

MKS 04-0001

Common Terms and Operations

Molecular Knowledge Systems
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ρ	ΔH_v	T_c	ΔG
η_l	D_{ab}	γ_{12}	Tf_{cc}
δ_h	P_{vp}	σ	C_p
T_b	λ_v	S_f	P_c

Helpful Prerequisites

Introductory Course

This course does not require any prerequisite courses. However, general knowledge of physical property estimation, chemical structures and computer applications is expected.

Additional Resources

1. Estimating the Properties of Chemicals ([video](#))
2. Estimating the Properties of Mixtures ([video](#))

Topics Presented

Common Operations

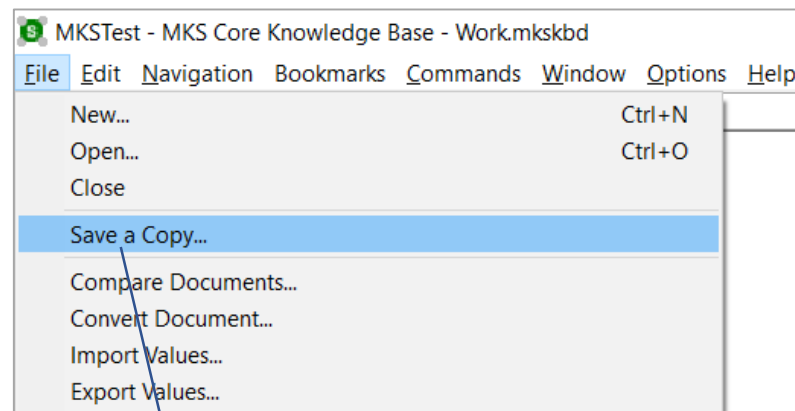
This course presents several terms and operations that are repeatedly used throughout Cranium and Synapse. These operations include navigation, editing data values, copying and pasting values, choosing units of measure, changing number formatting and printing.

- Basic Terminology
- Navigation
- Adding and Deleting Pages
- Editing Property Values
- Editing Special Characters
- Editing All Data Values
- Copying and Pasting Values
- Choosing Units of Measure
- Number Formatting
- Printing

Create a Working Copy

The actions taught in this course will permanently change the contents of the database file being used. It is highly recommended that a 'working copy' of a knowledge base be used.

To create a working copy, open a knowledge base and then select the Save a Copy command from the File menu. Enter a name for the working copy. Open and use the working copy once the copy operation is complete.



Save a copy of a knowledge base to be used for practice and experimentation.

Terminology: Document Window Structure

Document windows are divided into several sub-windows called panes. A typical window contains the following panes:

1. Chapters Pane
2. Identifier Pane
3. Data Pane
4. Status Pane

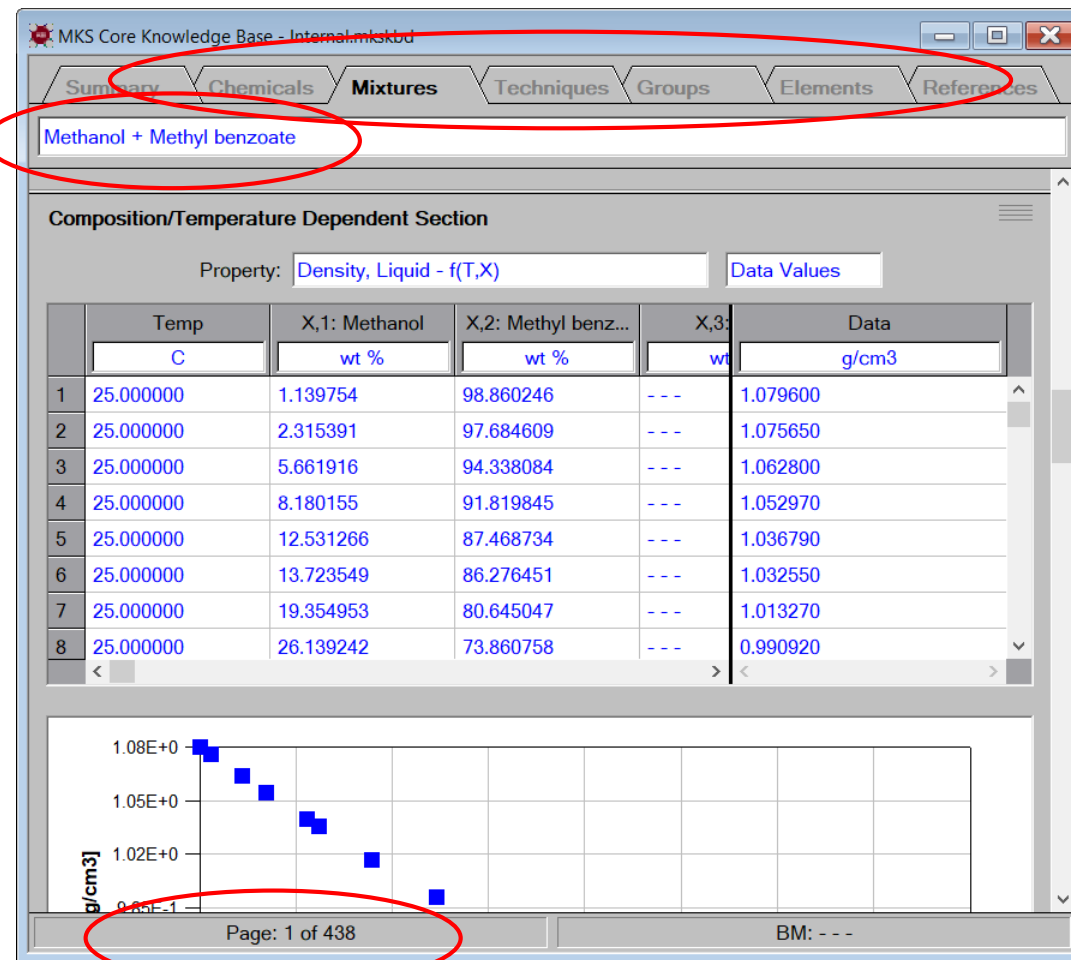
The screenshot displays the 'MKS Core Knowledge Base - Internal.mkskbd' window. The interface is divided into several panes, with four numbered callouts:

- 1**: Points to the 'Chapters Pane' at the top, which includes tabs for 'Summary', 'Chemical', 'Mixtures', 'Techniques', 'Groups', 'Elements', and 'References'.
- 2**: Points to the 'Identifier Pane' below the tabs, containing the text 'Trifluoroiodomethane'.
- 3**: Points to the 'Data Pane' in the center, which displays a chemical structure diagram of trifluoroiodomethane (I-CF₃).
- 4**: Points to the 'Status Pane' at the bottom, which shows 'Page: 411 of 2548' and 'BM: ---'.

