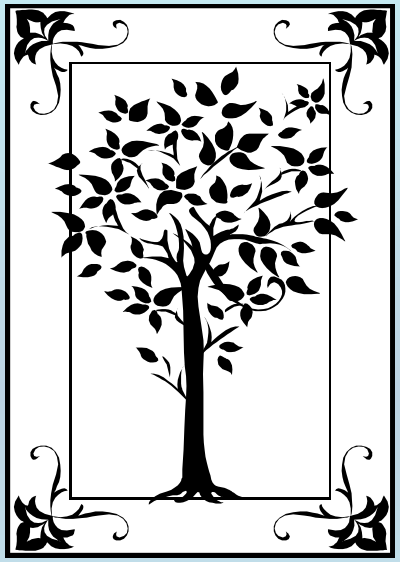
METADATA AND NUMERICAL DATA CAPTURE:
Normal Boiling Temperature (T_{bp})
(for 1 – Component; p = 101.325 kPa)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Boiling Point (T_{bp})**
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*, 271−273

Vapor−Liquid Equilibria of Binary Mixtures Containing Nitroethane with Five Alkyl Esters at 101.3 kPa

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Vapor−liquid equilibria (VLE) were measured at 101.3 kPa, in a range of temperatures from 350.28 to 387.00 K, for five binary mixtures formed by nitroethane with ethyl acetate, propyl acetate, isopropyl acetate, methyl propionate, and ethyl propionate. Calculations of nonideality of the vapor phase were made with the Soave−Redlich−Kwong equation of state. The thermodynamic consistency of the data was tested via Herington analysis. The experimental VLE data were reduced, and binary parameters for four liquid models, such as van Laar, Wilson, NRTL, and UNIQUAC, were fitted. A comparison of model performances was made by using the criterion of average absolute deviations in boiling point and in vapor-phase composition.

Normal Boiling Temperature (ì Pointî) for 1 component
nitroethane

Table 1. Densities, Refractive Indices, and Normal Boiling Points of Chemicals Used

	ρ(298.15K)/(kg·m^{-3})		n_D(298.15K)		T_b(101.3 kPa)/K	
compd	this work	lit.	this work	lit.	this work	lit.
nitroethane	1044.51	1044.64[a] 1043.8[b]	1.38987	1.38973[a]	387.00	387.22[a] 387.12[b]

