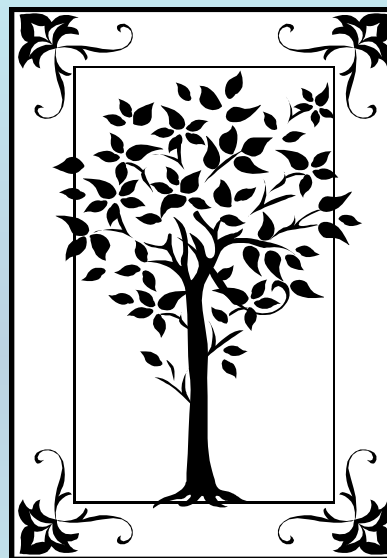


METADATA AND NUMERICAL DATA CAPTURE:

Enthalpy Increments

$$H(T, p) - H(T', p')$$

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Enthalpy Increments** $H(T,p) - H(T',p')$
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:

348

J. Chem. Eng. Data 2000, 45, 348–352

Specific Enthalpy Increments for Pentan-1-ol at Temperatures up to 623.2 K and 10.1 MPa

Christopher J. Wormald* and Gareth F. James

School of Chemistry, University of Bristol, Bristol BS8 1TS, U.K.

Measurements of specific enthalpy increments for pentan-1-ol are reported. A countercurrent water-cooled flow calorimeter was used to measure 102 enthalpy increments over the temperature range 448.2 K to 623.2 K at pressures from 0.1 MPa up to 10.1 MPa. Extrapolation of the gas-phase measurements to zero pressure gave values in excellent agreement with pure component ideal gas enthalpies calculated by extrapolating data on lower alcohols. Values of the specific enthalpy of vaporization derived from the measurements are in agreement with other work and are well fitted by a modification of the Watson equation. A method for the calculation of the two-phase enthalpy–pressure envelope is described.

Enthalpy Increments for Pentan-1-ol as a function of T and p

Table 1. Specific Enthalpy Increments Δh (kJ·kg⁻¹) for Pentan-1-ol Measured Relative to the Saturation Pressure p_s of the Liquid at the Standard Temperature 298.15 K

T K	p MPa	Δh kJ·kg ⁻¹	p MPa	Δh kJ·kg ⁻¹	p MPa	Δh kJ·kg ⁻¹	p MPa	Δh kJ·kg ⁻¹	p MPa	Δh kJ·kg ⁻¹
448.2	0.25	895	0.77	437	4.32	440	6.50	438	9.32	436
473.2	0.20	947	0.46	927	1.13	517	4.36	518	6.63	517
	0.35	937	0.64	527	2.94	519	5.61	517		
498.2	0.17	1005	0.47	995	0.74	970	2.10	600	7.15	604
	0.34	1000	0.57	991	1.20	600	2.78	598	10.1	595
523.2	0.15	1072	0.74	1044	1.35	1013	4.07	696	8.18	691
	0.49	1057	1.10	1022	2.33	703	5.38	690	10.1	685
548.2	0.12	1137	0.77	1123	1.88	1070	3.46	798	5.38	786
	0.52	1117	1.29	1103	2.52	800	4.03	790	8.38	785
573.2	0.11	1185	2.72	1112	3.96	905	5.67	885	7.62	872
	0.77	1175	3.50	918	5.12	889	5.98	883	8.31	871
	1.32	1162	3.75	910	5.23	888	6.63	881	9.50	870
586.2	0.11	1221	3.18	1127	4.50	942	5.67	937	8.31	924
	0.78	1210	3.50	1111	5.12	941	5.98	935	9.52	925
	1.33	1197	3.85	970	5.23	940	6.63	937		
	2.72	1152	3.96	957	5.48	938	7.63	934		
598.2	0.15	1259	4.13	1106	4.71	1015	5.96	957	10.1	966
	1.09	1232	4.32	1079	5.25	995	6.50	981		
	2.59	1200	4.51	1048	5.48	992	8.00	968		
	3.84	1135	4.66	1026	5.62	989	9.26	968		
623.2	0.40	1307	2.56	1274	5.35	1116	8.96	1075		
	1.33	1293	4.00	1222	6.63	1086	10.0	1070		

This data set is considered here.