Terminology: Reference Book Analogy

Documents are presented in a format analogous to a printed reference book:

1. Documents are divided into chapters
2. Chapters contain pages.
3. Each page contains data and attributes about a single entity.



Terminology: Entities

Cranium and Synapse and their documentation often use the term “entity” to refer to the objects used in each application. Examples of entities are shown in the lists to the right. Entities are typically displayed in document chapters.

Entity Examples	
Combinatorial Design	XY Data Set
Graphical Design	XY Graph
Triangular Graph	Function
Technique	Element
Reference	Mixture
Chemical	Report
Bookmark	Group

Navigation: Terminology

Document windows are divided into several sub-windows called panes. A typical window contains the following panes:

1. Chapters Pane
2. Identifier Pane
3. Data Pane
4. Status Pane

The screenshot displays the 'MKS Core Knowledge Base - Internal.mkskbd' window. The interface is divided into several panes, with four numbered callouts: 1. 'Chapters Pane' (Navigation tabs: Summary, Chemical, Mixtures, Techniques, Groups, Elements, References); 2. 'Identifier Pane' (Search bar containing 'Trifluoroiodomethane'); 3. 'Data Pane' (Chemical Structure Section containing a chemical structure of trifluoroiodomethane, CI(F)(F)F); 4. 'Status Pane' (Page: 411 of 2548, BM: ---).

Navigation: Chapters and Pages

Because Cranium and Synapse's user interface is analogous to a printed reference book, navigation typically consists of changing chapters and turning pages.

Chapters

The screenshot shows the MKS Core Knowledge Base interface. At the top, there is a navigation bar with tabs for Summary, Chemicals, Mixtures, Techniques, Groups, Elements, and References. The 'Mixtures' tab is selected and circled in red. Below the navigation bar, the search bar contains 'Methanol + Methyl benzoate'. The main content area is titled 'Composition/Temperature Dependent Section' and shows a table of density data for a liquid mixture at 25.000000 C. The table has columns for Temp (C), X,1: Methanol (wt %), X,2: Methyl benz... (wt %), X,3: (wt %), and Data (g/cm3). Below the table is a scatter plot of density vs. composition. At the bottom of the interface, the page number 'Page: 1 of 438' is circled in red.

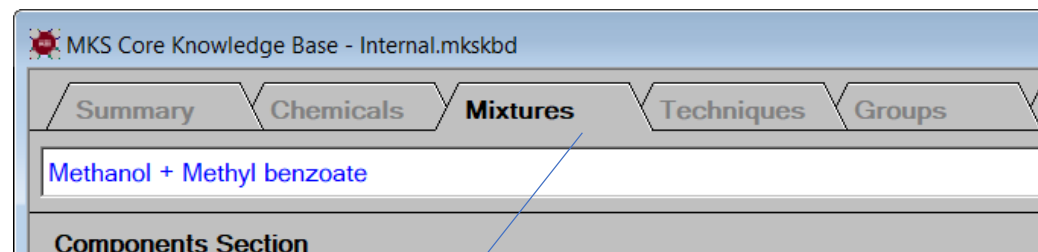
Pages

	Temp C	X,1: Methanol wt %	X,2: Methyl benz... wt %	X,3: wt %	Data g/cm3
1	25.000000	1.139754	98.860246	---	1.079600
2	25.000000	2.315391	97.684609	---	1.075650
3	25.000000	5.661916	94.338084	---	1.062800
4	25.000000	8.180155	91.819845	---	1.052970
5	25.000000	12.531266	87.468734	---	1.036790
6	25.000000	13.723549	86.276451	---	1.032550
7	25.000000	19.354953	80.645047	---	1.013270
8	25.000000	26.139242	73.860758	---	0.990920

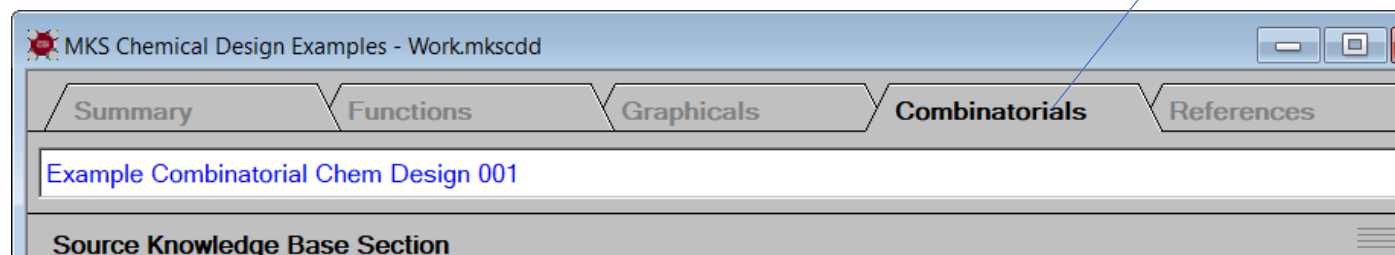
Page: 1 of 438

Navigation: Changing Chapters

To change to a different chapter simply click the left mouse button on the chapter's tab.

