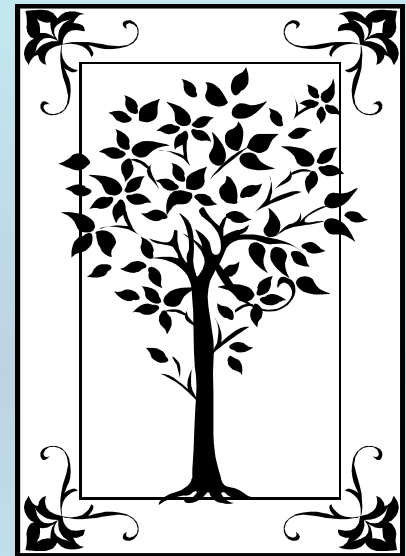


**METADATA AND NUMERICAL DATA CAPTURE:
Common pure-component properties
density d at 1 temperature and pressure**

**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

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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 %)	$d(298.15\text{ K})/(\text{g}\cdot\text{cm}^{-3})$		$n_D(298.15\text{ K})$		$T_b(101.3\text{ kPa})/\text{K}$	
	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 (99.9)	0.735 20	0.735 28 ^c	1.3664	1.3663 ^d	327.83	327.83 ^e

The data considered here.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

Sample

Mixture

Reaction

Property

Data Tables

1999 Ior auc 0

methanol

Sample 1 (cm,99.9w%,nc;x;99.9w%,glc)

methyl tert-butyl ether

Sample 1 (cm,99.8w%,nc;x;99.8w%,glc)

1. SELECT the *sample* of the *compound* (**methanol** here) for which the property is to be entered.

2. CLICK *Property*

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

The image shows a software dialog box titled "Property and experimental method for methanol + N-methylpiperazine". The dialog box contains several fields and a list of property groups. A red box highlights the "Property group:" dropdown menu. A red arrow points from this box to a yellow callout box containing the text "1. CLICK in the Property group field." A blue circle highlights the "Volumetric properties" option in the dropdown menu. A blue arrow points from this circle to another yellow callout box containing the text "2. SELECT Volumetric properties from the menu." Other fields in the dialog box include "Units:", "Method of measurement:", "Experimental purpose:", and "Comment (optional)". A "Cancel" button is located at the bottom right.

Property group:

Units:

Method of measurement:

Experimental purpose:

Comment (optional)

Cancel

1. **CLICK** in the **Property group** field.

2. **SELECT Volumetric properties** from the menu.

Property selection

Property and experimental method for methanol + N-methylpiperazine

Help

Property group: Volumetric properties

Property: **Specific density**

Units:

Method of measurement:

Experimental purpose:

Comment (optional)

Cancel

1. CLICK in the Property field.

2. SELECT Specific density from the menu.

Units selection

The image shows a software dialog box titled "Property and experimental method for methanol". It contains several fields: "Property group" (Volumetric properties), "Property" (Specific density), "Units" (highlighted with a red box), "Method of measurement", and "Experimental purpose". The "Units" dropdown menu is open, showing options: kg/m³, g/cm³, lb/ft³, and ALL OTHER UNITS. A blue circle highlights "g/cm³". A red arrow points from a yellow box with the instruction "1. CLICK in the Units field." to the "Units" dropdown. A blue arrow points from a yellow box with the instruction "2. SELECT from the menu; g/cm³ here" to the "g/cm³" option. At the bottom, there are buttons for "1-Variable data", "2-Variable data", "One data point", and "Cancel". A "Comment (optional)" text area is also present.

Property and experimental method for methanol

Help

Property group: Volumetric properties

Property: Specific density

Units:

- kg/m³
- g/cm³
- lb/ft³
- ALL OTHER UNITS

Method of measurement:

Experimental purpose:

Comment (optional)

1-Variable data 2-Variable data

One data point Cancel

1. CLICK in the Units field.

2. SELECT from the menu; g/cm³ here

Method selection

Property and experimental method for methanol

Help

Property group: Volumetric properties

Property: Specific density

Units: g/cm³

Method of measurement: Vibrating tube method

Experimental purpose:

- Pycnometric method
- Buoyancy method
- Vibrating tube method
- Isochoric PVT measurement
- Other PVT measurement
- Burnett expansion technique
- Constant-volume
- Other experimental

Comment (optional)

Details...

1. **CLICK** in the **Method of measurement** field.

2. **SELECT** the **Method of measurement** from the menu, which best describes your experiment; *Vibrating tube method*, here.

NOTE: *Other* is an option. A one sentence description or a reference is often adequate in this case.

Method detail selection

Experiment details

Select the statements, which are true for the reported measurement

More than two calibration points used

Accept

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

Experimental purpose selection

Property and experimental method for methanol

Help

Property group: Volumetric properties

Property: Specific density

Units: g/cm³

Method of measurement: Vibrating tube method

Experimental purpose:

- Principal objective of the work
- Secondary purpose (by-product of other objective)
- Determined for identification of a synthesized compound

1. **CLICK** in the **Experimental purpose** field.

2. **SELECT** the **Purpose** from the menu.

3. **CLICK One data point**

1-Variable data

2-Variable data

One data point

Cancel

Specification of phase, temperature, and value

1. **SELECT** the **Phase** for the property value from the list provided. (*Liquid* here)

The screenshot shows a software window titled "Specific density at fixed conditions". The interface includes the following fields and controls:

- Substance:** A dropdown menu with "methanol" selected.
- Sample #:** A dropdown menu with "1" selected.
- Property set #:** A text input field containing "1".
- Phase 1:** A dropdown menu with "Liquid" selected. This field is highlighted with a red box and a red arrow pointing to it from the first instruction box.
- Independent variable:** A dropdown menu with "Temperature" selected.
- Value:** A text input field containing "298.15".
- Unit:** A dropdown menu with "K" selected. This field is highlighted with a blue box and a blue arrow pointing to it from the second instruction box.
- Uncertainty:** An empty text input field.
- Property value:** A text input field containing "0.78732". This field is highlighted with a green box and a green arrow pointing to it from the third instruction box.
- Unit:** A dropdown menu with "g/cm3" selected.
- Precision:** An empty text input field.
- No of determinations:** An empty text input field.
- Comment to this record:** An empty text input field.
- Buttons:** "Accept" and "Cancel" buttons at the bottom right.

2. **TYPE** the temperature **Value** and **SELECT** the **Unit** from the menu.

3. **TYPE** the **Property value**; *0.78732* here.

Form is complete...

1. Include approximate **Uncertainties, if known.**

Substance: 1

Property set # Phase 1:

Independent variable: Temperature
Value:

Property value
 g/cm³

Uncertainty:

Precision: No of determinations:

Comment to this record:

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 Data

File Edit Tools Help

Reference

Compound

Sample

Mixture

Reaction

[-] 1999 lor auc 0

[-] methanol

[-] Sample 1 (cm:99.9w%ncw:99.9w%alc)

^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.