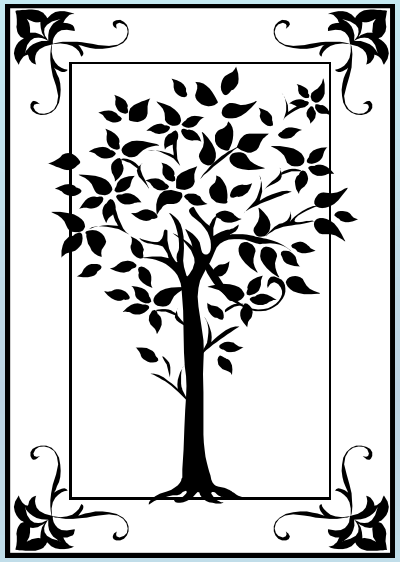
METADATA AND NUMERICAL DATA CAPTURE:
Critical Temperature
(for 1 – Component)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Critical Temperature (1 component)**
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 2000, *45*, 157−160

Critical Point and Vapor Pressure Measurements at High Temperatures by Means of a New Apparatus with Ultralow Residence Times

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Wiltec Research Company, Inc., 488 South 500 West, Provo, Utah 84601

A new flow method has been employed to obtain critical point and vapor pressure data at high temperatures for four compounds: squalane, toluene, ethylbenzene, and styrene. This new flow method allows the determination of reliable critical points and vapor pressures for thermally unstable or otherwise reactive compounds. The critical point is inferred from other measurements in the critical region. The measurement accuracy is less than that obtained by more conventional methods, but this method has been used where conventional methods fail.

Critical Temperature for 1 component
squalane

Table 1. Results of Critical Point Measurements

	T_c/K			P_c/MPa		
compound	meas	previous	est[a]	meas	previous	est[a]
squalane	795.9		882.5	0.59		0.83
toluene	591.8	591.90[a]	598.4	4.11	4.111[b]	4.13
		591.79[c]			4.109[c]	
		591.75[d]			4.108[d]	
ethylbenzene	618.0	617.26[b]	623.3	3.62	3.616[b]	3.66
		617.20[c]			3.606[c]	
		617.15[d]			3.609[d]	
styrene	635.2		644.1	3.87		3.86