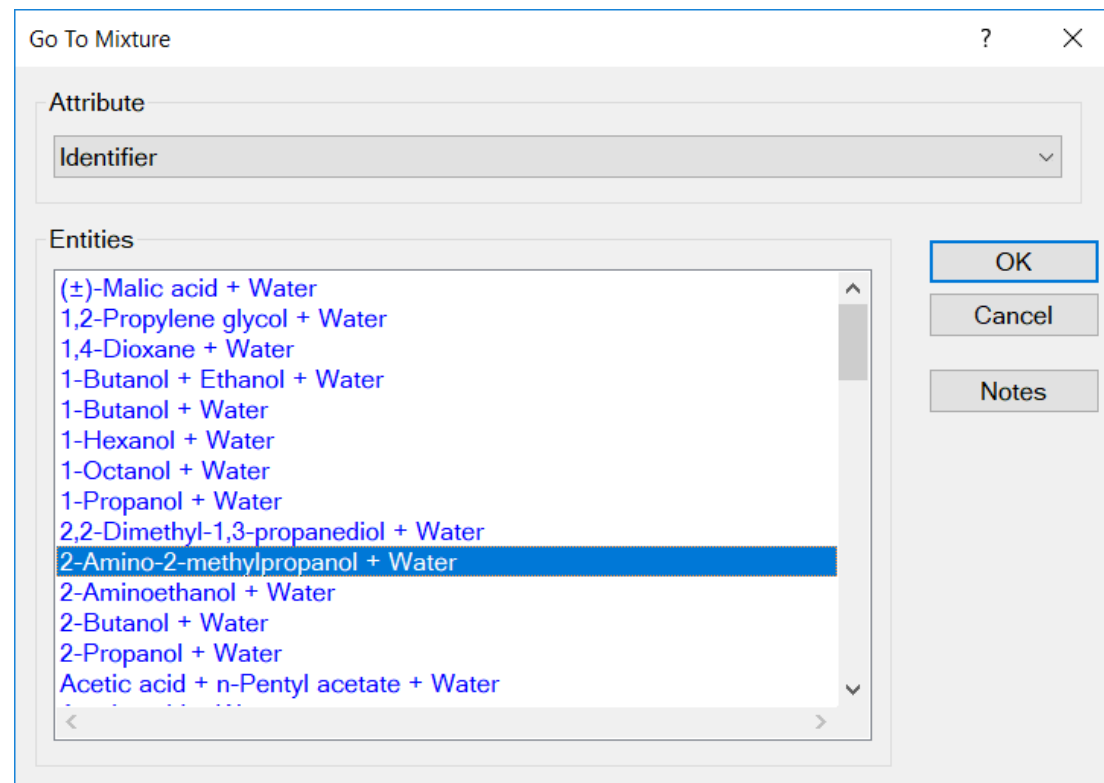
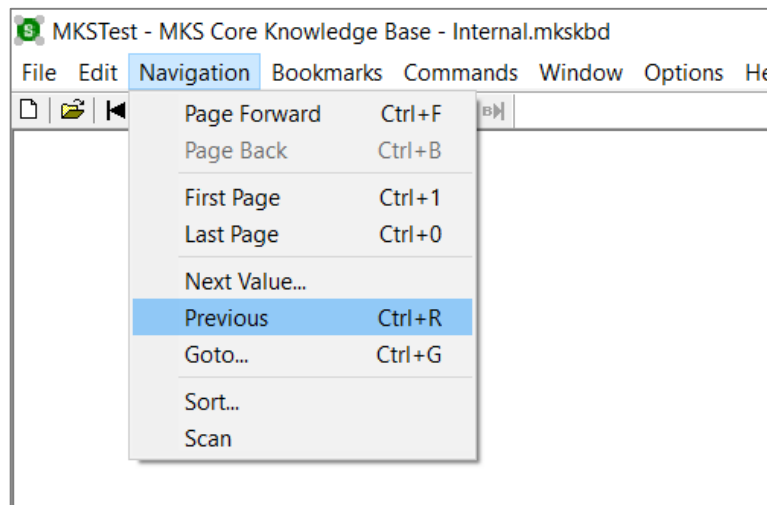


Click the left mouse button on the chapter's tab



Navigation: Changing Pages

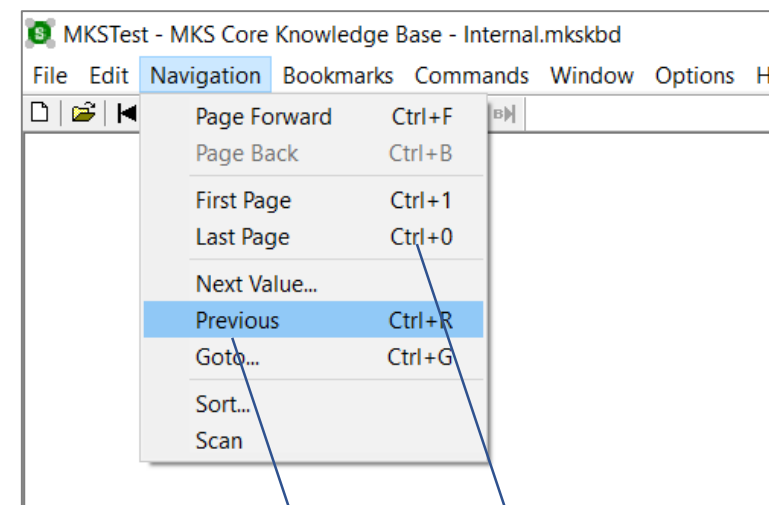
From within a chapter, changing to a new page can be done using menu commands, toolbar buttons or keyboard shortcuts.



Navigation: Menu Commands and Shortcuts

Every chapter of every document has a Navigation menu. The menu's commands allow you to page forward and backward through the chapter. (If the chapter has no pages or only one page then most commands will be disabled.)

Associated with many menu commands is a keyboard shortcut shown to the right of each command.



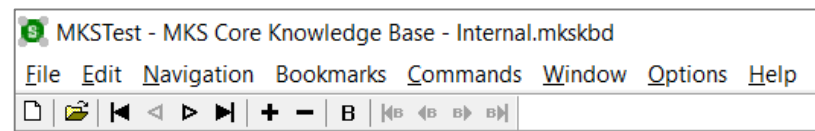
Keyboard Shortcut

Menu Command

Navigation: Toolbar Buttons

The toolbar contains four navigation buttons enabling. Simply pressing the button will run the navigation command.

Toolbar buttons may be disabled if the navigation operation cannot be performed, e.g., you cannot go back one page if you are on the first page of the chapter.