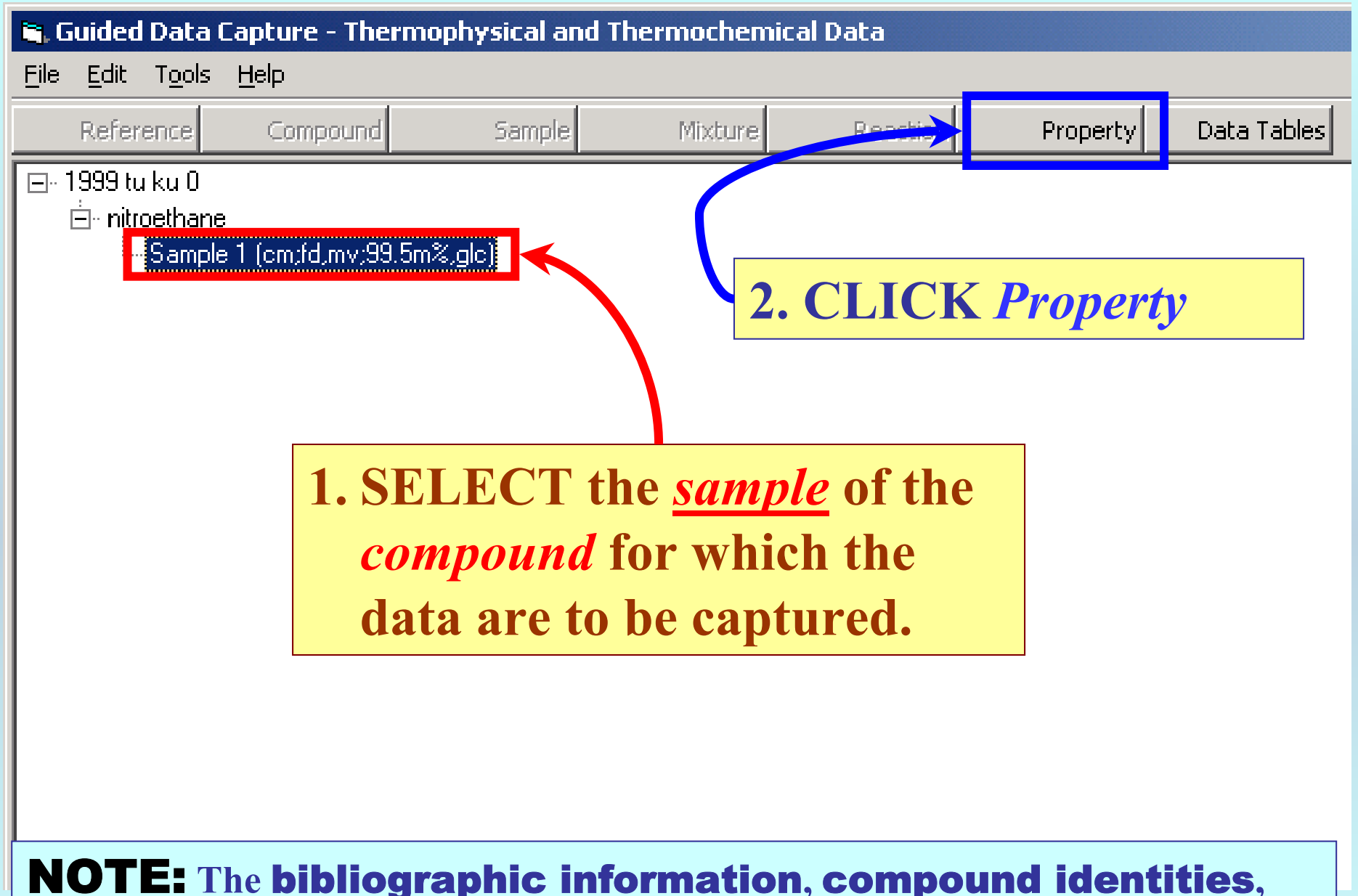
This data point is considered here.

Experimental Method Info :