NOTE: For $T = 298.15$ K,
 $p_{sat} = 0.2$ kPa

Experimental Method and Uncertainty Information:

Enthalpy increments were measured with the counter-current heat-exchange calorimetric apparatus described previously (Wormald and Yerlett, 1985).

Systematic errors on the measurements are estimated to be no greater than $\pm 1 \text{ kJ}\cdot\text{kg}^{-1}$. Random errors arose mainly from fluctuations in the operation of the metering pump supplying the alcohol and were estimated to be $\pm 3 \text{ kJ}\cdot\text{kg}^{-1}$.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

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

2000 wor jam 0
1-pentanol
Sample 1 (cm,99.5m%,nc:)

1. SELECT the *Sample* for which 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 1-pentanol

Help

Property group: Heat capacity and derived properties

Property: Standard enthalpy $H(T)-H(0)$

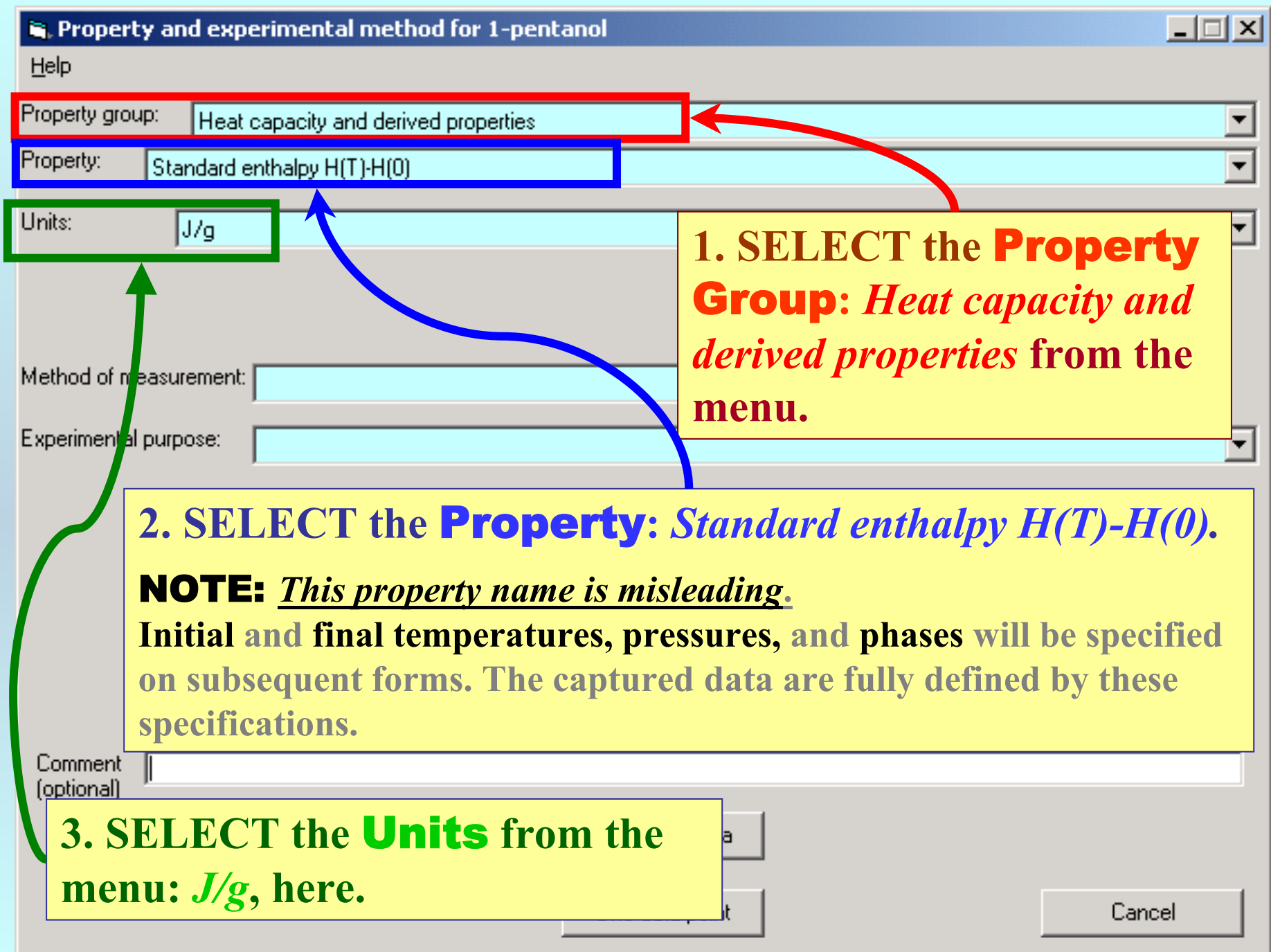
Units: J/g

Method of measurement:

Experimental purpose:

Comment (optional)

Cancel



1. SELECT the **Property Group**: *Heat capacity and derived properties* from the menu.

2. SELECT the **Property**: *Standard enthalpy $H(T)-H(0)$* .
NOTE: *This property name is misleading.*
Initial and final temperatures, pressures, and phases will be specified on subsequent forms. The captured data are fully defined by these specifications.

3. SELECT the **Units** from the menu: *J/g*, here.

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.

Units: J/g

Method of measurement: Flow calorimetry

Experimental purpose: Principal objective of the work

2. SELECT the Experimental Purpose from the list provided.

3. CLICK *2-Variable Data* for the example

Comment (optional): Method described in: Wormald and Yerlett, J. Chem. Thermodyn, 1985, 17, 1171-1186.