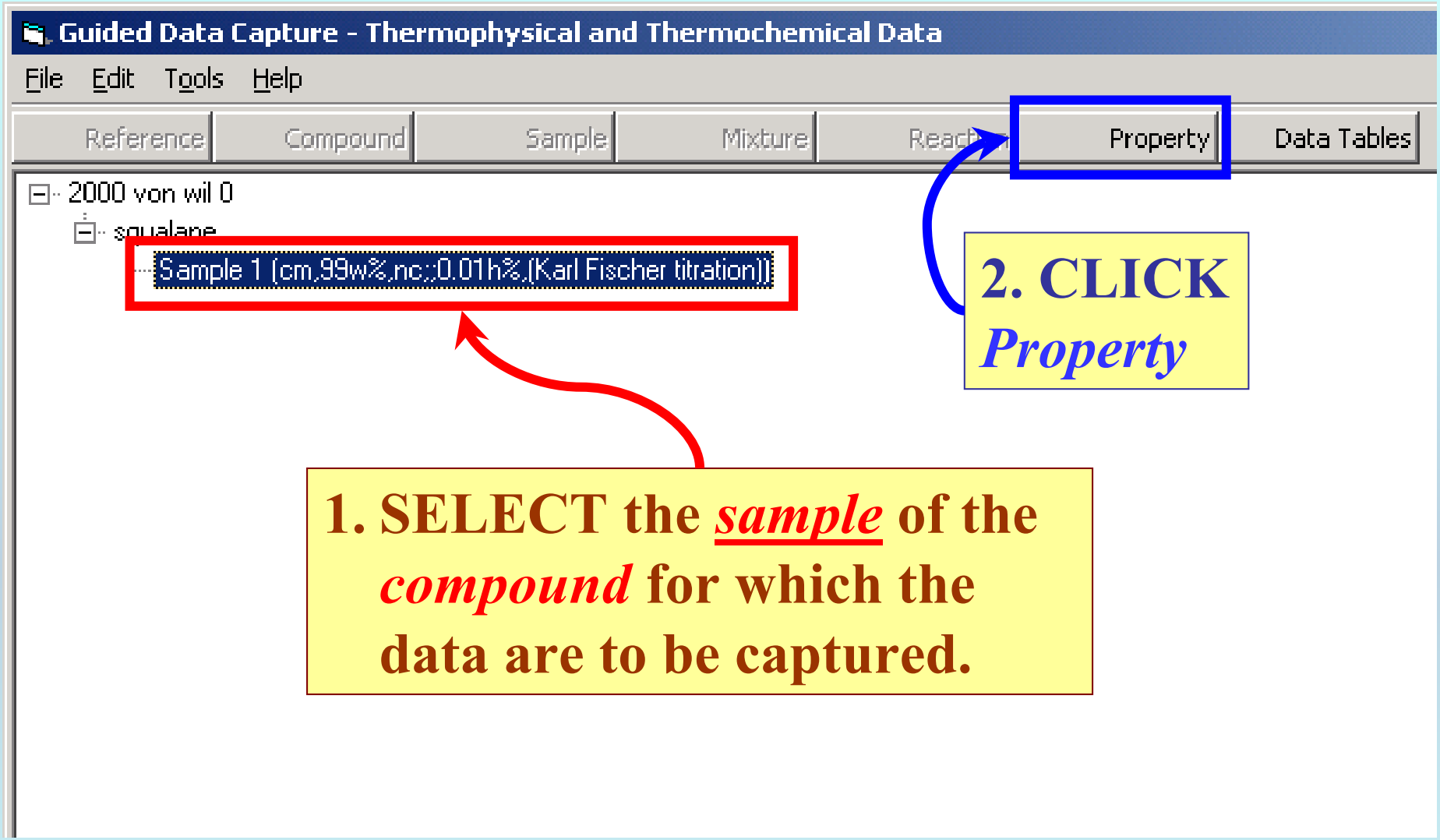
This experimental value is considered here.

Experimental Method Info :