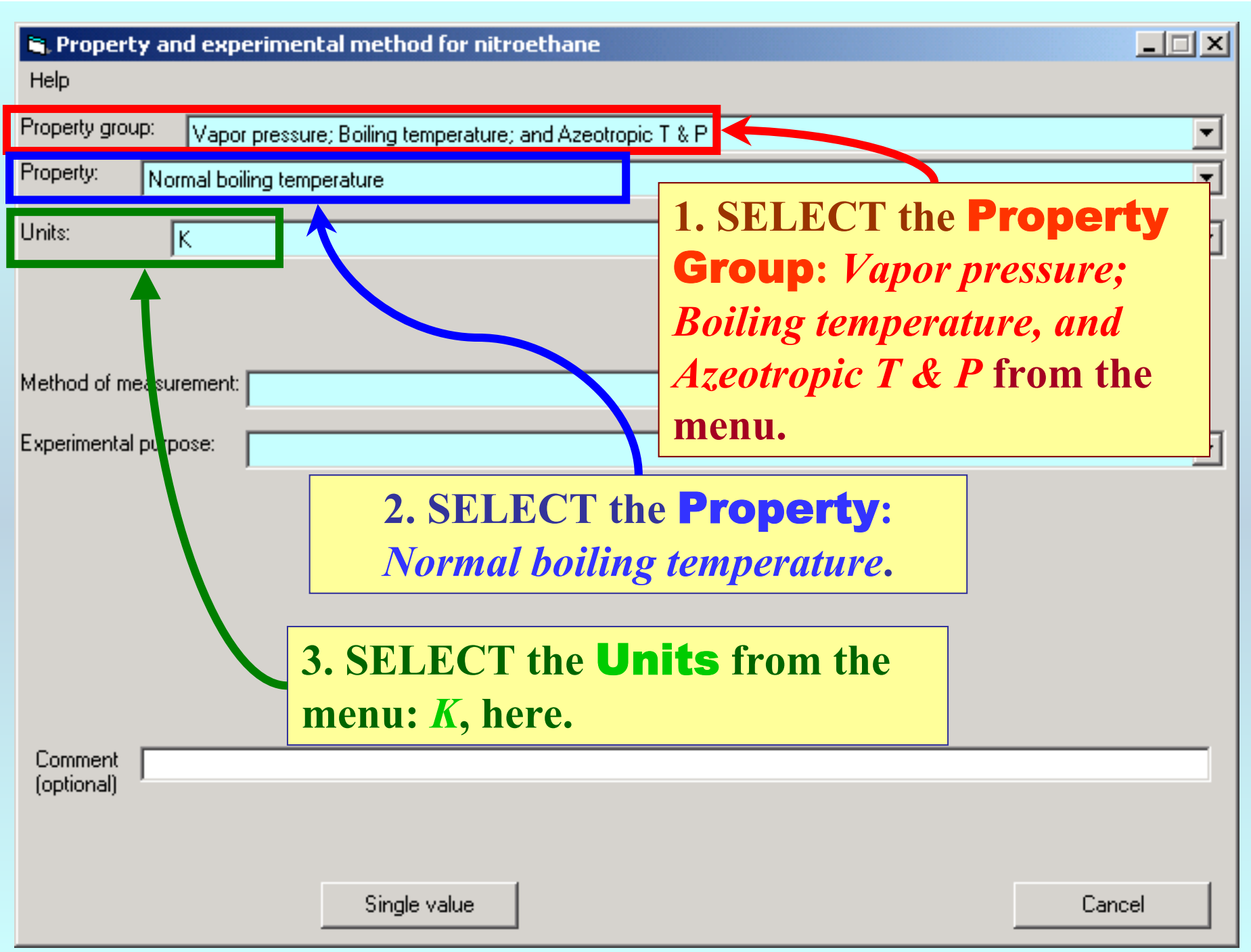
Recirculating still