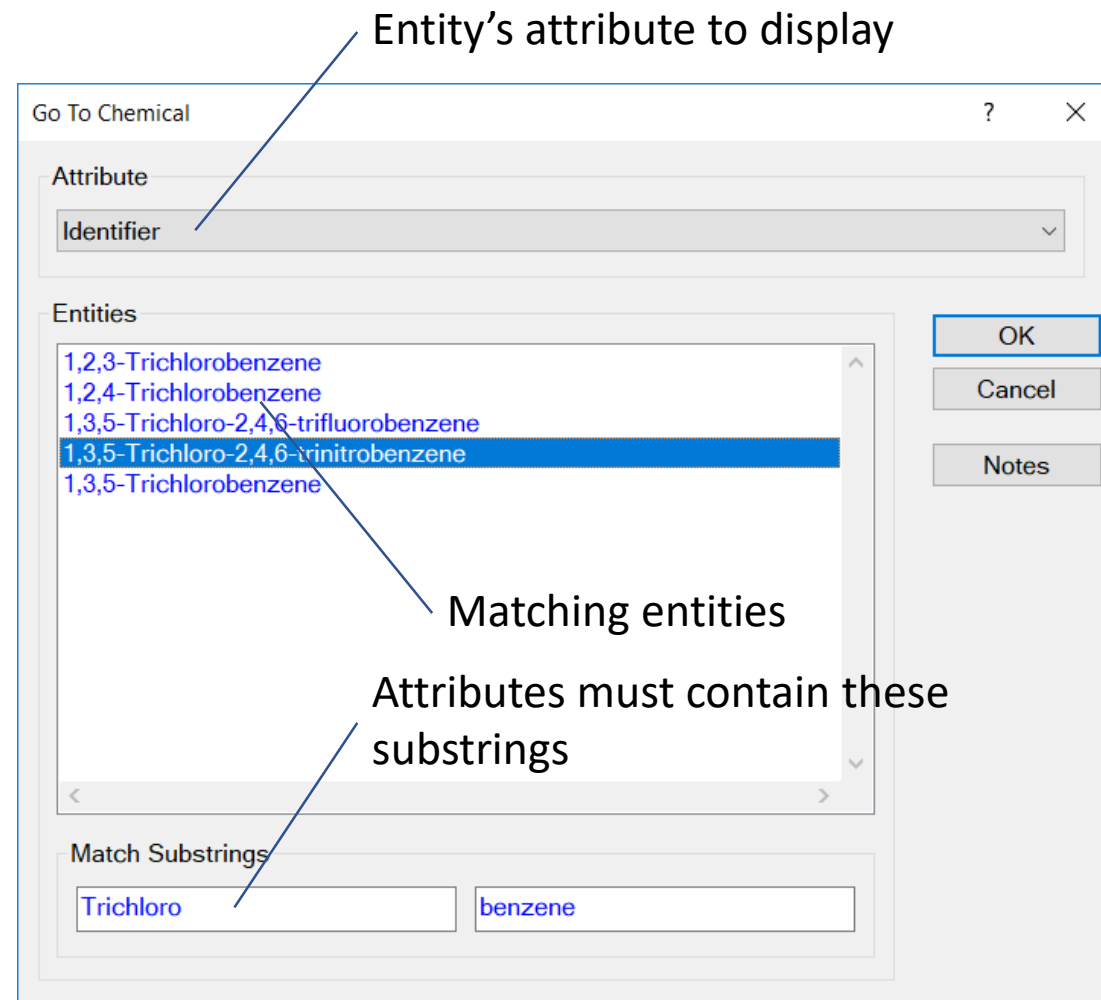


- Go to the last page
- Go forward one page
- Go back one page
- Go to the first page

Navigation: Go To Entity Dialog

The Go To Entity dialog gives you the ability to change to any page within the current document. You can select the page using the entity's name or, depending upon the entity's type, another attribute.

For example, the Go To Dialog for the Chemicals chapter enables you to select by name, formula, synonym, etc.



Navigation: Scan Dialog

The Navigation Menu's Scan command activates the Scan Dialog. This dialog will page forward through the current chapter displaying each entity.

The speed at which pages are turned can be controlled by the dialog's slider control.

MKS Core Knowledge Base - Internal.mkskbd

Summary Chemic... Mixtures Techniq... Groups Elements Referen...

4-(4-Methoxyphenyl)-2-butanone

Descriptive Information Section

Formula: C11H14O2 CAS #: 104-20-1

Beilstein: --- EC #: 203-184-2

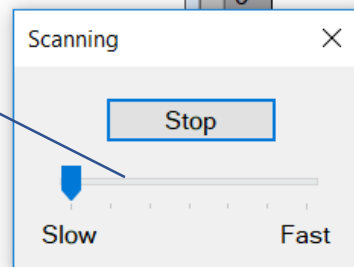
RTECS #: EL9085500 Merck: ---

Synonyms Section

1	Anisylacetone
2	FEMA Number: 2672
3	Flavis Number: 7.029
4	---
5	---

Page: 175 of 2548 BM: ---

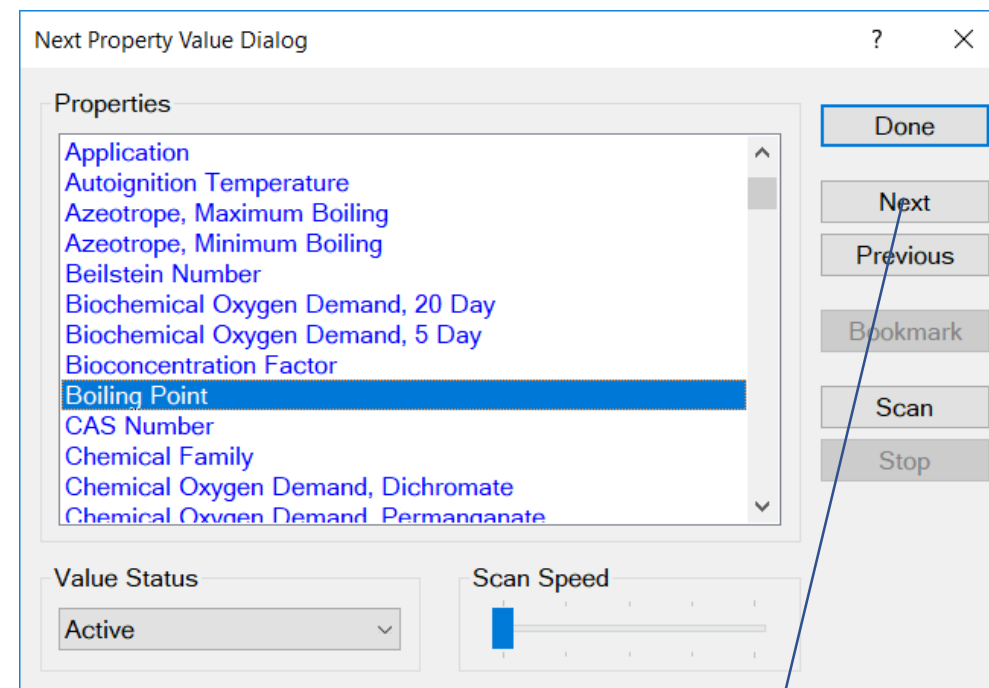
Speed control



Each page of the current chapter is shown

Navigation: Next Value Dialog

The Navigation Menu's Next Value command activates the Next Value dialog. This dialog enables you to go forward or backward to the next entity that has a value for the selected property.

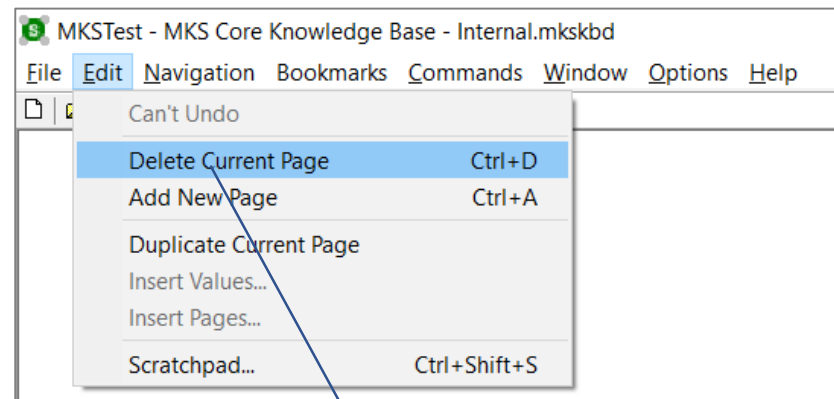


Pressing the Next button will display the next chemical that has a value for the normal boiling point.