1-Variable data **2-Variable data** One data point Cancel

1. SELECT the **Independent variable(s)** with **Units**; *Temperature (K)* and *Pressure (MegaPa)*, here. Include **Uncertainties**, if known.

Substance: 1-pentanol Sample # 1

Independent variable 1
Temperature Units: K Uncert: K %

Independent variable 2
Pressure Units: MegaPa Uncert: MegaPa %

Definition of Measurement Results (Absolute vs Relative)

- Direct value
- Direct value
- Rel. to ref. phase at fixed T and P
- Rel. to ref. phase at fixed T and same P
- Rel. to ref. phase at same T and fixed P
- Rel. to ref. phase at same T and P
- Rel. to ref. phase in equil. with Phase 1
- The reference state described in a comment
- Difference between Upper and Lower T

Phase 1:

Precision of the Property Value(s)

Comment to this record: Method described in: Wormald and Yerlett, J. Chem. Thermodyn, 1985, 17, 1171-1186.

Property and method Numerical Data Cancel

2. SELECT the **Definition of Measurement Results (Absolute vs Relative)** from the menu. Here, SELECT *Rel. to ref. phase at fixed T and P*.

NOTE: Additional fields appear

Standard enthalpy $H(T)-H(0)$ (J/g) as function of 2 variable(s)

Substance: 1-pentanol Sample # 1

Independent variable 1
Temperature Units: K Uncert: K %

Independent variable 2
Pressure Units: MegaPa Uncert: MegaPa %

Definition of Measurement Results (Absolute vs Relative)

Rel. to ref. phase at fixed T and P Relation: Difference X-Xref

Reference T: 298.15 K Reference pressure: 0.2 kPa Reference phase: Liquid

Data presentation

ENTER the:

- (1) **Reference T** in K (298.15, here)
- (2) **Reference pressure** in kPa (0.2, here)

SELECT the:

- (1) **Reference phase** (*Liquid*, here)
- (2) **Relation** (*Difference X-Xref*, for enthalpy increments)