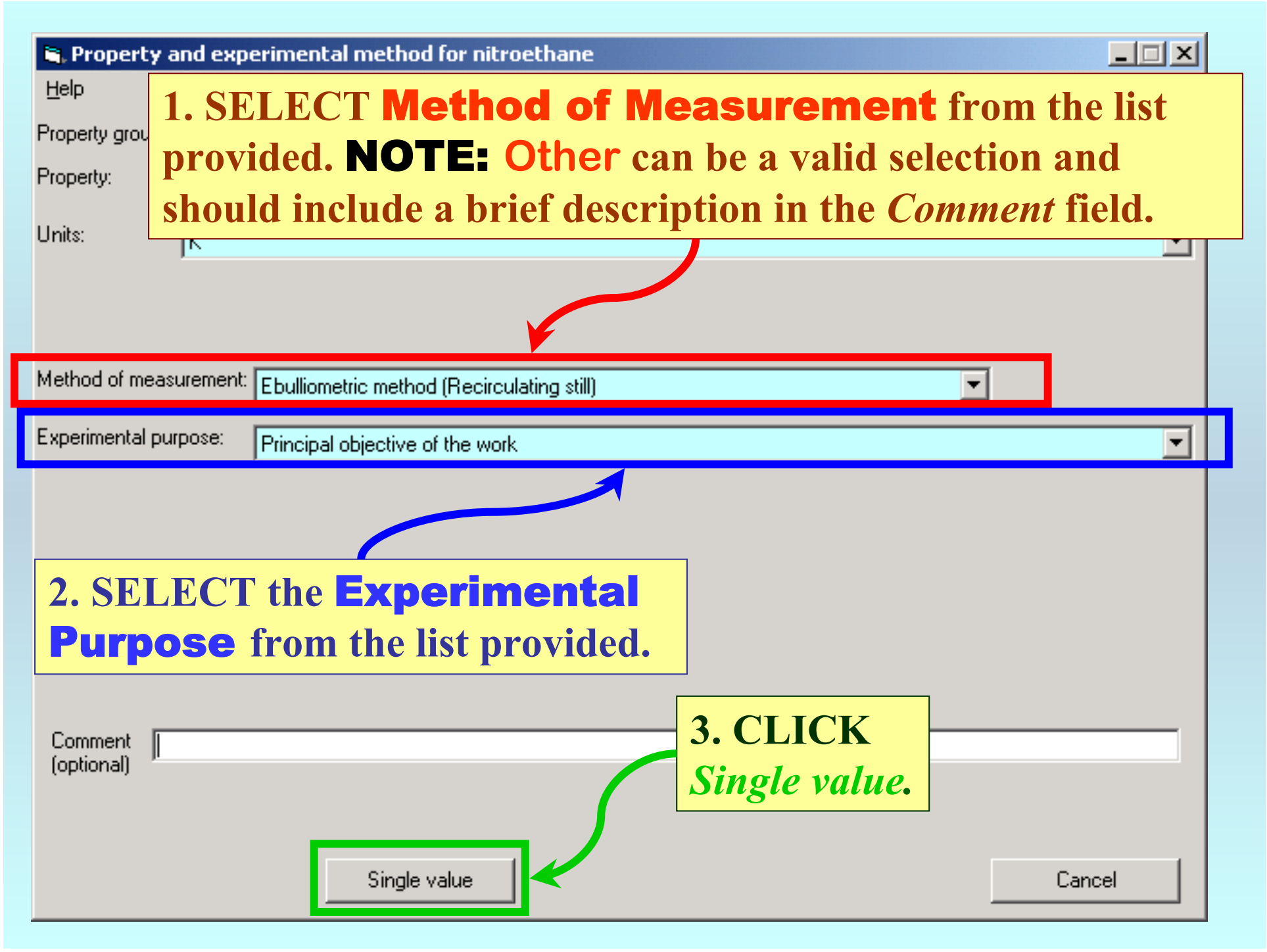
Authorís uncertainty estimates:

***T*: 0.02 K**

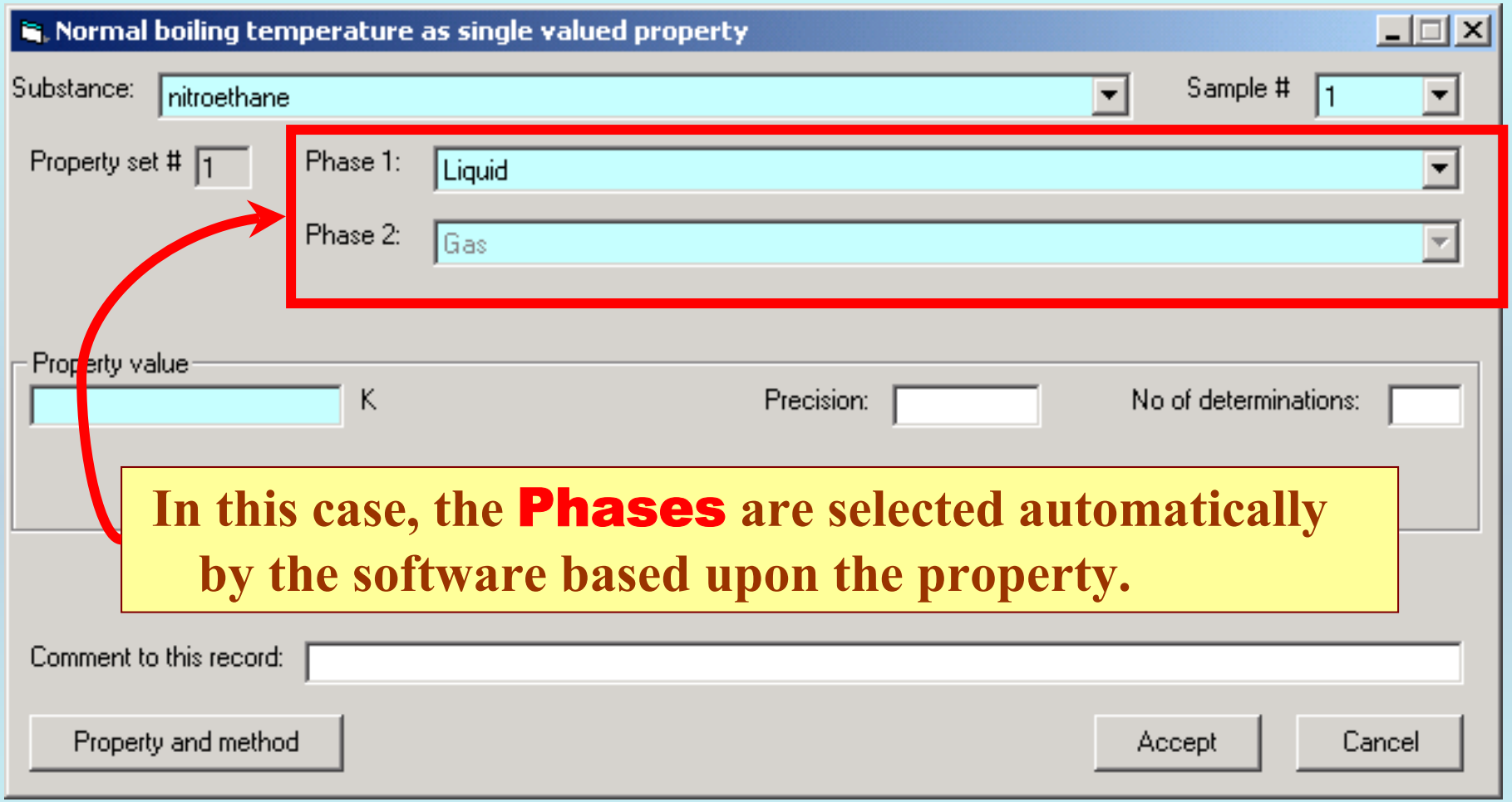


