

The **Compound** module

- Use **Compound** for the administration of a private compound database, i.e. enter, edit, delete pure substance data in a database.

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The *Compound* module



- Click on *Compound* in the main *FactSage* window to activate this module.

Create a private **Compound** database

Before you can start entering compound data in a **private database** you must first create the **database file** with the basic information.

A directory must be chosen and a file name be given, a nick name must be defined and a short database description may be entered.

At the end of this procedure the Compound module will give a status of the new database showing

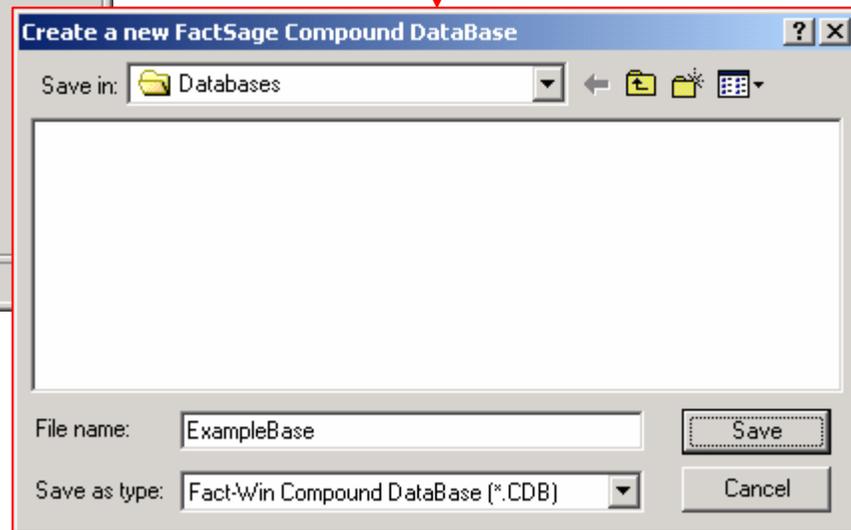
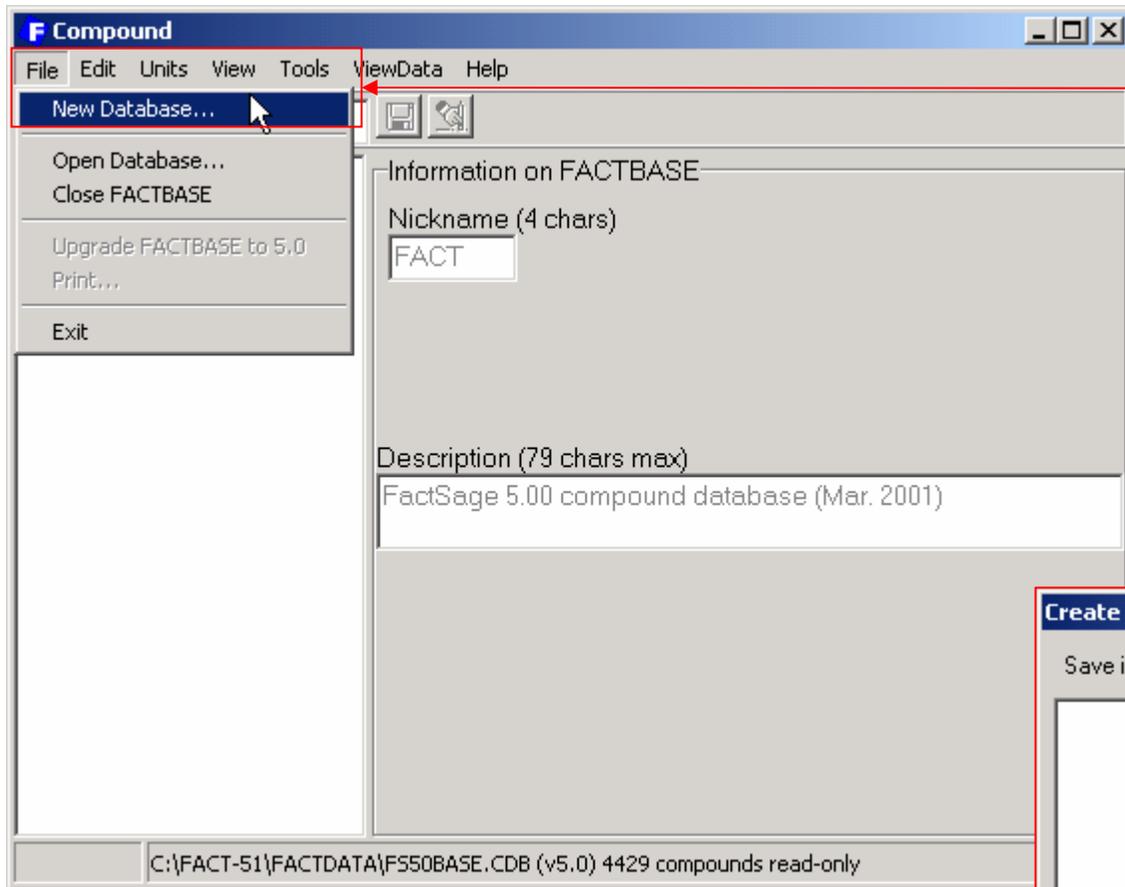
- its location: **path\name**
- the number of compounds it contains: **0 compound(s)** initially;
- the **FactSage** version it goes with: **5.0**
- and its access permission: **read/write.**

