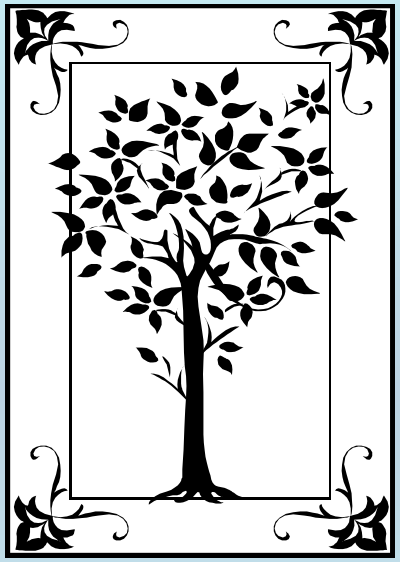
METADATA AND NUMERICAL DATA CAPTURE:
Triple Point Temperature (T_{tp})
(for 1 – Component)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Triple Point Temperature (T_{tp})**
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 1997, *42*, 475−487

Thermodynamic Equilibria in Xylene Isomerization. 2. The Thermodynamic Properties of *m*-Xylene†

R. D. Chirico,* S. E. Knipmeyer, A. Nguyen, J. W. Reynolds, and W. V. Steele

Bartlesville Thermodynamics Group, BDM Petroleum Technologies, P.O. Box 2543, Bartlesville, Oklahoma 74005

Measurements leading to the calculation of the ideal-gas thermodynamic properties for *m*-xylene are reported. Experimental methods included adiabatic heat-capacity calorimetry (5 K to 430 K), vibrating-tube densitometry (323 K to 523 K), comparative ebulliometry (309 K to 453 K), and differential-scanning calorimetry (DSC). The critical temperature was measured by DSC. Saturation heat capacities for the liquid phase between 430 K and 550 K and the critical pressure were derived with the vapor-pressure and DSC results. Results were combined with an enthalpy of combustion reported in the literature to derive standard molar entropies, enthalpies, and Gibbs free energies of formation at selected temperatures between 250 K and 550 K. The standard state is defined as the ideal gas at the pressure $p = p^{\circ} =$ 101.325 kPa. Standard entropies are compared with those calculated statistically on the basis of assigned vibrational spectra for the vapor phase. All results are compared with literature values.

Triple Point Temperature for 1 component
m-xylene (i.e., 1,3-dimethylbenzene)

Table 4. Measurements of Molar Enthalpy Increment, $\Delta_{tot}U_m$, for *m*-Xylene ($R = 8.314\ 51\ J \cdot K^{-1} \cdot mol^{-1}$)

N^a	H^b	T_i/K	T_f/K	T_{trs}/K	$\Delta_{tot}U_m^c$/ (kJ·mol^{-1})	$\Delta_{trs}H_m^d$/ (kJ·mol^{-1})
		Single-Phase Measurements in the Crystal Phase				
5	1	101.515	164.591		5.382	−0.001
5	1	164.599	211.048		4.985	−0.002
		Crystals to Liquid				
1	7	213.566	228.234	225.30	13.538	11.644
2	2	222.024	228.561		12.573	11.644
5	3	211.085	227.940		13.782	11.644
					Average:	11.644
		Single-Phase Measurements in the Liquid Phase				
5	1	227.941	310.367		14.244	−0.001
7	1	294.786	395.440		20.003	−0.003
7	1	395.410	427.130		7.118	−0.001

This data set is considered here.

