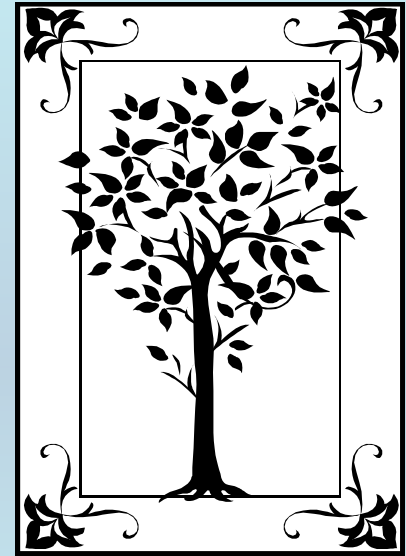


METADATA AND NUMERICAL DATA CAPTURE:

Common pure-component properties

Melting Point near 101.3 kPa pressure

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Common pure-component properties:**
Melting Point at approximately 101.3 kPa 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:

1220

J. Chem. Eng. Data 2002, 47, 1220–1221

Solid–Liquid Equilibria of Terephthalaldehydic Acid in Different Solvents

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Solubilities of terephthalaldehydic acid in water, acetic acid, chloroform, *N, N*-dimethylformamide, and *N*-methyl-2-pyrrolidone were determined by a static analytical method at temperatures ranging from 293.15 K to 371.15 K at atmospheric pressure. The Buchowski equation was used to correlate the solubility data with standard deviations in the range 0.006–3.438 g of terephthalaldehydic acid/100 g of solvent.

Melting Point

Melting Point for terephthalaldehydic acid

Shimadzu). The melting point of terephthalaldehydic acid measured with a NETZSCH STA449C differential scanning calorimeter was **522.8 K** and compares with the literature value 520.2 K.³

The data considered here.

Method: Differential Scanning Calorimetry

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction **Property** Data Tables

2002 li eva 0

terephthalaldehydic acid

Sample 1 (cm,98.0w%,nc;ch,cs,se;99.8w%,hplc)

1. SELECT the *sample* of the *compound* 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 & Units selection

The image shows a software dialog box titled "Property and experimental method for terephthaladehydric acid". It contains several input fields and buttons. Three callout boxes provide instructions: a red box for selecting the property group, a blue box for selecting the property, and a green box for selecting the units. The "Property group" is set to "Phase transition properties", the "Property" is "Triple point temperature", and the "Units" are "K".

Property group: Phase transition properties

Property: Triple point temperature

Units: K

Method of measurement:

Experimental purpose:

Comment (optional)

Single value Cancel

1. SELECT the **Property group:** *Phase transition properties*

2. SELECT the **Property:** *Triple point temperature*

3. SELECT the **Units:** *K*, here

Method selection

Property and experimental method for terephthalaldehydic acid

Help

Property group: Phase transition

Property: Triple point temperature

Units: K

Method of measurement: DSC/DTA

Experimental purpose: Principal objective of the work

Single value

Cancel

1. SELECT the **Method of measurement** from the menu. SELECT "*Other*" and provide a short *Comment*, if needed.

2. SELECT the **Experimental purpose**

3. CLICK *Single Value*

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*.

Specification of phases and value

1. SELECT the **Phases** for the property value
(*Crystal, Liquid, Air at 1 atm*) for the Melting Point

Triple point temperature

Substance: terephthalaldehydic acid

Property set # 1

Phase 1: Crystal

Phase 2: Liquid

Phase 3: Air at 1 atmosphere

Property value: 522.8 K

Precision:

No. of determinations:

Comment to this record:

Property and method

Accept

Cancel

2. TYPE the temperature **Value** and
Precision, if known.

3. CLICK *Accept*

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

NOTE: The new *Property* appears below the *Sample* of the appropriate *Compound* in the navigation tree.

[-] 2002 li eva 0

[-] terephthalaldehydic acid

[-] Sample 1 (cm,98.0w%,nc;ch,cs,se;99.8w%,hplc)

... ^0: T(C,L,air), Set 1, B Method:DTA

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.