Create a private **Compound** database, I

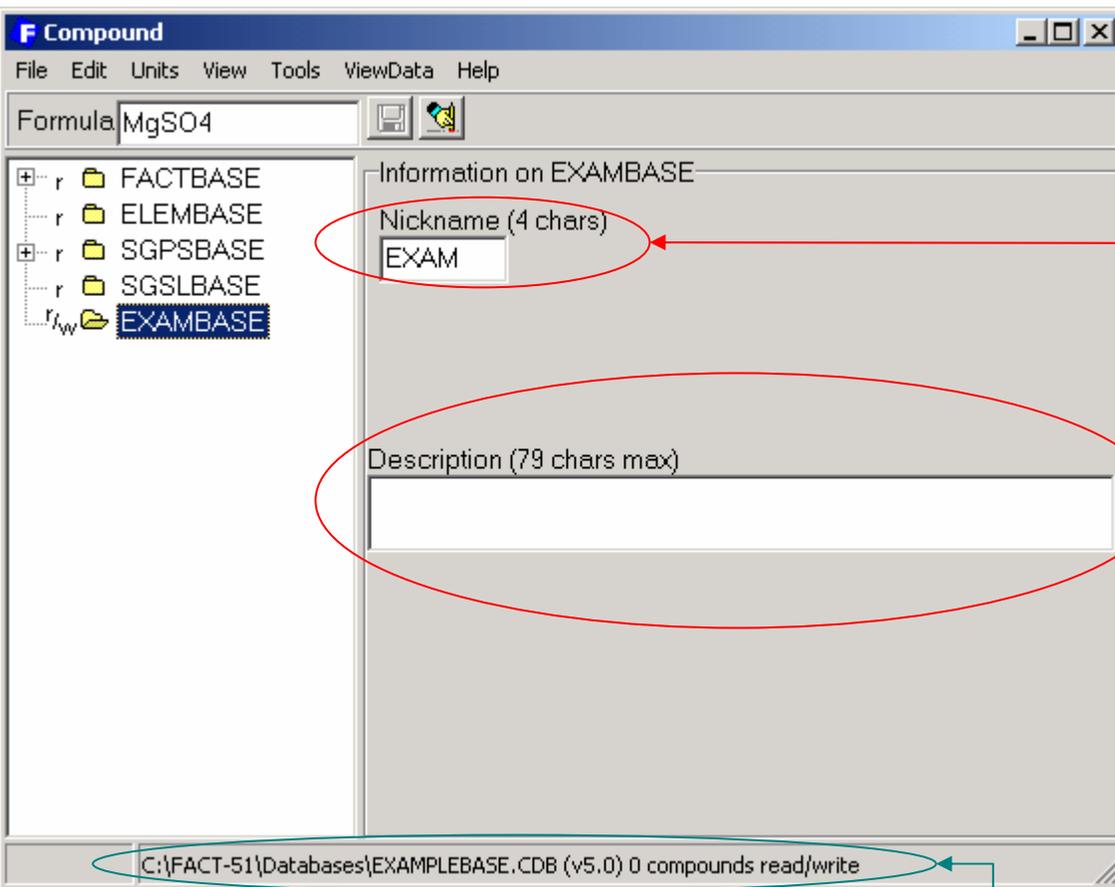
To create a read and write (r/w) database:

1. Click on «**New Database...**» from the «**File**» Menu

2. Choose a **filename** and select a **directory** for your new database



Create a private *Compound* database, II



The program selects automatically a four character nickname and adds the suffix **-BASE** to complete the name of your private database. You can edit the nickname.