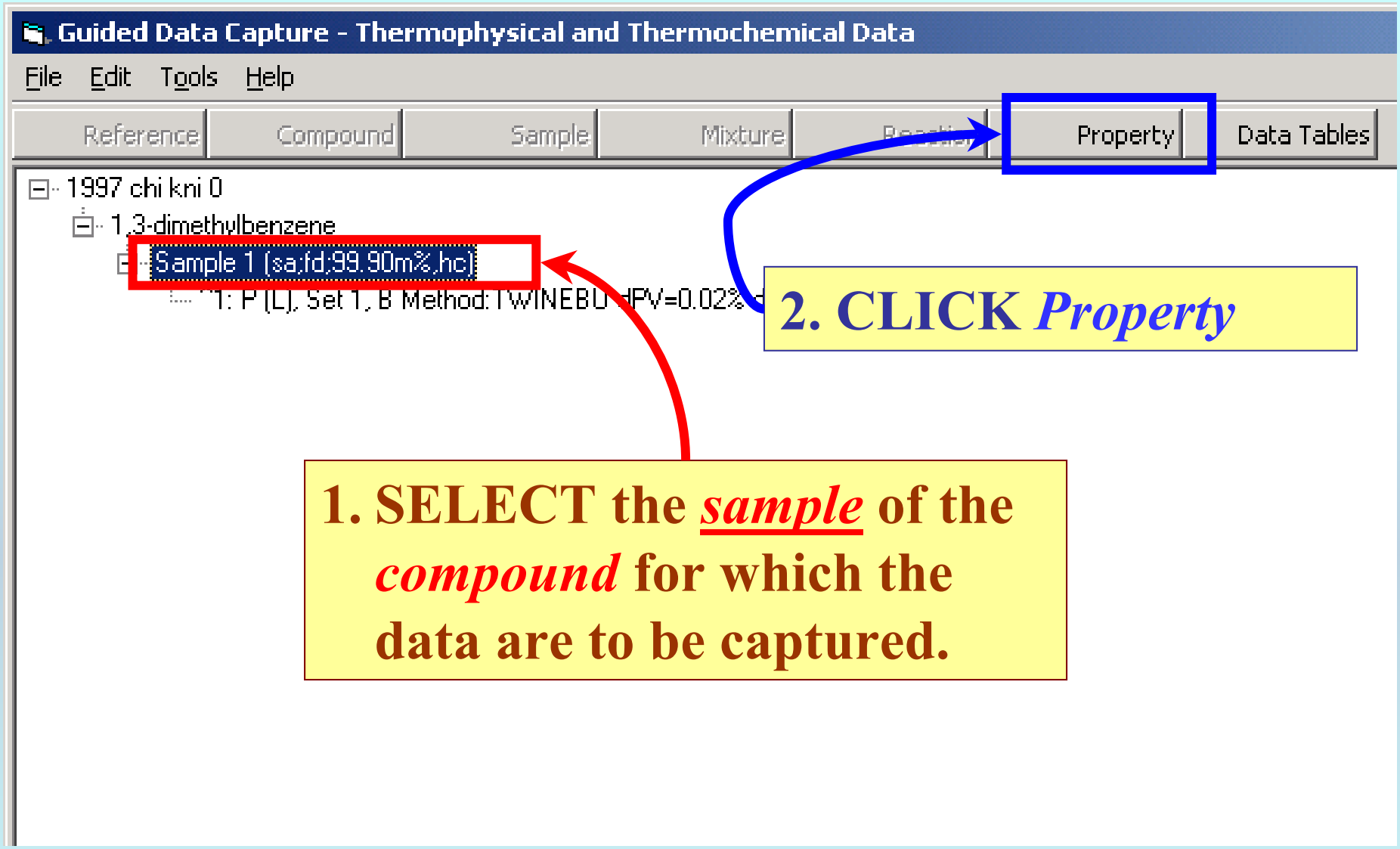
Experimental Method Info :