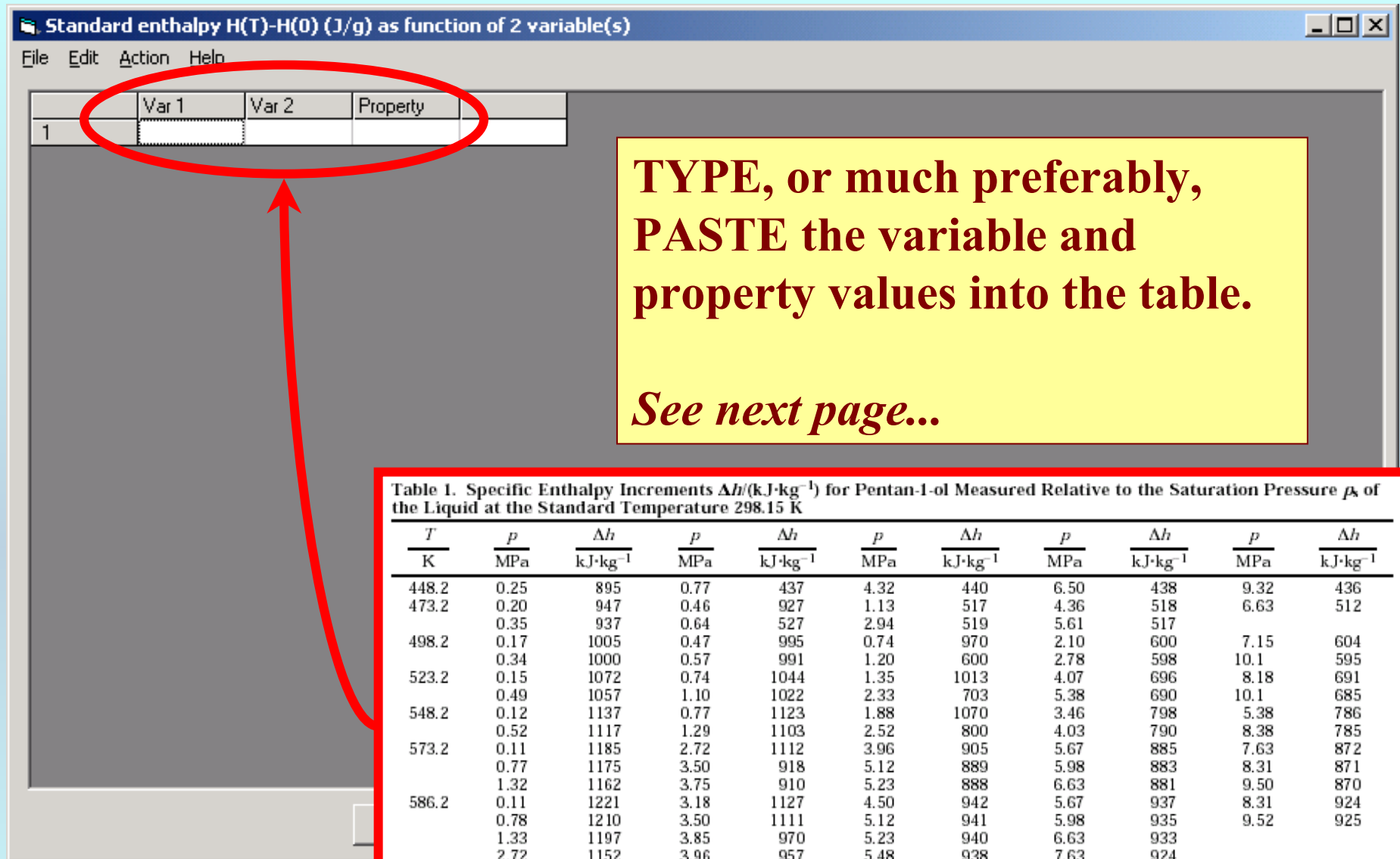
1. SELECT the **Data presentation** method, *Experimental values*