You can enter a short **description** of your private database (with a maximum of 79 characters).

The status bar provides information on the database:

- its location: **C:\FACT-51\DATABASE\EXAMPLEBASE.CDB;**
- the number of compounds it contains: **0 compound(s)** (for now);
- its version: **5.0;**
- and its access permission: **read/write.**

Add a **compound** to the database

The following 20 slides (sections 4 to 9) show how to enter the data for a **new compound with three phases** (solid, liquid, gas) into a **private database**.

MgCl₂ is taken as an example. The data for this compound are summarized in [slide 4.3](#). All entries are made using the values in this figure.

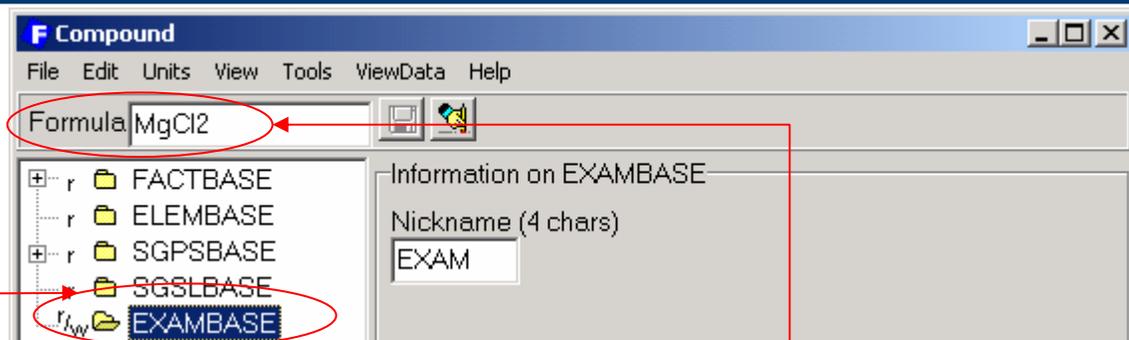
The two different variants of entering data are demonstrated:

- 1) **H₂₉₈, S₂₉₈ and C_p with transition data** for the high temperature phase (using data for solid and liquid MgCl₂)
- 2) **H₂₉₈, S₂₉₈ and C_p** for the **high temperature phase** itself (using data for the gas).

Add a **compound** to the database, I

To enter a new compound, for example **MgCl₂**, in the **EXAMBASE**:

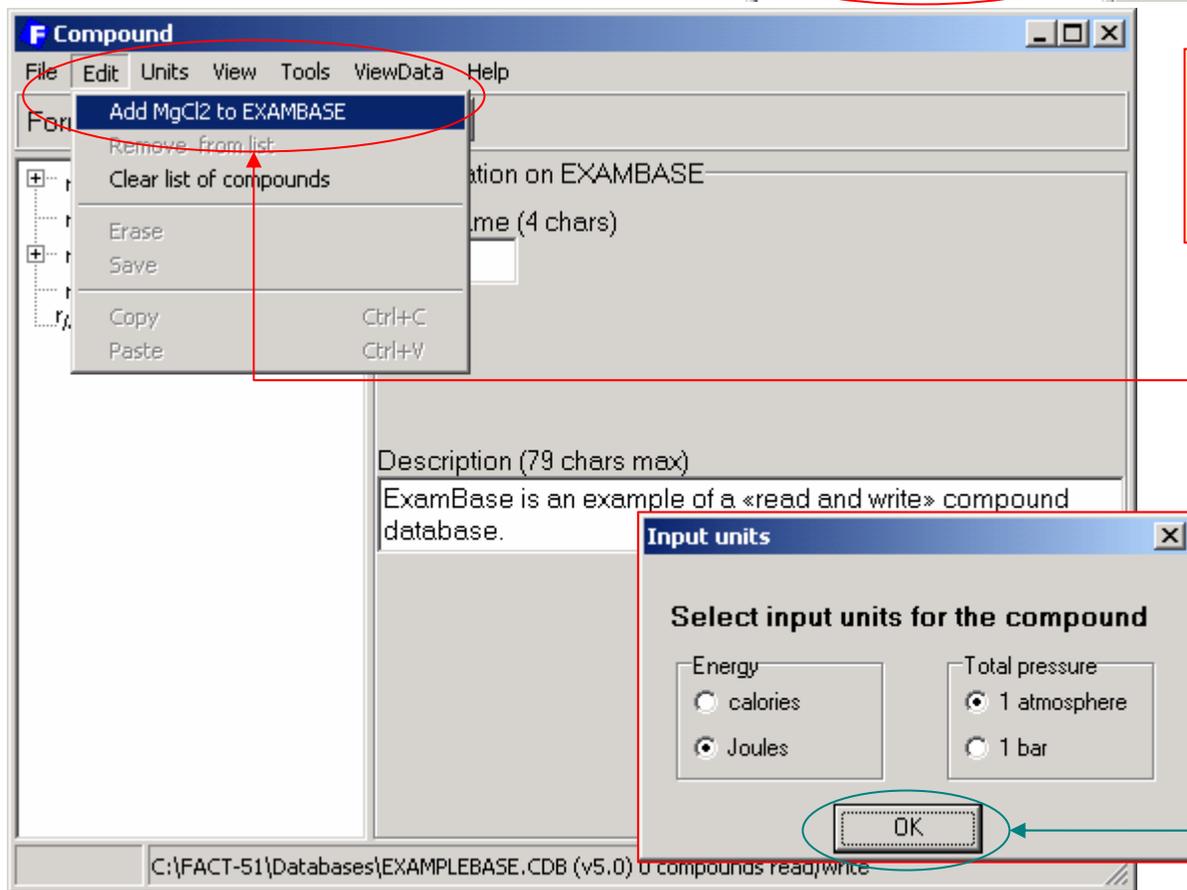
1. Select **EXAMBASE** database



2. Type the chemical formula of the compound: **MgCl₂**, in the **Formula** input box

3. Select the function «**Add MgCl₂ to EXAMBASE**» from the **Edit** Menu.

4. Select **input units** for the compound.



5. Press «**OK**»

Add a **compound** to the database, II

Your database is now ready for a new entry or for a modification of a compound's data.

Energy: Joules Pressure: atm MgCl2

File Edit Units View Tools ViewData Help

Formula: MgCl2

FACTBASE
ELEMBASE
SGPSBASE
SGSLBASE
EXAMBASE

MgCl2

MgCl2 properties
Weight: 95.2104 g/mol Modified: 2002 May 13

Compound Name Reference no.
magnesium chloride

Comments
Example for the COMPOUND program's help.

Real Stoichiometry (for advanced users only)
Cl 2 Mg 1

Modified C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 0 compounds read/write

6. If you want, you can enter:
- the **compound name**;
 - reference number(s)**;
 - and **comments**.

7. Right click on **MgCl2** to access the following pop-up menu.

Add phase ...
Add Cp range
Delete phase
Delete Cp range
Erase MgCl2 from EXAMBASE