Adiabatic heat-capacity calorimetry

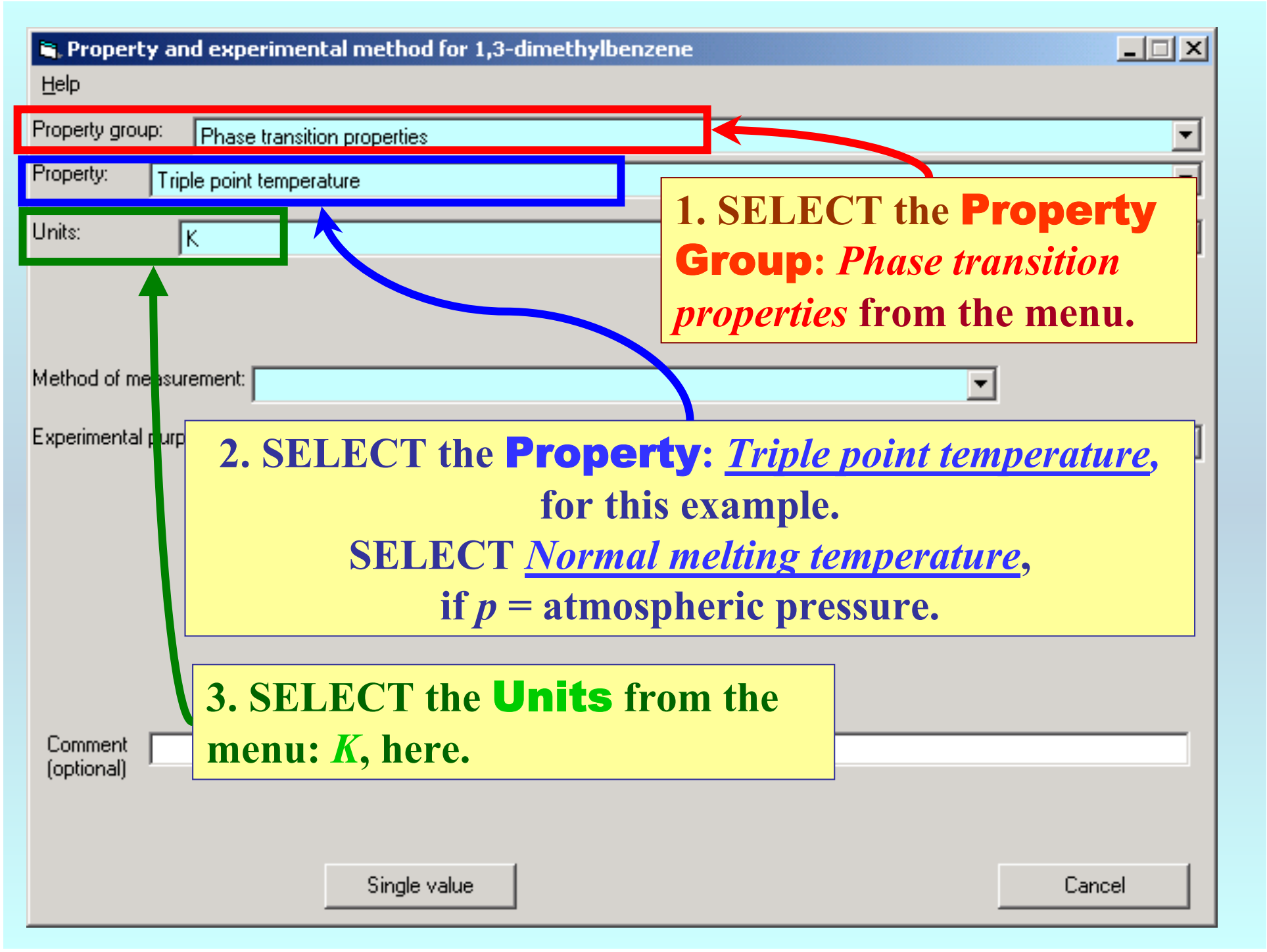
Uncertainty estimates:

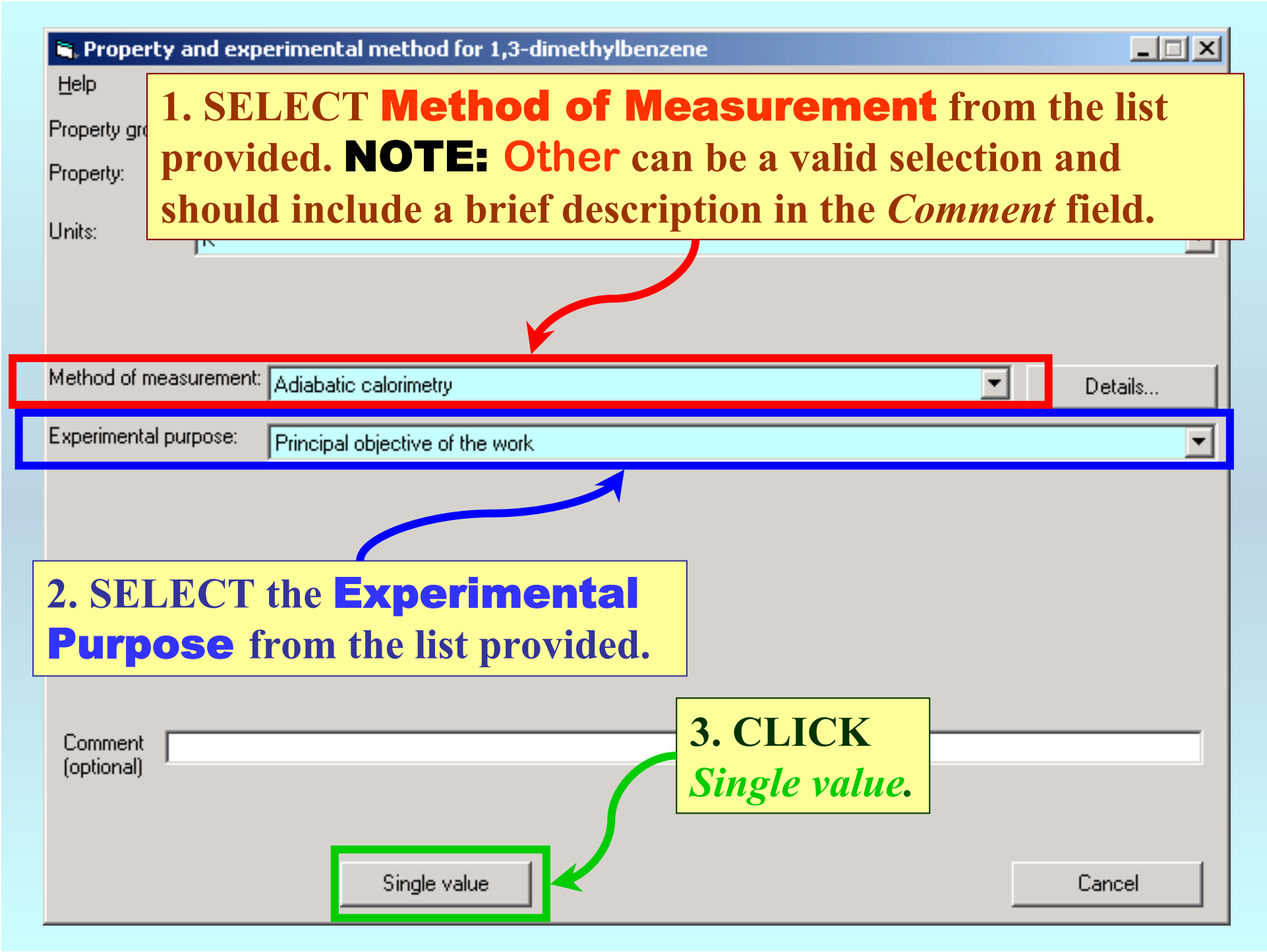
Table 3. Melting-Study Summary for *m*-Xylene[a]

F	$T(F)$/K
0.1596	225.069
0.2587	225.158
0.4073	225.209
0.6550	225.242
0.8037	225.252
T_{tp}/K	(225.30 ± 0.01)
x	0.0010