2. SELECT **Phase 1** (i.e., the phase associated with **Independent variables**: *Liquid*, here).

3. ENTER the **Precision of the Property Value(s)**, if known.

4. CLICK *Numerical Data*

The image shows a software window for data entry. At the top right, there is a 'Sample #' dropdown menu set to '1'. Below this, there are two 'Independent variable' fields: 'Temperature' and 'Pressure'. The 'Definition of Measurement Results' section includes a dropdown for 'Rel. to ref. phase at fixed T and P', a 'Relation' dropdown set to 'Difference X-Xref', and input fields for 'Reference T: 298.15 K', 'Reference pressure: 0.2 kPa', and 'Reference phase: Liquid'. The 'Data presentation' dropdown is highlighted with a red box and contains 'Experimental values'. Below it, 'Property set #' is '1' and 'Constraint' is 'Single phase'. The 'Phase 1:' dropdown is highlighted with a blue box and contains 'Liquid'. The 'Precision of the Property Value(s)' section has a text input field with '3', a radio button selected for 'J/g', and another radio button for '%'. At the bottom, there is a 'Comment to this record:' field with a text entry. The 'Numerical Data' button is highlighted with a green box. A red arrow points from the first callout to the 'Data presentation' dropdown. A blue arrow points from the second callout to the 'Phase 1:' dropdown. A black arrow points from the third callout to the 'Precision of the Property Value(s)' section. A green arrow points from the fourth callout to the 'Numerical Data' button.



**TYPE, or much preferably,
PASTE the variable and
property values into the table.**

See next page...

Table 1. Specific Enthalpy Increments Δh /(kJ·kg⁻¹) for Pentan-1-ol Measured Relative to the Saturation Pressure p_s of the Liquid at the Standard Temperature 298.15 K

T K	p MPa	Δh kJ·kg ⁻¹	p MPa	Δh kJ·kg ⁻¹	p MPa	Δh kJ·kg ⁻¹	p MPa	Δh kJ·kg ⁻¹	p MPa	Δh kJ·kg ⁻¹
448.2	0.25	895	0.77	437	4.32	440	6.50	438	9.32	436
473.2	0.20	947	0.46	927	1.13	517	4.36	518	6.63	512
498.2	0.35	937	0.64	527	2.94	519	5.61	517		
	0.17	1005	0.47	995	0.74	970	2.10	600	7.15	604
523.2	0.34	1000	0.57	991	1.20	600	2.78	598	10.1	595
	0.15	1072	0.74	1044	1.35	1013	4.07	696	8.18	691
548.2	0.49	1057	1.10	1022	2.33	703	5.38	690	10.1	685
	0.12	1137	0.77	1123	1.88	1070	3.46	798	5.38	786
573.2	0.52	1117	1.29	1103	2.52	800	4.03	790	8.38	785
	0.11	1185	2.72	1112	3.96	905	5.67	885	7.63	872
586.2	0.77	1175	3.50	918	5.12	889	5.98	883	8.31	871
	1.32	1162	3.75	910	5.23	888	6.63	881	9.50	870
598.2	0.11	1221	3.18	1127	4.50	942	5.67	937	8.31	924
	0.78	1210	3.50	1111	5.12	941	5.98	935	9.52	925
598.2	1.33	1197	3.85	970	5.23	940	6.63	933		
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623.2	0.15	1259	4.13	1106	4.71	1015	5.96	987	10.1	966
	1.09	1232	4.32	1079	5.25	995	6.50	981		
623.2	2.59	1200	4.51	1048	5.48	992	8.00	968		
	3.84	1135	4.66	1026	5.62	989	9.26	968		
623.2	0.40	1307	2.56	1274	5.35	1116	8.96	1075		
	1.33	1293	4.00	1222	6.63	1086	10.0	1070		

Standard enthalpy $H(T)-H(0)$ (J/g) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	448.2	0.25	895
2	448.2	0.77	437
3	448.2	4.32	440
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5	448.2	9.32	436
6	473.2	0.20	947
7	473.2	0.35	937
8	473.2	0.46	927
9	473.2	0.64	527
10	473.2	1.13	517
11	473.2	2.94	519
12	473.2	4.36	518
13	473.2	5.61	517
14	473.2	6.63	512
15	498.2	0.17	1005
16	498.2	0.34	1000
17	498.2	0.47	995
18	498.2	0.57	991
19	498.2	0.74	970
20	498.2	1.20	600
21	498.2	2.10	600
22	498.2	2.78	598
23	498.2	7.15	604
24	498.2	10.10	595
25	523.2	0.15	1072