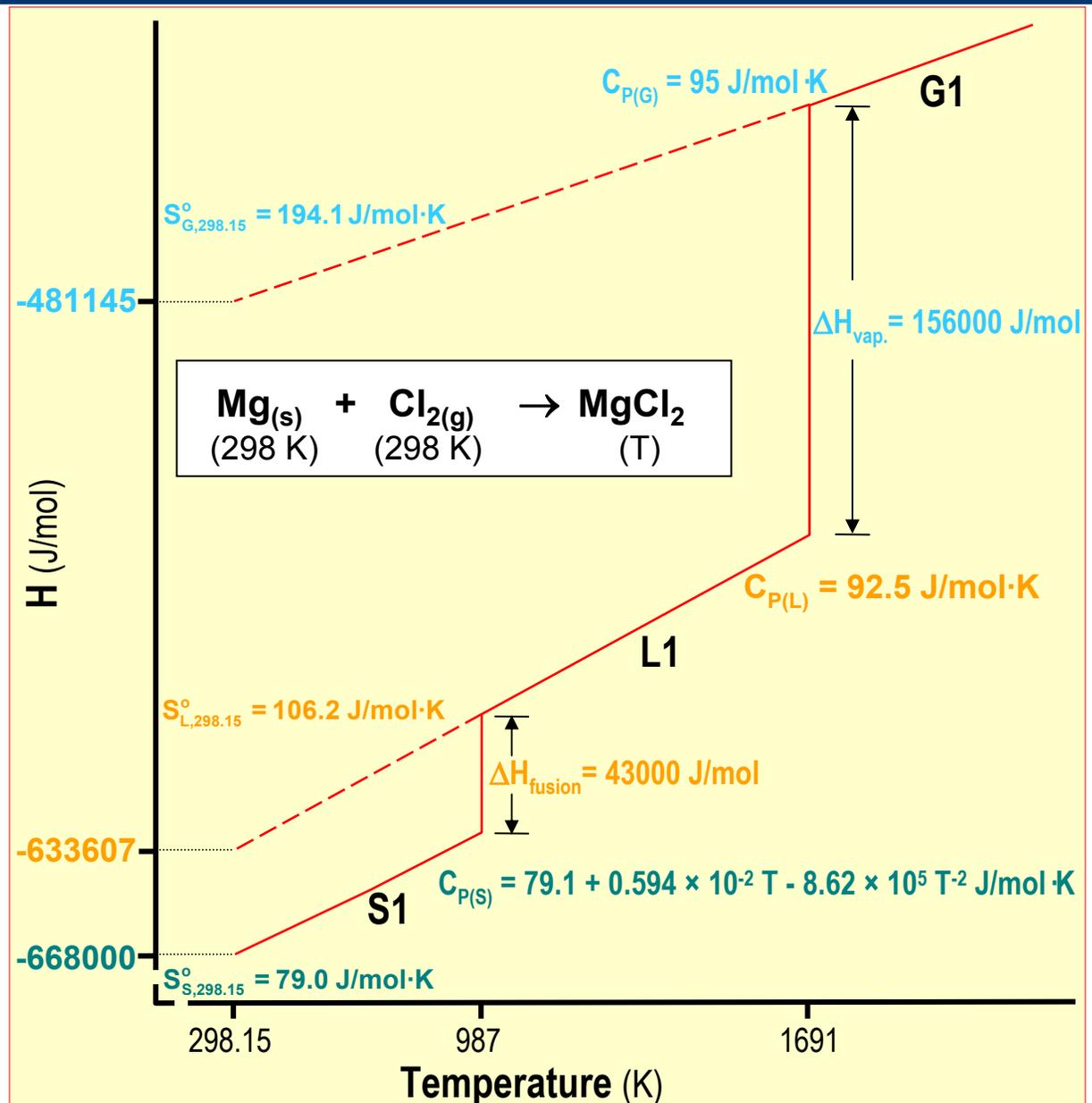
The **Real Stoichiometry** input box appears if you have checked «**Real stoichiometry**» in the menu **View**. This feature is for **advanced users only** and applies to **every phase of the compound** (it does not apply to elements).

View

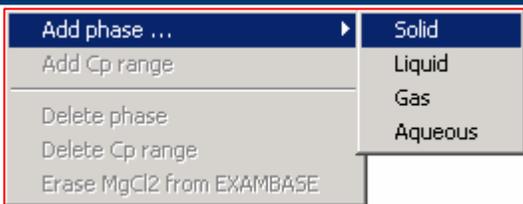
Extended properties
✓ Real stoichiometry
List of products
Entire FACTBASE
Mixer ...