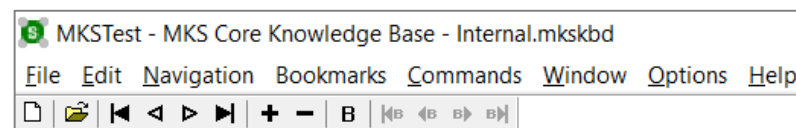
Adding and Deleting Pages

To add a new entity to a document's chapter you simply insert a new, blank page and then enter the entity's information on that page.

Adding and deleting pages can be done using Edit menu commands, toolbar buttons and keyboard shortcuts.



Add and delete pages using the Edit Menu's commands



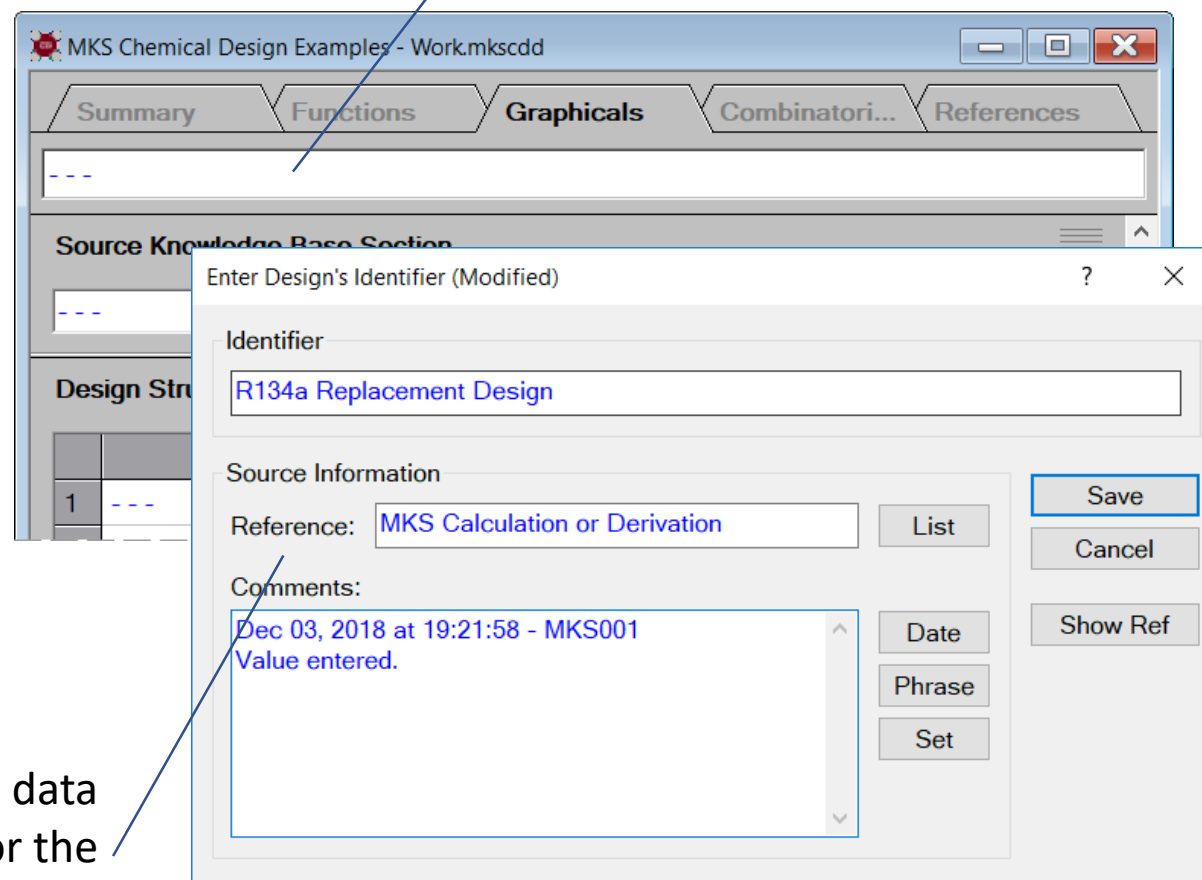
Delete the current page
Add a new blank page

Editing Property Values

After adding a new page you must enter property values. Property values are displayed in fields, tables and graphs.

To edit any of these property values, simply click the left mouse button on the field, table or graph.

Click the left mouse button on a field, table or graph to edit its associated property.



The application activates a data entry dialog tailored for the property being edited.

Data Entry Dialogs

Dialogs used for editing values typically have commands tailored for the particular property being edited. In addition, these dialogs perform numerous checks to ensure the values being entered are valid.

Values for the temperature, pressure and composition are checked for validity.

Enter the Mixture's Density, Liquid - f(T,P,X)

Composition (in original units) Units: mol frac

Methanol	X: 0.4983	±	
n-Butylamine	X: 0.5017	±	
---	X:	±	

Molality/Molarity, Solvent: n-Butylamine

Molarity, Solution Density: kg/m3

Datum (in original units)

Temp: 298.15 ± Units: K

Pres: 159.6 ± Units: bar

Value: 0.777200 ± 0.0001 Units: g/cm3

Source Information

Reference: Papaioannou + Bridakis + Panayiotou (1993) List

Comments: Jul 16, 2013 at 12:45:05 - MKS001 Value entered.

