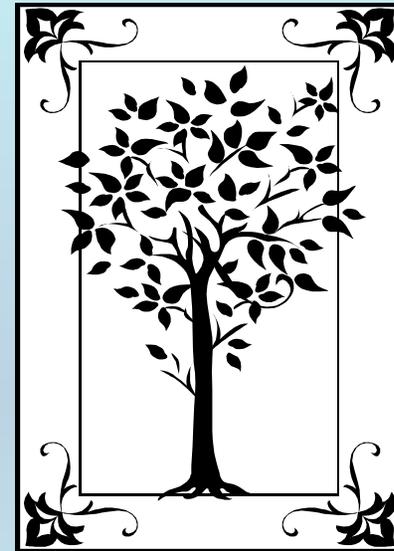


METADATA AND NUMERICAL DATA CAPTURE:  
**Normal Boiling Temperature ( $T_{bp}$ )**  
(for 1 – Component;  $p = 101.325$  kPa)

*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

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## **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 (i Pointi) for 1 component nitroethane

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

compd	$\rho(298.15\text{K})/(\text{kg}\cdot\text{m}^{-3})$		$n_D(298.15\text{K})$		$T_b(101.3\text{ kPa})/\text{K}$	
	this work	lit.	this work	lit.	this work	lit.
nitroethane	1044.51	1044.64 <sup>a</sup> 1043.8 <sup>b</sup>	1.38987	1.38973 <sup>a</sup>	<u>387.00</u>	387.22 <sup>a</sup> 387.12 <sup>b</sup>

This data point is  
considered here.

## **Experimental Method Info :**

**Recirculating still**

## **Author's uncertainty estimates:**

**$T$ : 0.02 K**

The screenshot shows the 'Guided Data Capture - Thermophysical and Thermochemical Data' application. The menu bar includes 'File', 'Edit', 'Tools', and 'Help'. The main window has several tabs: 'Reference', 'Compound', 'Sample', 'Mixture', 'Reaction', 'Property', and 'Data Tables'. The 'Property' tab is highlighted with a blue box and a blue arrow. In the tree view on the left, '1999 tu ku 0' is expanded to show 'nitroethane', which is further expanded to show 'Sample 1 (cm:fd,mv:99.5m%,glo)'. This sample name is highlighted with a red box and a red arrow. A yellow callout box with blue text says '2. CLICK *Property*'. Another yellow callout box with red text says '1. SELECT the *sample* of the *compound* for which the data are to be captured.'

1. SELECT the *sample* of the *compound* for which the data are to be captured.

2. CLICK *Property*

**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:

Comment (optional)

Single value

Cancel

The image shows a software window titled "Property and experimental method for nitroethane". It contains several input fields: "Property group" (set to "Vapor pressure; Boiling temperature; and Azeotropic T & P"), "Property" (set to "Normal boiling temperature"), "Units" (set to "K"), "Method of measurement", "Experimental purpose", and "Comment (optional)". At the bottom are "Single value" and "Cancel" buttons. Three numbered instructions with arrows point to the "Property group", "Property", and "Units" fields respectively.

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.

Property and experimental method for nitroethane

Help  
Property group  
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:  Sample #

Property set #

Phase 1:

Phase 2:

Property value  K Precision:  No of determinations:

Comment to this record:

**In this case, the **Phases** are selected automatically by the software based upon the property.**

**Normal boiling temperature as single valued property**

Substance:  Sample #

Property set #  Phase 1:

Phase 2:

Property value:  K Precision:  No of determinations:

Comment to this record:

**1. TYPE the Property Value and Precision (if known).**

**2. CLICK ì Acceptî**

# Guided Data Capture - Thermophysical and Thermochemical

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.***