Add a **compound** to the database, III

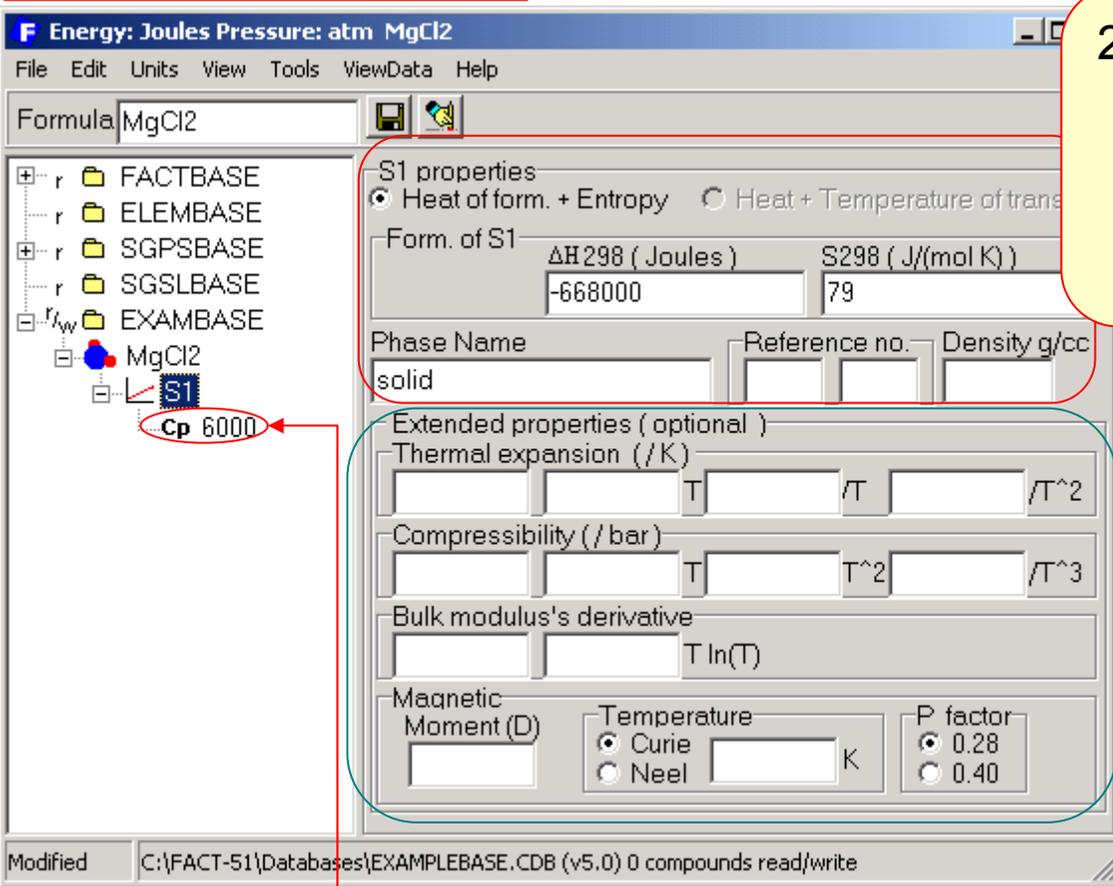
Data for **MgCl₂** are taken from this graph and entered into a **private database**.



Add a **compound** to the database: H_{298} and S_{298} for **1st** phase, IV



1. In the pop-up menu, point the arrow to «**Add phase...**» and select «**Solid**» from the sub menu with a left click.



2. Enter the values for the **enthalpy of formation** ($\Delta H^{\circ}_{s,298.15}$) and **entropy** ($S^{\circ}_{s,298.15}$). **Compound** only takes these values when entering data for the **first** phase.

The **Extended properties** input box appears if you have checked «**Extended properties**» in the menu **View**. This feature applies to a **phase exclusively**.

View
Extended properties
Real stoichiometry
List of products
Entire FACTBASE
Mixer ...

3. Left click on **Cp 6000** to open the input box for C_p .

Values of $\Delta H^{\circ}_{s,298.15}$ and $S^{\circ}_{s,298.15}$ were obtained from the graph (see previous slide)

Add a **compound** to the database: **extended properties**, V

Thermal expansion expression: $a + bT + \frac{c}{T} + \frac{d}{T^2} [K^{-1}]$

Compressibility expression:

$$a + bT + cT^2 + \frac{d}{T^3} [bar^{-1}]$$

Bulk modulus derivative expression: $a + bT \ln T$

Magnetic contribution expression to the **Gibbs free energy** G_{mag} :

$$G_{mag} = RT \ln(\beta + 1) g(\tau) \quad \text{where} \quad \tau = \frac{T}{T_c} \quad \text{and} \quad \beta \text{ is the magnetic moment.}$$

$$g(\tau) = \frac{1}{D} \left\{ 1 - \left[\frac{79\tau^{-1}}{140p} + \frac{474}{497} (p^{-1} - 1) \left(\frac{\tau^3}{6} + \frac{\tau^9}{135} + \frac{\tau^{15}}{600} \right) \right] \right\} \quad \text{when} \quad \tau \leq 1$$

$$g(\tau) = \frac{1}{D} \left[\frac{\tau^{-5}}{10} + \frac{\tau^{-15}}{315} + \frac{\tau^{-25}}{1500} \right] \quad \text{when} \quad \tau > 1$$

where $D = \frac{518}{1125} + \frac{11692}{15975} (p^{-1} - 1)$, p is a phase (structure) dependent factor.

Add a **compound** to the database: C_p values for the **1st** phase, VI

Energy: Joules Pressure: atm MgCl2

Formula MgCl2

FACTBASE
ELEMBASE
SGPSBASE
SGSLBASE
EXAMBASE
MgCl2
S1
Cp 6000

Cp expression for S1
 ΔH_{298} : -668000 J/mol
 S_{298} : 79 J/(mol K)
 from 298.150 K to 6000.000 K
 $C_p(T) =$ $T^{\wedge} 0.00$

Buttons: Cp, H, S, G, Edit

1. Left click on **Cp 6000** to open the input box «**Cp expression for S1**».

You can enter expressions for C_p and list those of H , S or G .