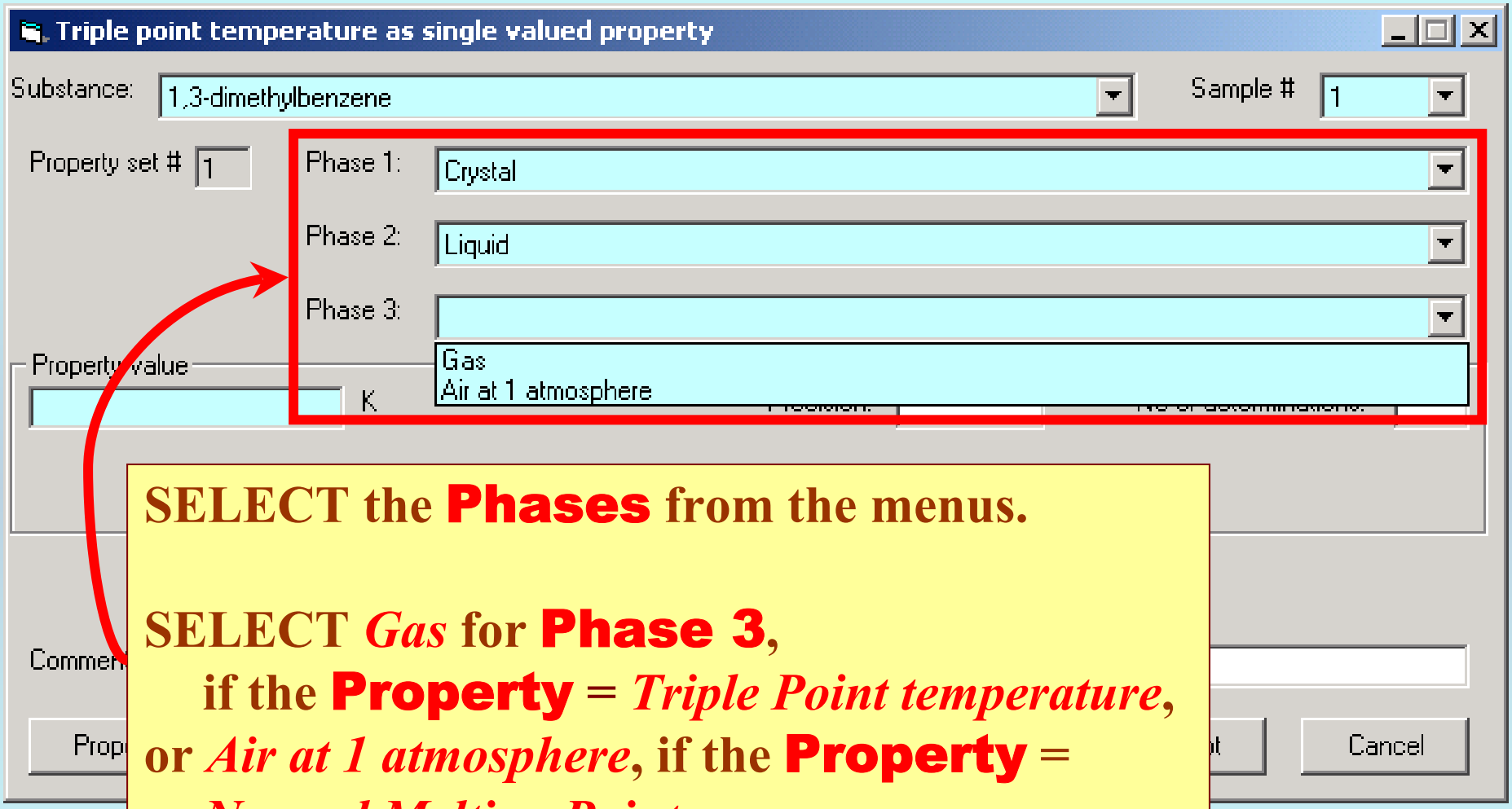


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for 1,3-dimethylbenzene
Help
Property group:
Phase transition properties
Property:
Triple point temperature
Units:
K
Method of measurement:
Experimental purp
Comment (optional)
Single value
Cancel
1. SELECT the Property Group: Phase transition properties from the menu.
2. SELECT the Property: Triple point temperature, for this example.
SELECT Normal melting temperature, if p = atmospheric pressure.
3. SELECT the Units from the menu: K, here.