Date Phrase Set

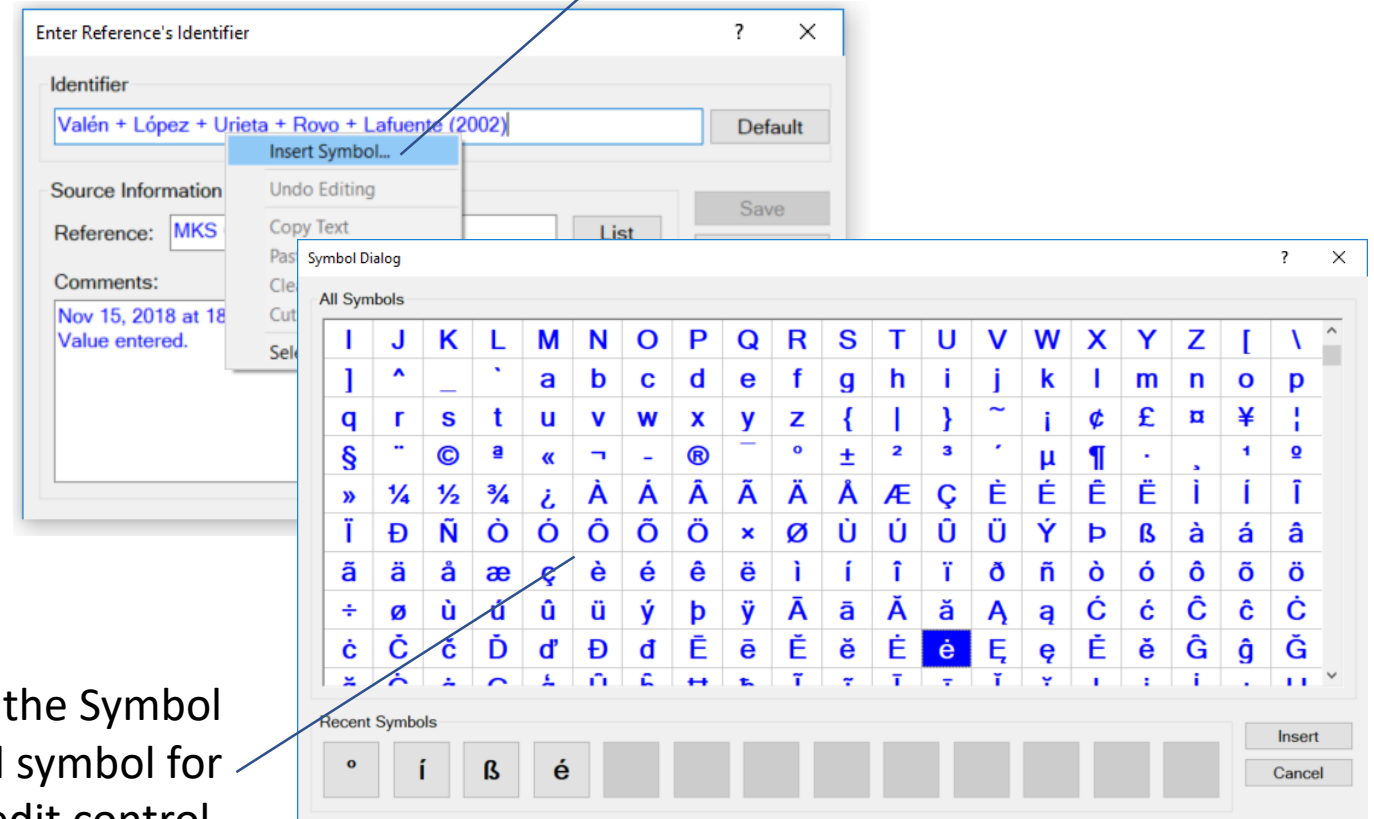
OK OK & Next Cancel X Default X Total Show Ref

Tailored commands for each property.

Editing Special Characters

Special characters can be entered into an edit control by clicking the right mouse button and selecting the Insert Symbol menu command.

Click the right mouse button in an edit control and select the Insert Symbol command.

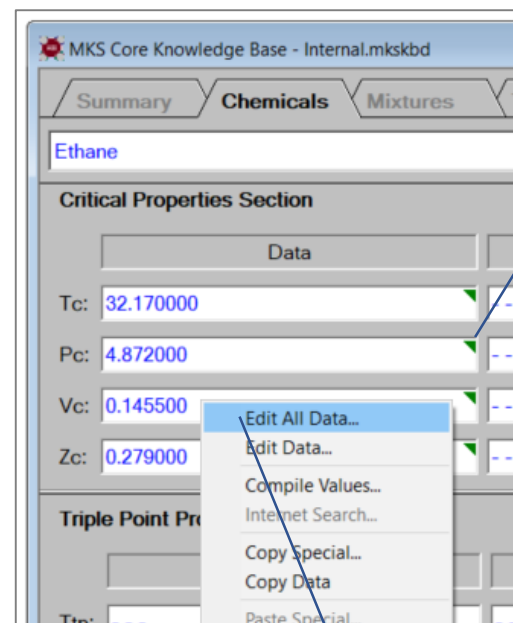


The application activates the Symbol dialog. Select a special symbol for insertion into the edit control.

Editing All Data

It is very common that multiple values are available for a property's value. For example, many researchers have measured the boiling point of acetone.

Click the right mouse button in a field and choose the Edit All Data command to enter multiple property values.



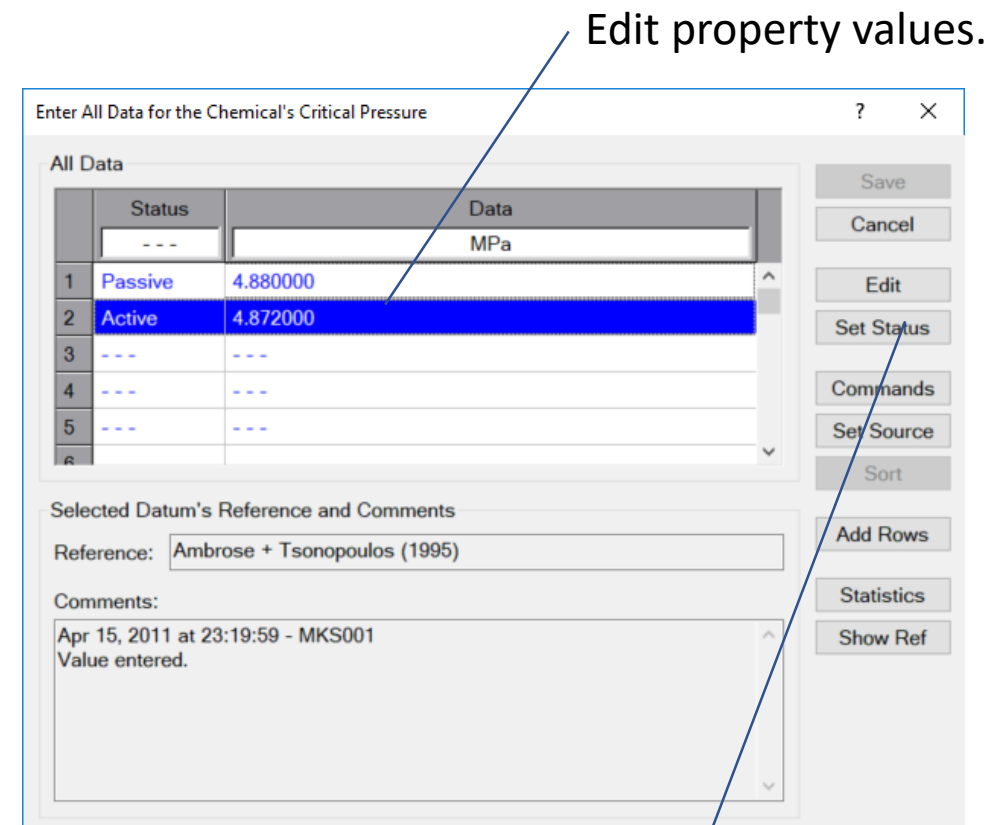
A green triangle in a field's upper right corner indicates that additional data is available for the property.

Select the Edit All Data command to add property values having different status.

Editing All Data

Cranium and Synapse can store property values having four status values: active; passive; rejected; unknown.