Energy: Joules Pressure: atm MgCl2

Formula MgCl2

FACTBASE
ELEMBASE
SGPSBASE
SGSLBASE
EXAMBASE
MgCl2
S1
Cp 987

Cp expression for S1
 ΔH_{298} : -667999.9999999983 J/mol
 S_{298} : 78.99999999998367 J/(mol K)
 from 298.150 K to 987.000 K
 $C_p(T) =$ 79.1 $T^{\wedge} 0.00$
 0.00594 $T^{\wedge} 1.00$
 -862000 $T^{\wedge} -2.00$

Buttons: Cp, H, S, G, Edit

2. Enter the C_p range from **298.15 K** to **987 K** and the C_p expression for **MgCl₂ S1** (see [slide 4.3](#))
 $C_{p(S)} = 79.1 + 5.94 \times 10^{-3} T - 8.62 \times 10^5 T^{-2} \text{ J/mol}\cdot\text{K}$

Show data as H, S and G functions

Compound permits the conversion of H_{298} , S_{298} and C_p input data into enthalpy, entropy and Gibbs energy functions.

The coefficients of these H, S and G functions can be viewed directly.

Show data as H, S and G functions

Compound calculates automatically the expressions of **H**, **S** and **G** from your entry of the **Cp** expression.

H expression for S1

ΔH_{298} : -668000 J/mol
 S_{298} : 79.00000000000001 J/(mol K)

from 298.150 K to 987.000 K

H(T) =

-694738.84063152	T ^{0.00}
79.1	T ^{1.00}
0.00297	T ^{2.00}
862000	

Note: T⁹⁹ => ln T

Cp
H
S
G Edit

S expression for S1

ΔH_{298} : -668000 J/mol
 S_{298} : 79.00000000000001 J/(mol K)

from 298.150 K to 987.000 K

S(T) =

-378.299413912727	T ^{0.00}	
79.1	T ^{99.00}	ln T
0.00594	T ^{1.00}	
431000	T ^{-2.00}	
	T	

Note: T⁹⁹ => ln T

Cp
H
S
G Edit

G expression for S1

ΔH_{298} : -668000 J/mol
 S_{298} : 79.00000000000001 J/(mol K)

from 298.150 K to 987.000 K

G(T) =

-694738.84063152	T ^{0.00}
457.399413912727	T ^{1.00}
-79.1	T ln T
-0.00297	T ^{2.00}
431000	T ^{-1.00}
	T

Note: T⁹⁹ => ln T

Cp
H
S
G Edit

The data colored in **gray** indicates that you can not edit these expressions.

Edit the **Gibbs Energy** function

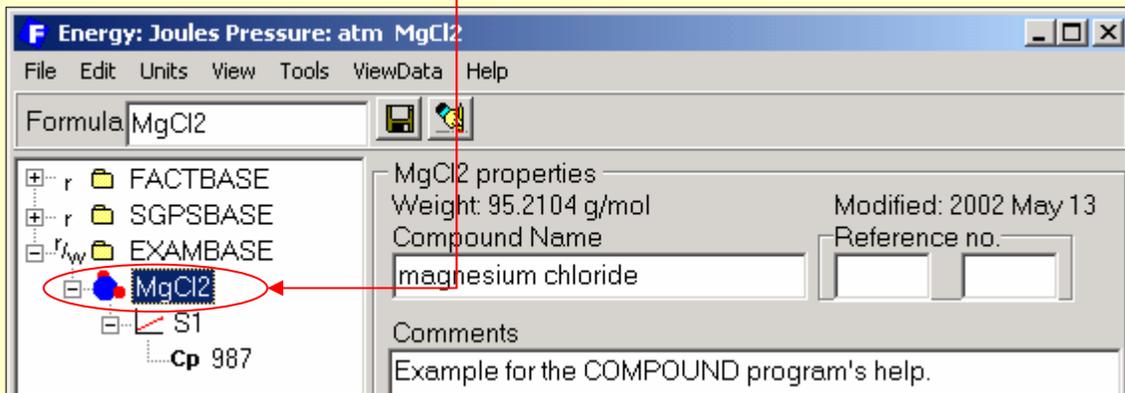
The following slide shows how to **edit** the data of a compound phase when using the **Gibbs energy** coefficients instead of H, S and C_p data.