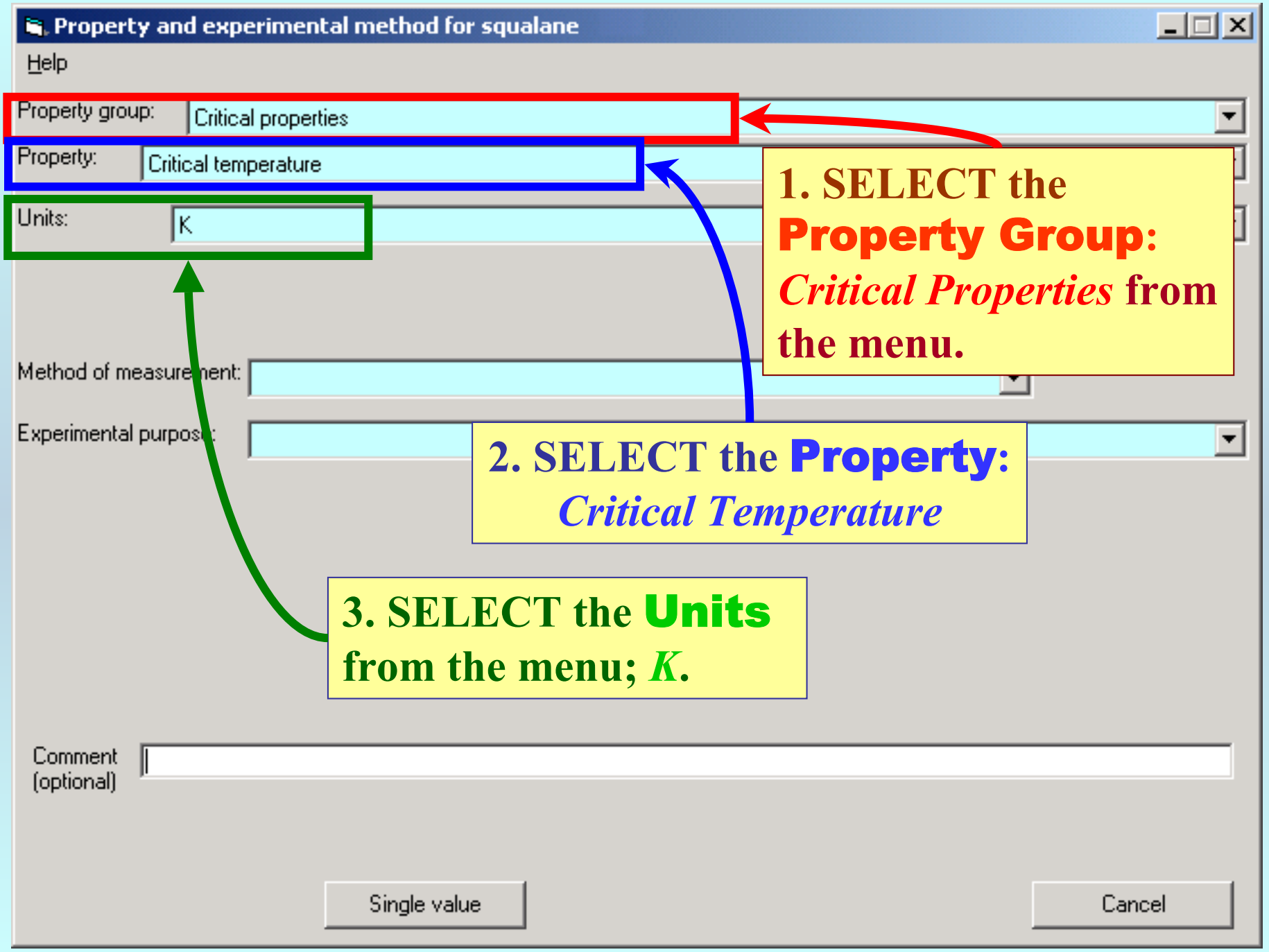
Flow Method