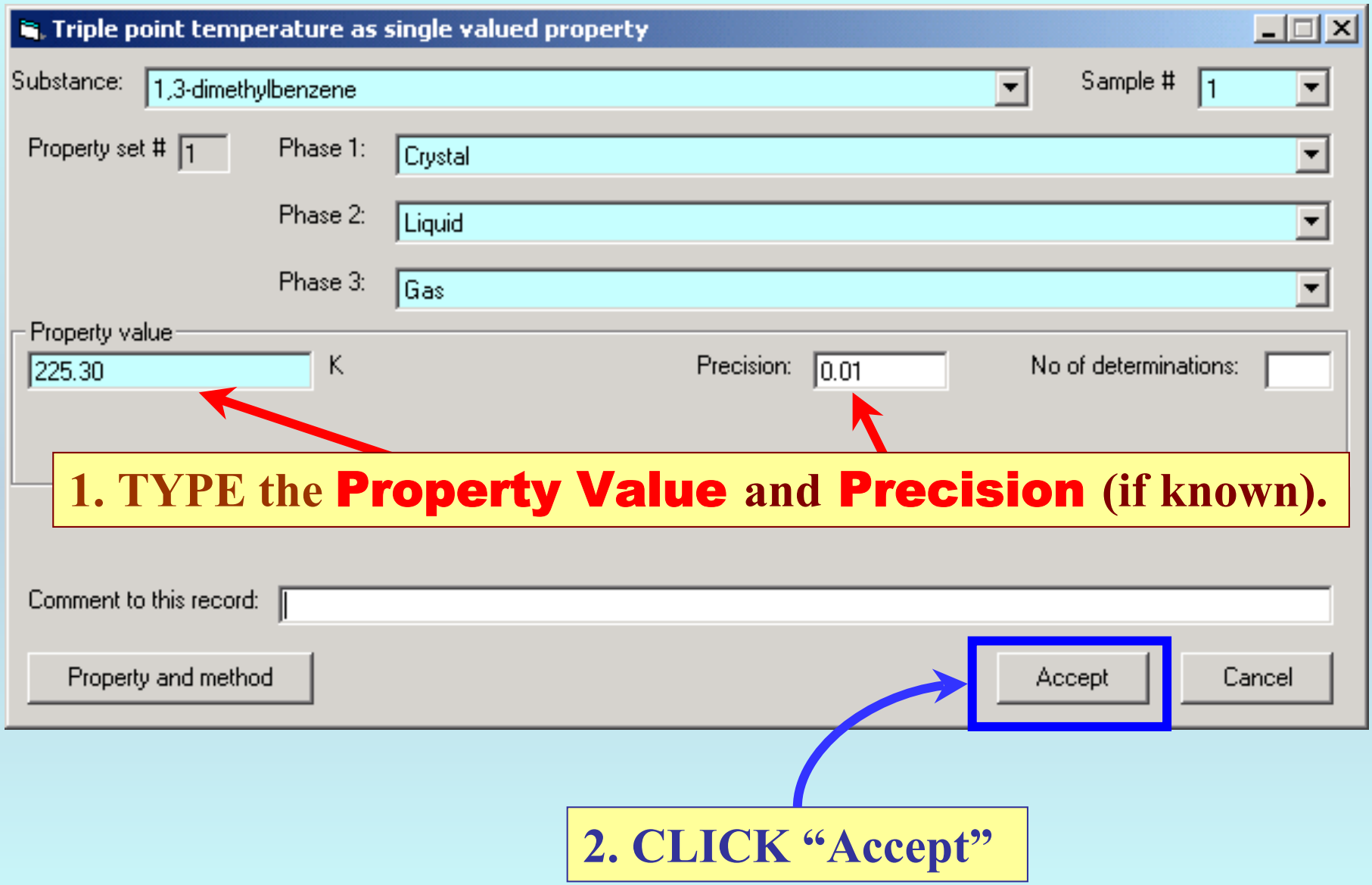

Property and experimental method for 1,3-dimethylbenzene
Help
Property gr
Property:
Units:
1. SELECT Method of Measurement from the list provided. NOTE: Other can be a valid selection and should include a brief description in the Comment field.
Method of measurement:
Adiabatic calorimetry
Details...
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

