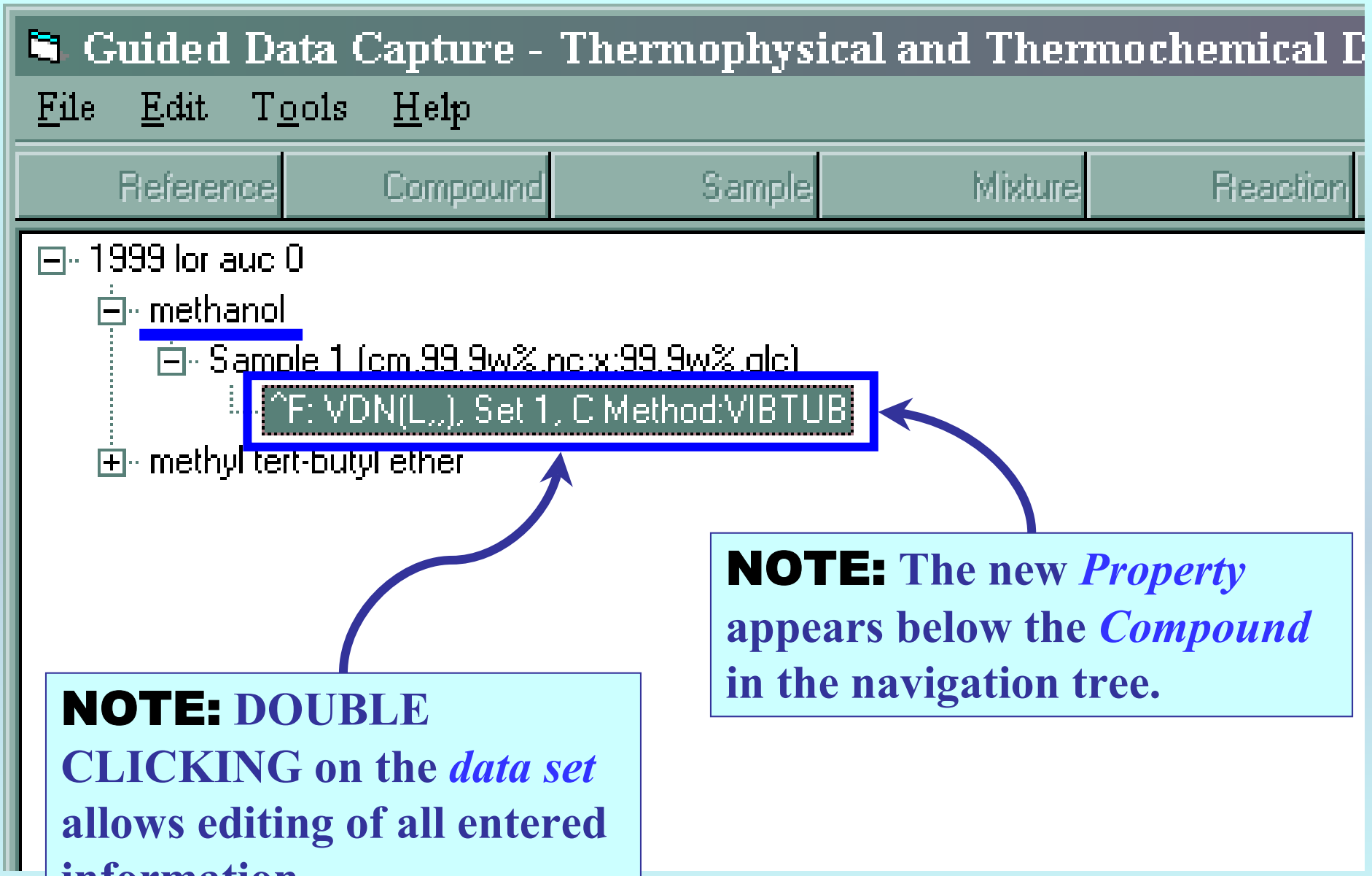
Form is complete...



1. Include approximate Uncertainties, if known.

2. CLICK *Accept*

NOTE: For a single density value, the pressure is assumed to be p = 101.3 kPa.


Guided Data Capture - Thermophysical and Thermochemical D
File Edit Tools Help
Reference Compound Sample Mixture Reaction
1999 lor auc 0
methanol
Sample 1 (cm,99.9w%,nc:x:99.9w%,olc)
^F: VDN(L,,), Set 1, C Method:VIBTUB
methyl tert-butyl ether
NOTE: DOUBLE CLICKING on the data set allows editing of all entered information.
NOTE: The new Property appears below the Compound in the navigation tree.

END

Continue with other compounds, samples, properties, reactions, etc...

***or* save your file and exit the program.**