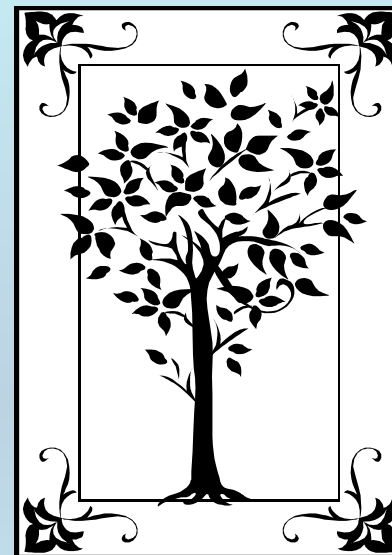


METADATA AND NUMERICAL DATA CAPTURE:
Enthalpy of Vaporization (ΔH_{vap})
(for 1 – Component; 1 Value)

Guided Data
Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Enthalpy of Vaporization (ΔH_{vap})**
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:

1372

J. Chem. Eng. Data 2002, 47, 1372–1378

Vapor Pressures and Enthalpies of Vaporization of Benzyl Halides and Benzyl Ethers

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Molar enthalpies of vaporization $\Delta_1^{\text{g}}H_m^{\text{o}}$ of seven benzyl halides and seven benzyl ethers have been obtained from the temperature dependence of the vapor pressure measured by the transpiration method. These values and the correlation-gas chromatography method, based on Kovat's index, have been applied for the determination of $\Delta_1^{\text{g}}H_m^{\text{o}}$ of three cumyl halides (Cl, Br, and I). The data obtained for $\Delta_1^{\text{g}}H_m^{\text{o}}$ of benzyl derivatives have been checked successfully for internal consistency using enthalpies of formation of alkyl halides and alkyl ethers available from the literature.

Enthalpy of Vaporization Benzyl fluoride

Benzyl Fluoride (1a), $\Delta_{\text{vap}}^{\text{H}}(298.15 \text{ K}) = (46.22 \pm 0.26) \text{ kJ}\cdot\text{mol}^{-1}$

Experimental Method Info :

Derived from vapor pressures
measured by the transpiration method

The screenshot shows the 'Guided Data Capture - Thermophysical and Thermochemical Data' application. The menu bar includes 'File', 'Edit', 'Tools', and 'Help'. Below the menu bar is a tabbed interface with tabs for 'Reference', 'Compound', 'Sample', 'Mixture', 'Reaction', 'Property', and 'Data Tables'. The 'Property' tab is highlighted with a blue box and a blue arrow. In the main workspace, a tree view shows a hierarchy: '2002 kra vas 0' (expanded) -> 'benzyl fluoride' (expanded) -> 'Sample 1 (cm,fd;99.9m% glc)' (selected and highlighted with a red box). A red arrow points from the 'Sample 1' entry to a yellow instruction box. Another yellow instruction box points to the 'Property' tab.

2. *CLICK Property*

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

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 benzyl fluoride

Help

Property group: Phase transition properties

Property: Enthalpy of vaporization or sublimation

Units: kJ/mol

Method of measurement:

Experimental purpose:

Comment (optional)

One data point Cancel

1. SELECT the **Property Group**: *Phase transition properties* from the menu.

2. SELECT the **Property**: *Enthalpy of vaporization or sublimation*, for this example.

3. SELECT the **Units** from the menu: *kJ/mol*, here.

Property and experimental method for benzyl fluoride

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: Derived by Second law

Experimental purpose: Principal objective of the work

2. SELECT the **Experimental Purpose** from the list provided.

Comment (optional)

3. CLICK *One data point*.

One data point

Cancel

1. **SELECT** the condensed **Phase** (liquid or solid); *liquid*, here. The second phase is *gas* by definition of the property.

2. **TYPE** the **Temperature** value and **Uncertainty**, if known.

Substance: benzyl fluoride

Sample # 1

Property set # 1

Phase 1: Liquid

Independent variable: Temperature

Value: 298.15 K

Uncertainty:

Property value: 46.22 kJ/mol

Precision: 0.26

No of determinations:

Property and method

Accept

Cancel

3. **TYPE** the **Property value** and **Uncertainty**, if known.

4. **CLICK**
Accept.

Guided Data Capture - Thermophysical and Thermochemical

File Edit Tools Help

Reference

Compound

[-] 2002 kra vas 0

[-] benzyl fluoride

[-] Sample 1 [cm;fd;99.9m%;glc]

[-] ^F: HVP(L...), Set 1, B Method:SECLAW

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.