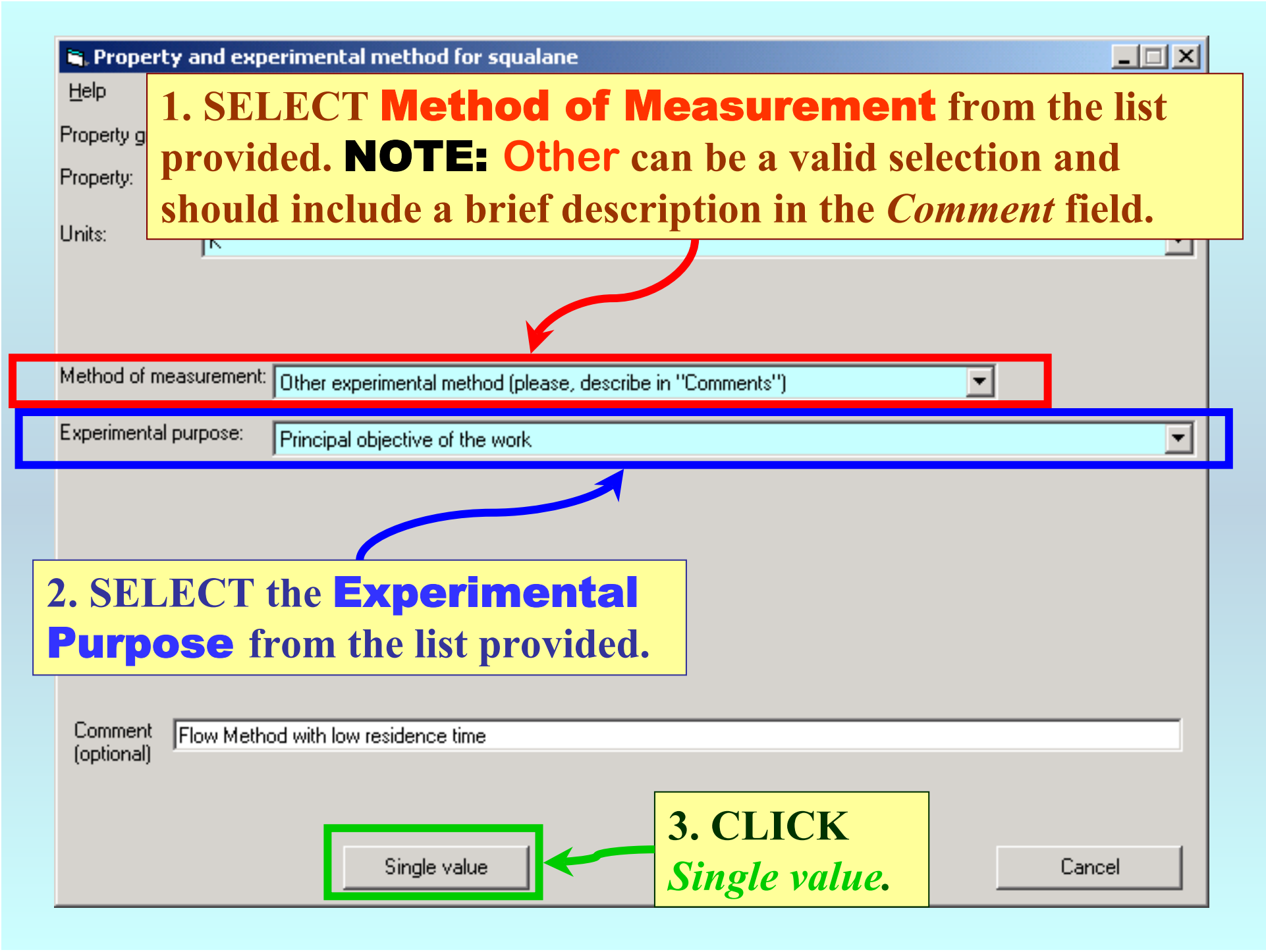
Authorís uncertainty estimates:

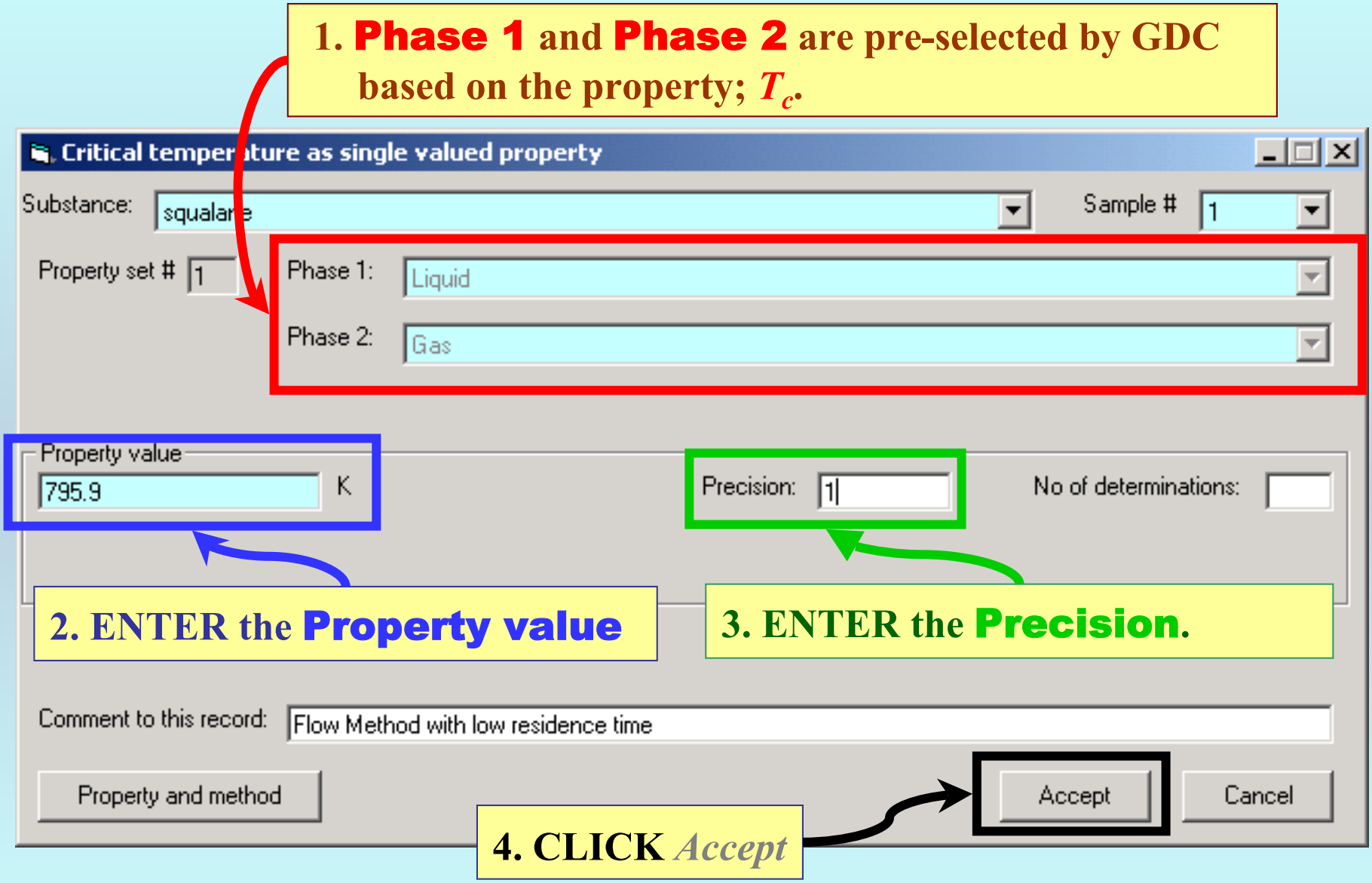
T_c: 1 K

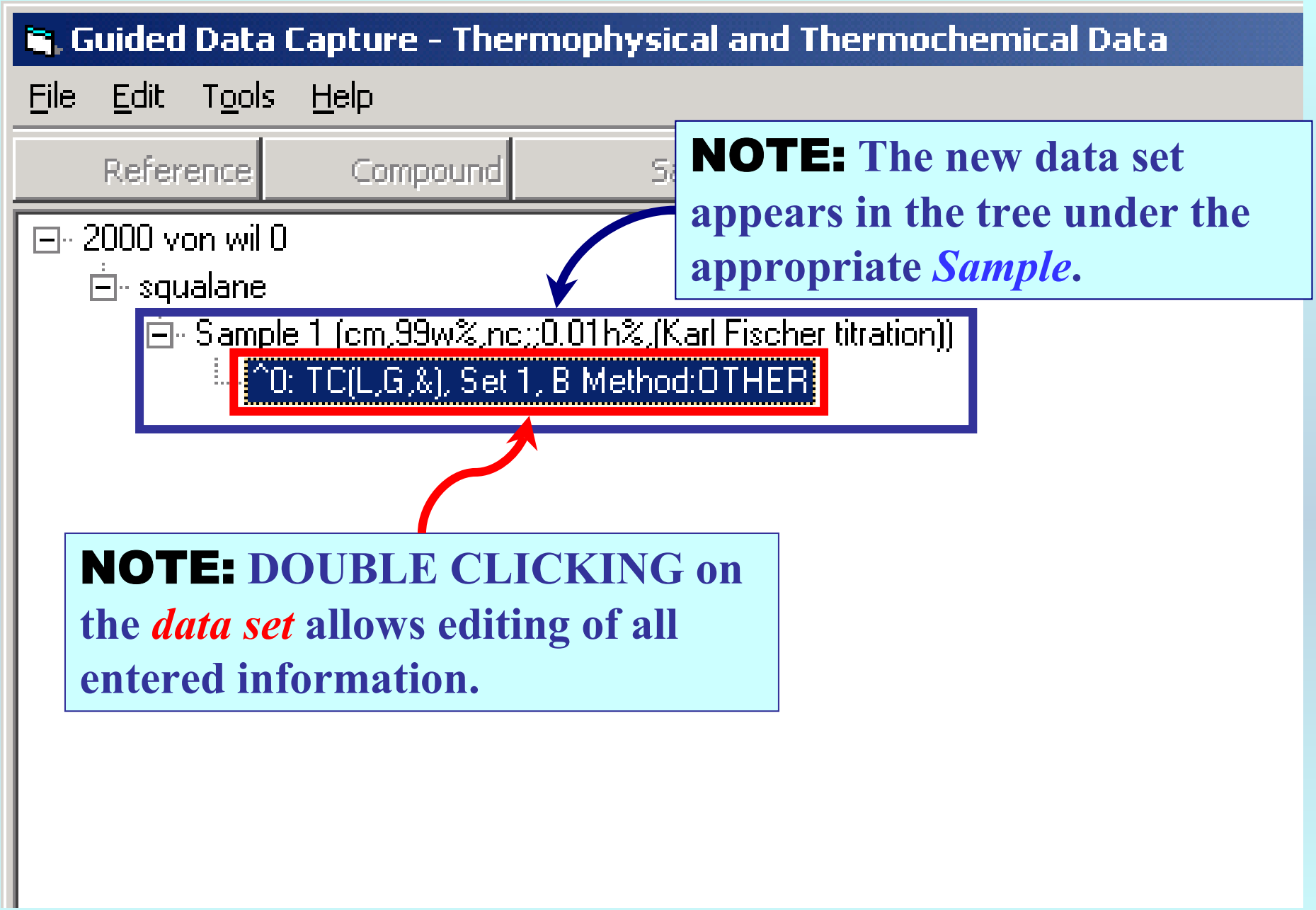


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for squalane
Help
Property group:
Critical properties
Property:
Critical temperature
Units:
K
Method of measurement:
Experimental purpose:
Comment (optional)
Single value
Cancel
1. SELECT the Property Group: Critical Properties from the menu.
2. SELECT the Property: Critical Temperature
3. SELECT the Units from the menu; K.


Property and experimental method for squalane
Help
Property g
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.
Comment (optional)
Flow Method with low residence time
Single value
3. CLICK Single value.
Cancel


1. Phase 1 and Phase 2 are pre-selected by GDC based on the property; T_c.
Critical temperature as single valued property
Substance:
squalane
Sample #
1
Property set #
1
Phase 1:
Liquid
Phase 2:
Gas
Property value
795.9
K
Precision:
1
No of determinations:
2. ENTER the Property value
3. ENTER the Precision.
Comment to this record:
Flow Method with low residence time
Property and method
Accept
Cancel
4. CLICK Accept


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
2000 von wil 0
squalane
Sample 1 (cm,99w%,nc;;0.01h%,(Karl Fischer titration))
^0: TC(L,G,&), Set 1, B Method:OTHER
NOTE: The new data set appears in the tree under the appropriate Sample.
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.**