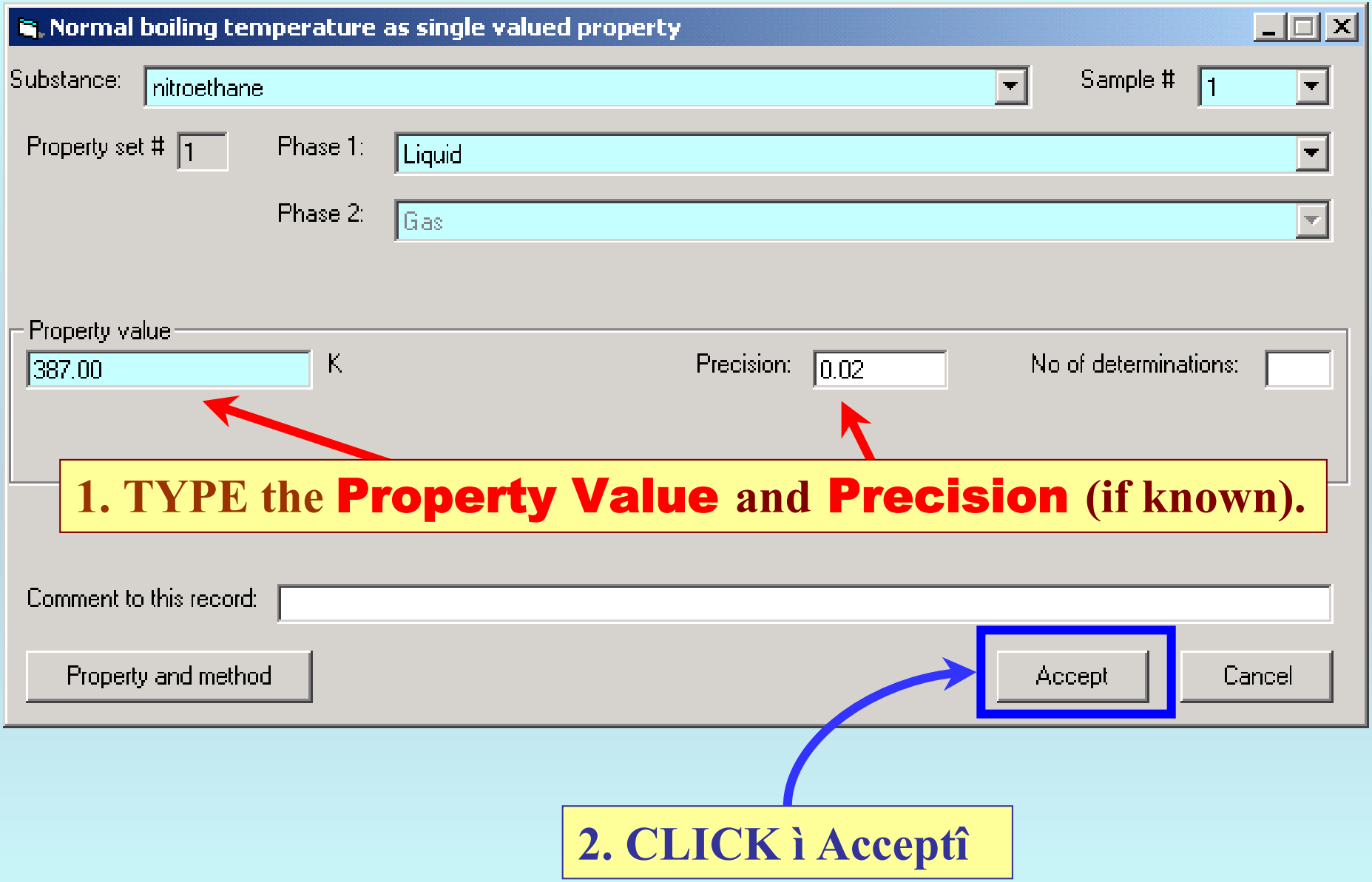
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