Click the right mouse button on a field or table and select the Edit All Data command to activate the Edit All Data dialog. This dialog enables you to enter property values and set their status.



Press the status button to change the status of the selected data to active, passive, rejected or unknown.

Copying and Pasting Values

Property values must often be copied from one application and pasted into Cranium or Synapse. Clicking the right mouse button on a field, table or graph activates a commands window the provides several copy and paste commands.

Click the right mouse button to activate a menu containing copy and paste commands.

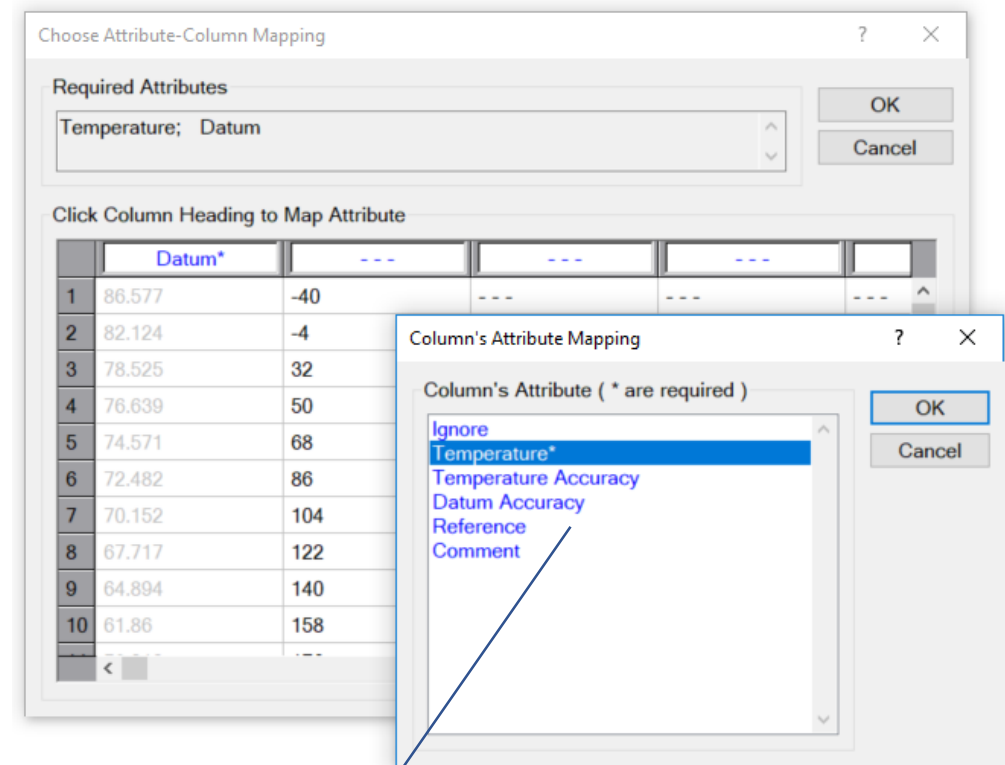
The screenshot shows the 'MKS Core Knowledge Base - Internal.mkskbd' window. The 'Chemicals' tab is active, and 'Ethane' is selected. The 'Temperature Dependent Section' is displayed, showing a table of density values for 'Density, Liquid - f(T)'. The table has two columns: 'Temp (C)' and 'Data (kg/m3)'. A context menu is open over the table, with 'Copy Data' selected. Below the table is a graph showing the density values plotted against temperature.

	Temp (C)	Data (kg/m3)
1	-173.150000	641.717856
2	-168.150000	636.236095
3	-163.150000	630.706222
4	-159.750000	623.600000
5	-158.150000	625.236489
6	-153.750000	617.100000
7	-153.150000	619.508154
8	-149.950000	610.500000
9	-148.150000	613.087300

Copying and Pasting Values

Values must often be pasted in a very specific order. For example, liquid density must be entered as set of temperature, value pairs.

The Paste Special menu command activates the Paste Special dialog that enables you to associate attributes with different data columns.



Use the Paste Special functionality to associate attributes with specific columns of data values.

Scratchpad Dialog

Sometimes copied values must be significantly rearranged before they can be pasted. The Edit menu's Scratchpad command activates the Scratchpad dialog that provides functionality for values rearrangement.

Scratchpad Dialog

	01	02	03	04	05
1	42.264	376.347	---	---	---
2	42.259	376.335	---	---	---
3	51.089	489.000	---	---	---
4	51.076	489.029	---	---	---
5	51.099	489.001	---	---	---
6	51.081	488.901	---	---	---
7	58.467	601.034	---	---	---
8	58.394	600.886	---	---	---
9	---	64.962	720.591	---	---
10	---	64.907	720.290	---	---
11	---	64.889	719.912	---	---
12	---	64.868	717.043	---	---
13	---	64.860	717.024	---	---
14	---	76.442	962.158	---	---
15	---	76.369	962.054	---	---
16	---	76.350	962.152	---	---

Text Delimiters: Tab Space Comma Semicolon Period

Paste Delimiter Options: Process consecutive delimiters as one

Done Edit Replace Clear Clear All Undo Cut Copy Paste Transpose Function Statistics Regress Add Rows Add Columns

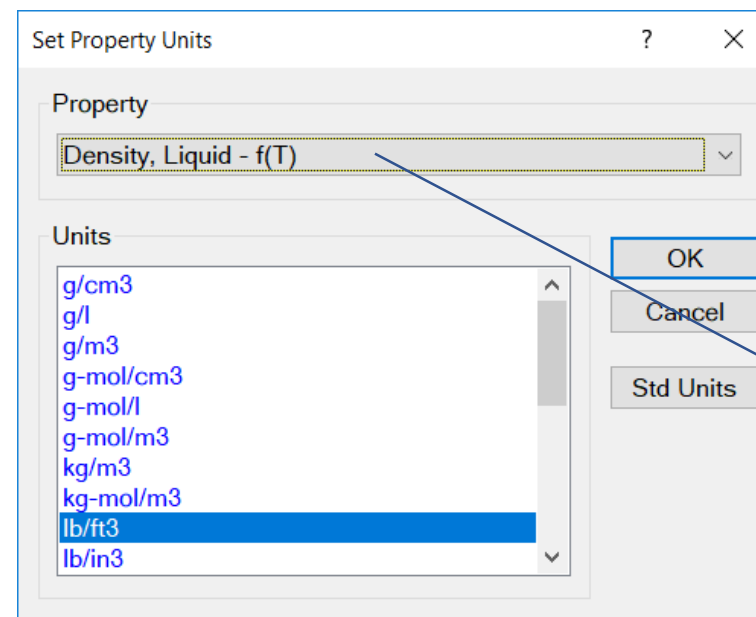
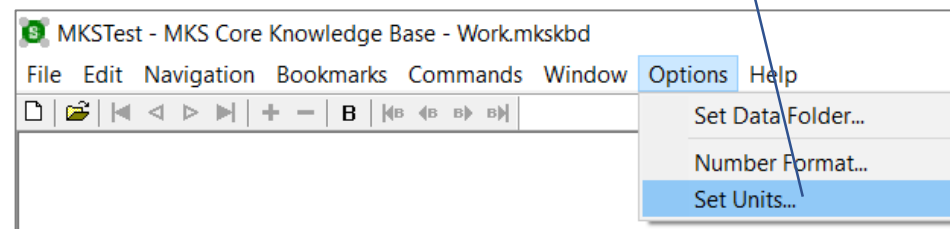
Use the Scratchpad Dialog to rearrange data values before pasting.

