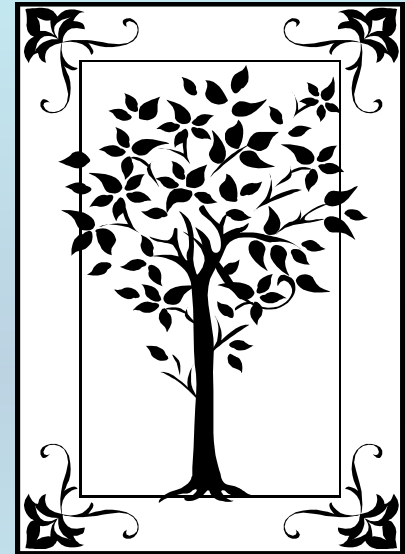


METADATA AND NUMERICAL DATA CAPTURE: **SL₁L₂G – Quadruple Point Temperature**

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for :
SL₁L₂G – Quadruple Point Temperature
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:

Solubility of Imidazoles in Ethers

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Quadruple Point – (Solid-Liquid₁-Liquid₂-Vapor)

Quadruple Point for 1,2-Dimethylimidazole (1) + Dibutyl ether (2)

Table 5. Experimental Solid-Liquid Equilibrium Temperatures, T and Liquid-Liquid Equilibrium temperatures, T_{LLE} for {1,2-Dimethylimidazole (1) + an Ether (2)} Systems; γ_1 , Experimental Activity Coefficient of Solute

x_1	T/K	T_{LLE}/K	γ_1	x_1	T/K	T_{LLE}/K	γ_1	x_1	T/K	T_{LLE}/K	γ_1
Dibutyl ether											
0.1521	290.63		5.2	0.3555	303.17	307.77	2.6	0.6150	303.17	303.35	1.5
0.1809	292.65		4.5	0.3907	303.17	307.18	2.3	0.6675	303.17	303.27	1.4
0.2052	294.65		4.1	0.4392	303.17	306.42	2.1	0.7342	303.83		1.3
0.2410	298.23		3.6	0.4853	303.17	305.31	1.9	0.7889	304.37		1.2
0.2823	303.17	305.40	3.3	0.5288	303.17	304.23	1.7	0.8690	306.04		1.1
0.3221	303.17	307.33	2.8	0.5687	303.17	303.44	1.6	1.0000	311.50		1.0

The data considered here.

Method: Dynamic Method / Visual Observation
Precision: 0.1 K

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

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

- 2002 dom koz 0
 - 1,2-dimethylimidazole
 - Sample 1 (cm,98m%,nc;fd,mv;99.8w%,glc)
 - dibutyl ether
 - Sample 1 (cm,99m%,nc;99.8w%,glc)
 - dibutyl ether + 1,2-dimethylimidazole**

1. SELECT the *mixture* 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 screenshot shows a dialog box titled "Property and experimental method for dibutyl ether + 1,2-dimethylimidazole". It contains several fields: "Property group" (set to "Phase transition properties"), "Property" (set to "Quadruple (quintuple) point temperature"), and "Units" (set to "K"). A "Method of measurement" field is also present but empty. At the bottom, there is a "Comment (optional)" text area and "OK" and "Cancel" buttons. Three callout boxes provide instructions: a red box points to the "Property group" dropdown, a blue box points to the "Property" dropdown, and a green box points to the "Units" dropdown.

Property group: Phase transition properties

Property: Quadruple (quintuple) point temperature

Units: K

Method of measurement:

Comment (optional)

OK Cancel

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

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

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

Method selection

Property and experimental method for data set 10: dmth101010

Help

Property group: Phase transition

Property: Quadruple (quintuple)

Units: K

Method of measurement: Other experimental method (please, describe in "Comments")

Experimental purpose: Principal objective of the work

Comment (optional): Dynamic Method with visual observation. See Fluid Phase Equilib., 1986, 26, 201-220.

OK 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 *OK*

Specification of phases and value

Quadruple (quintuple) point temperature

Mixture: dibutyl ether

Sample # 1

Sample # 1

Phase 1: Crystal of pure 1,2-dimethylimidazole

Phase 2: Liquid mixture 2

Phase 3: Liquid mixture 1

Phase 4: Air at 1 atmosphere

Property value: 303.17

Precision: 0.1

No of determinations:

Comment to this record: Dynamic Method with visual observation. See Fluid Phase Equilib., 1986, 26, 201-220.

Property and method

Accept

Cancel

1. SELECT the **Phases for the property value (*Crystal, Liquid 1, Liquid 2, Air at 1 atm*) for the Melting Point**

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

3. CLICK *Accept*

Guided Data Capture - Thermophysical and Thermochemical

File Edit Tools Help

Reference

Compound

Sample

Mixture

[-] 2002 dom koz 0

[-] 1,2-dimethylimidazole

... Sample

[-] dibutyl ether

... Sample 1 (cm.99m%nc::99.8w%alc)

[-] dibutyl ether + 1,2-dimethylimidazole

... ^Z: T (Cp2, L2, L1, air, , Set 1), B Method:OTHER

NOTE: The new *Property* appears below the *Mixture* in the navigation tree.

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.