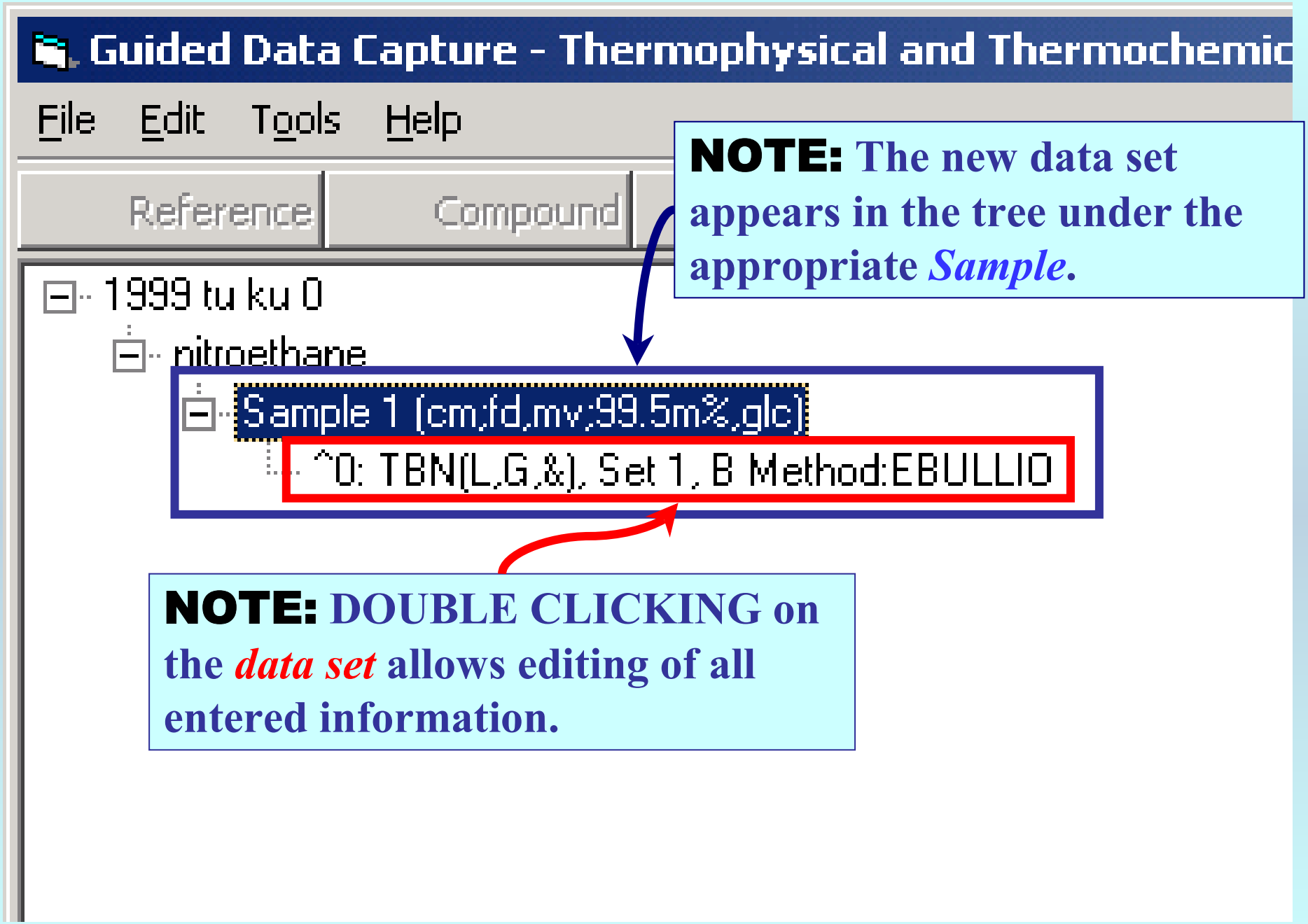

Property and experimental method for nitroethane
Help
Property group:
Vapor pressure; Boiling temperature; and Azeotropic T & P
Property:
Normal boiling temperature
Units:
K
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Vapor pressure; Boiling temperature, and Azeotropic T & P from the menu.
2. SELECT the Property: Normal boiling temperature.
3. SELECT the Units from the menu: K, here.
Comment (optional)
Single value
Cancel


Property and experimental method for nitroethane
Help
Property grou
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:
Ebulliometric method (Recirculating still)
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK Single value.
Single value
Cancel

Phase specification:




Normal boiling temperature as single valued property
Substance:
nitroethane
Sample #
1
Property set #
1
Phase 1:
Liquid
Phase 2:
Gas
Property value
387.00
K
Precision:
0.02
No of determinations:
1. TYPE the Property Value and Precision (if known).
Comment to this record:
Property and method
Accept
Cancel
2. CLICK ì Acceptî


Guided Data Capture - Thermophysical and Thermochemic
File Edit Tools Help
Reference
Compound
1999 tu ku 0
nitroethane
Sample 1 (cm;fd,mv;99.5m%,glc)
^0: TBN(L,G,&), Set 1, B Method:EBULLIO
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.**