Choosing Units of Measure

Data values are stored in their original units. However, the units in which values are displayed are specified by the user.

Selecting the Set Units command from the Options menu will activate the Set Property Units dialog. Select the property and its desired units of measure.

Select the Set Units command from the Options menu to assign units of measure.



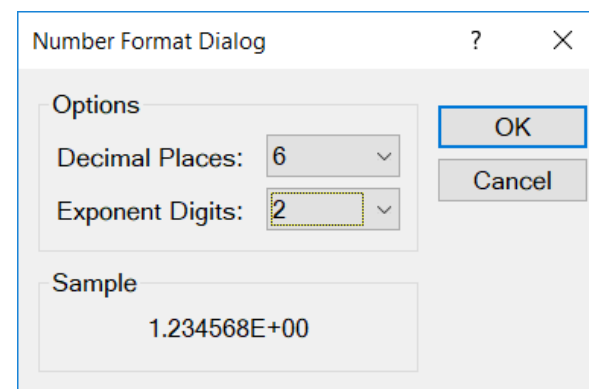
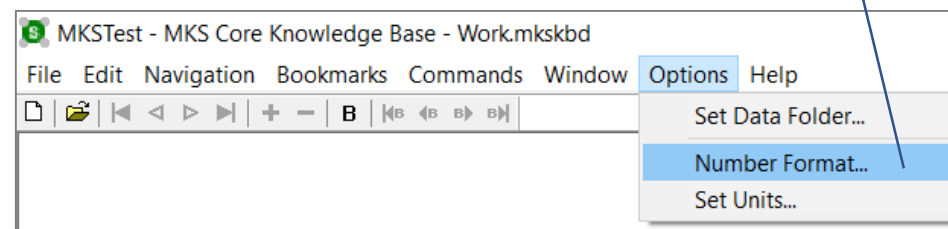
Select a property and its desired units of measure.

Number Formatting

The format of displayed numbers, e.g., the number of decimal places, is changed by selecting the Number Format command from the Options menu.

The Number Format command activates the Number Format dialog enabling you to choose the number of decimal places and exponent digits in displayed values.

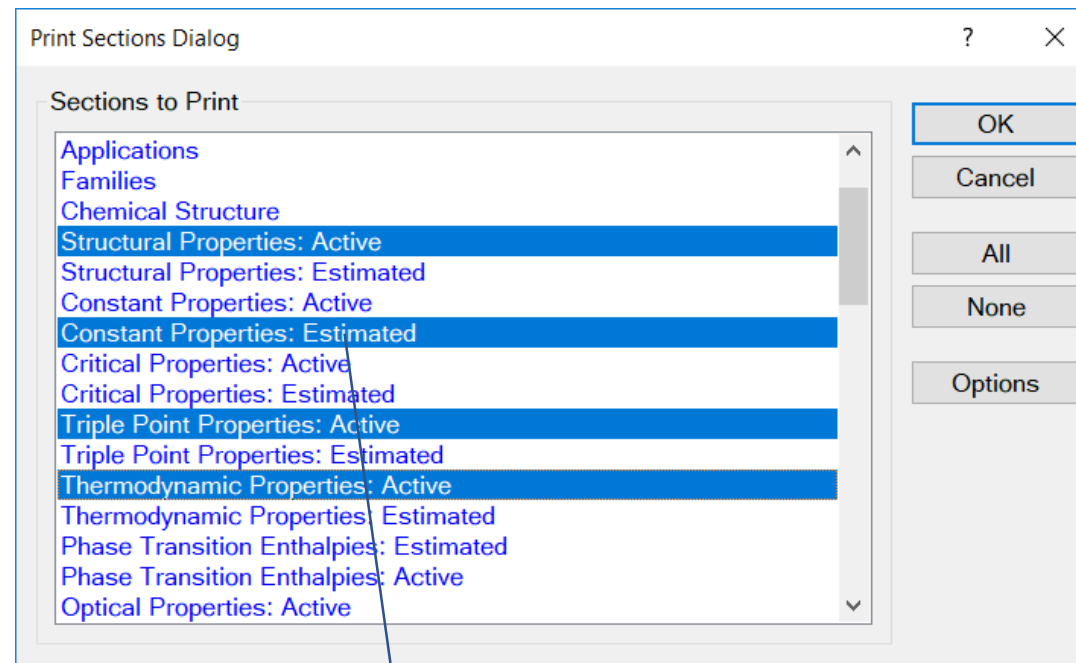
Select the Number Format command to change the format of displayed values.



Printing

Each document provides commands for page setup, print preview and printing. A standard report format is used to print data, estimates, molecular structure, graphs, etc.

When the Print command is selected from the File menu, the application will request the sections to be printed.



First select those sections who values you wish to print. Pressing the OK button will print the selected sections.

Printing

Selecting the Print Preview command will also activate the Print Section dialog. However, selecting the desired sections and pressing the OK button will not print those sections. Instead a preview of the printed page will be displayed in the document's window.

The screenshot shows a software window titled "MKS Core Knowledge Base - Work.mkskbd". At the top, there is a toolbar with buttons for "Print..", "Next Page", "Prev Page", "Two Page", "Zoom In", "Zoom Out", and "Close". The main content area displays the following information:

(+)-1-Phenylethanol

Synonyms:

Value	Reference
FEMA Number: 2685	1
Flavis Number: 2.064	1
Methyl phenyl carbinol	1

Chemical Structure

Constant Properties: Active

Property	Value	Units	Reference
Dipole Moment	1.510954	debye	2
Acentric Factor	---	---	---
Molecular Weight	122.167000	---	2
Melting Point	19.500000	C	2
Boiling Point	204.000000	C	2
Glass Transition Temperature	---	K	---
Radius of Gyration	4.131000E-10	m	2

References

- 1) "Sigma-Aldrich Chemical Catalog."
- 2) T.E. Daubert and R.P. Danner. "Physical and Thermodynamic Properties of Pure Chemicals." Hemisphere Publishing Corporation, Washington, DC, USA, Year 1982.

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Questions or Comments

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Thank You