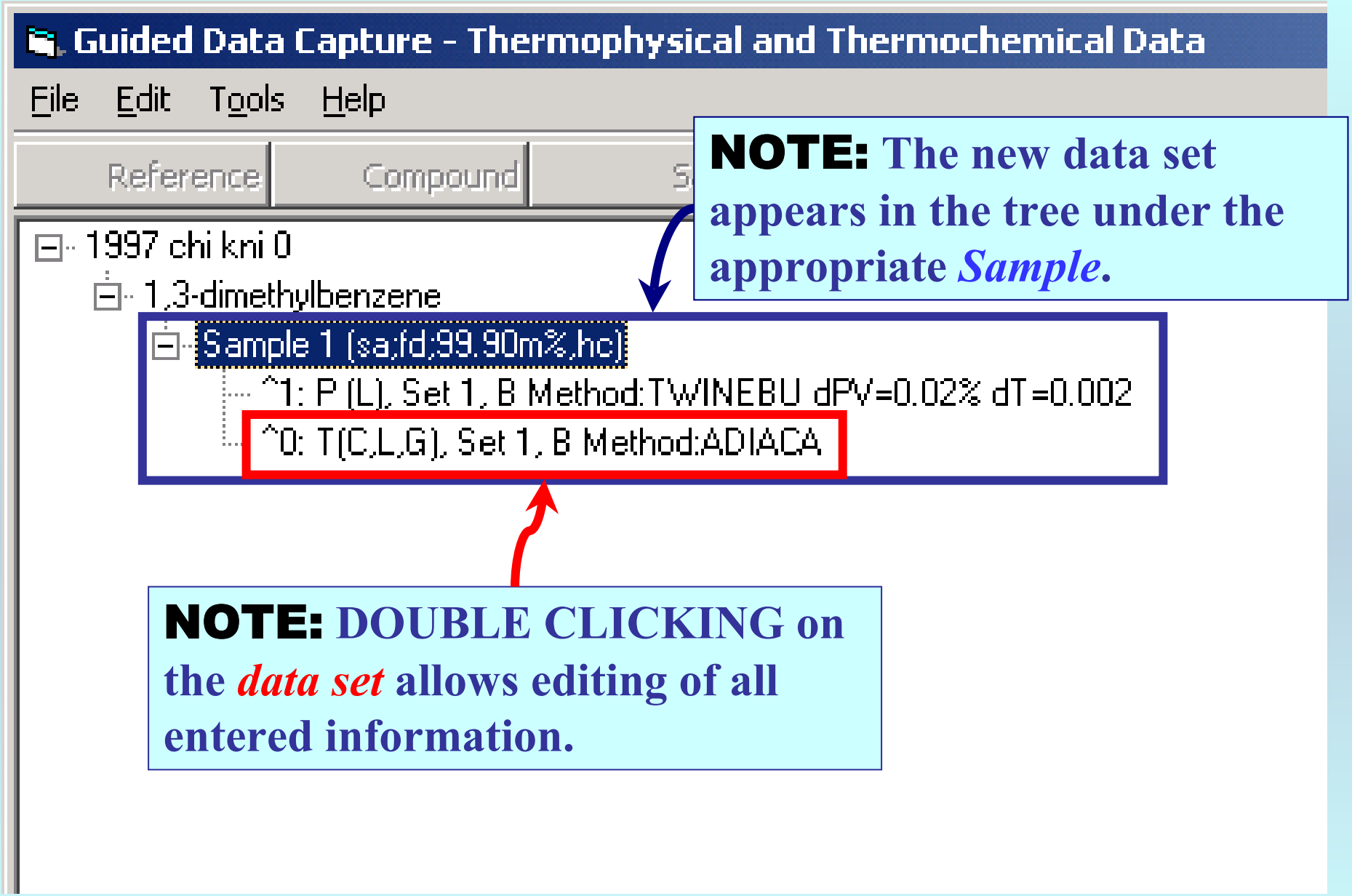
Phase specification:



SELECT the Phases from the menus.

SELECT *Gas* for Phase 3,
if the Property = *Triple Point temperature*,
or *Air at 1 atmosphere*, if the Property =
***Normal Melting Point*.**


Triple point temperature as single valued property
Substance:
1,3-dimethylbenzene
Sample #
1
Property set #
1
Phase 1:
Crystal
Phase 2:
Liquid
Phase 3:
Gas
Property value
225.30
K
Precision:
0.01
No of determinations:
1. TYPE the Property Value and Precision (if known).
Comment to this record:
Property and method
Accept
Cancel
2. CLICK "Accept"


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
1997 chi kni 0
1,3-dimethylbenzene
Sample 1 [sa;fd;99.90m%,hc]
^1: P (L), Set 1, B Method:TWINEBU dPV=0.02% dT=0.002
^0: T(C,L,G), Set 1, B Method:ADIACA
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.**