Table 1. Specific Enthalpy Increments Δh /(kJ·kg⁻¹) for Pentan-1-ol Measured Relative to the Saturation Pressure p_s of the Liquid at the Standard Temperature 298.15 K

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623.2	1.33	1293	4.00	1222	6.63	1086	10.0	1070		

Clear the

NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)

Standard enthalpy $H(T)-H(0)$ (J/g) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	448.2	0.25	895
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Clear the Table

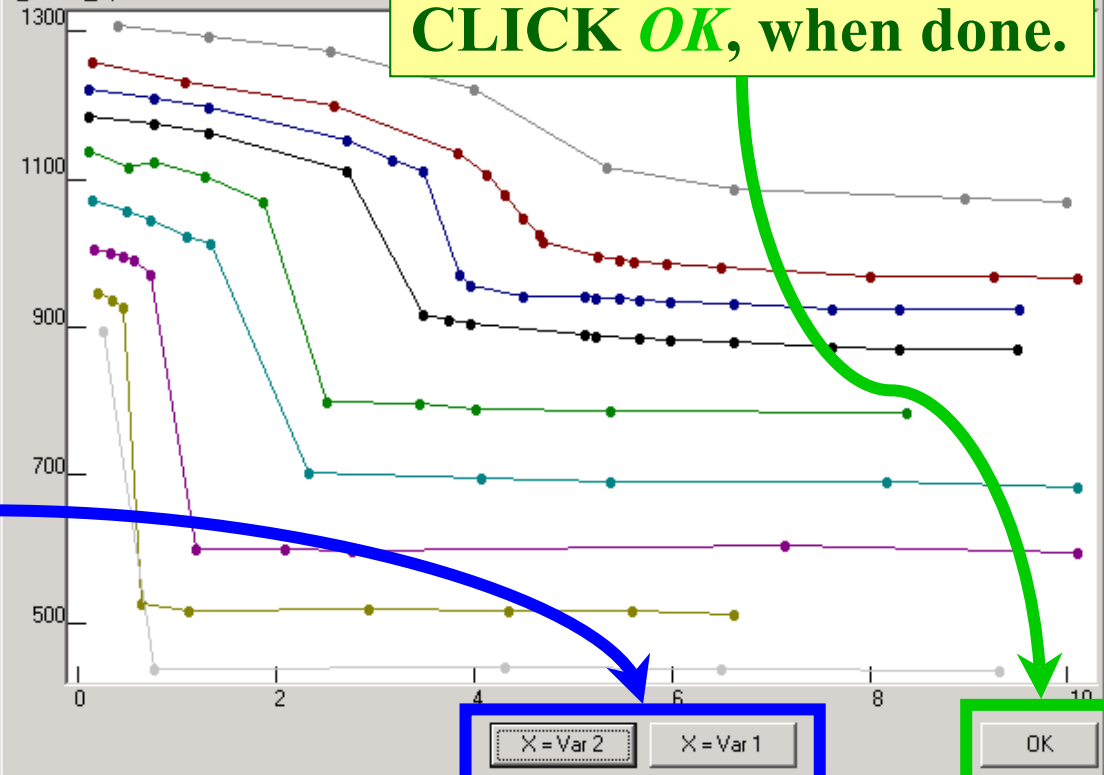
1. **CLICK *View plot*** to see a graphical representation of the data.

View plot

2. **SELECT** alternative plotting variables to optimize the view.

Standard enthalpy $H(T)-H(0)$ as fu

Tools Help



3. Check for typographical errors. **CLICK *OK***, when done.

X = Var 2

X = Var 1

OK

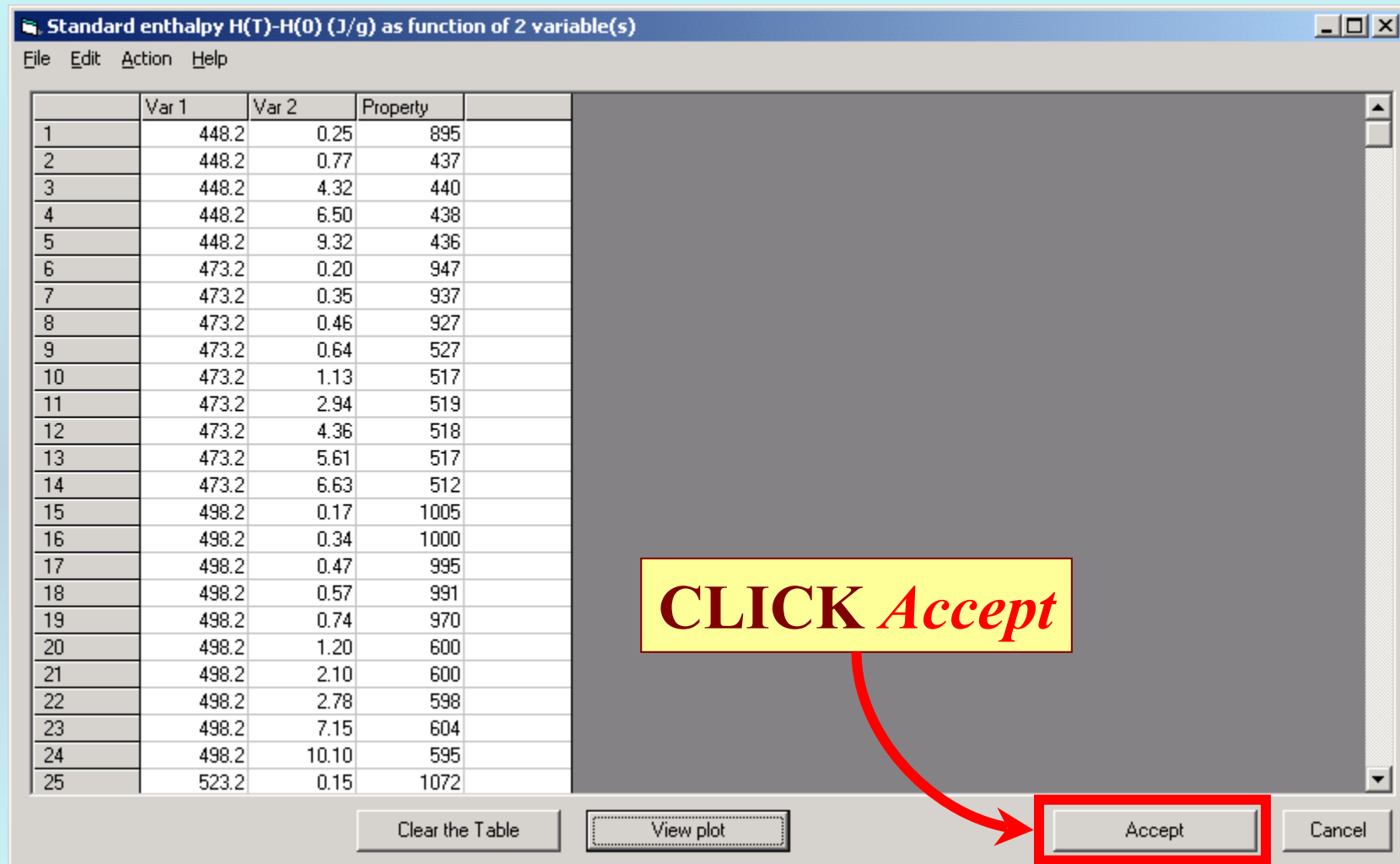
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File Edit Action Help

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23	498.2	7.15	604
24	498.2	10.10	595
25	523.2	0.15	1072

CLICK *Accept*

Clear the Table View plot **Accept** Cancel



Guided Data Capture - Thermophysical and Thermochemical

File Edit Tools Help

Reference

Compound

NOTE: The new data set appears in the tree under the appropriate *Sample*.

[-] 2000 wor jam 0

[-] 1-pentanol

[-] Sample 1 (cm,99.5m%,nc::)

^2: H (L), Set 1, B Method:FLOW dH=3

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.