Entering phase transition data: the **liquid** phase

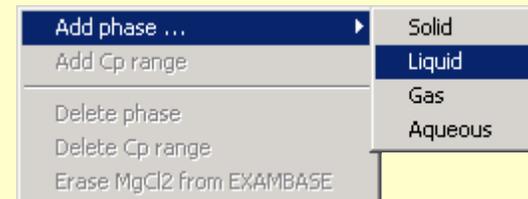
- The next three slides illustrate how to enter a new phase (here the **liquid**) if the data for the **phase transition** between the previous phase (here the **solid**) and the new phase, i.e. ΔH and T_{trans} , as well as the C_p data of the new phase are available.

Entering phase transition data: the **liquid** phase, I

1. Right click on «  » to open a **pop-up menu**.

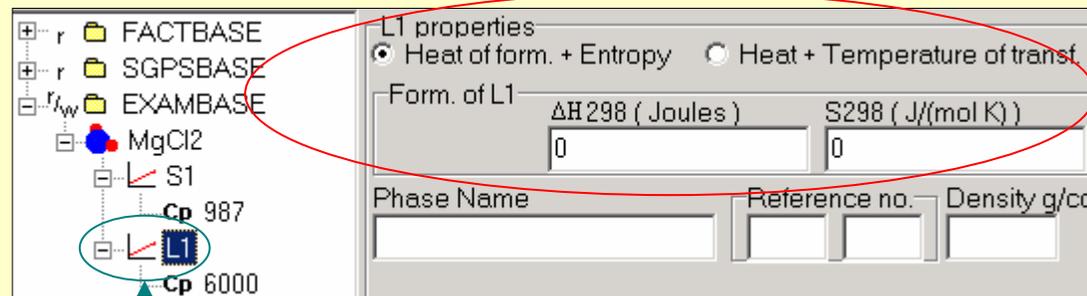


2. Point the arrow to « **Add phase...** » and select « **Liquid** » from the sub menu with a click.

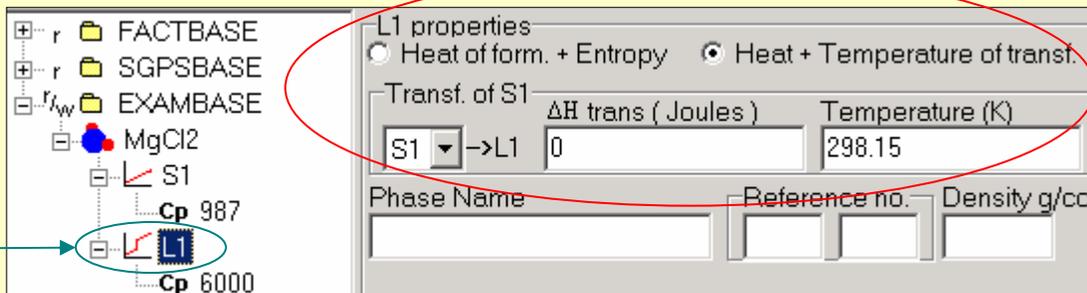


3. **Compound** proposes two ways to enter the data:

- either you enter the **enthalpy of formation** ($\Delta H^\circ_{L, 298.15}$) and **entropy** ($S^\circ_{L, 298.15}$) and the entry is flagged by the **icon** 



- or you enter the **enthalpy and temperature of transformation** and the entry is flagged by the **icon** 



Entering phase transition data: the **liquid** phase, II

3.(continued)

Entering the **enthalpy** and **temperature** of transformation.

4. Click on **C_p 6000** to open the box «**Cp expression for L1**»

Energy: Joules Pressure: atm MgCl2

File Edit Units View Tools ViewData Help

Formula MgCl2

FACTBASE
SGPSBASE
EXAMBASE
MgCl2
S1
Cp 987
Cp 6000

L1 properties
 Heat of form. + Entropy Heat + Temperature of transf.

Transf. of S1

	ΔH trans (Joules)	Temperature (K)
S1 → L1	43000	987

Phase Name Reference no. Density g/cc

liquid

Extended properties (optional)

Thermal expansion (/K)

	T	T	T ²

Compressibility (/bar)

	T	T ²	T ³

Modified C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 1 compounds read/write

View

- Extended properties
- Real stoichiometry
- List of products
- Entire FACTBASE
- Mixer ...

The **Extended properties** input box appears if you have checked «**Extended properties**» in the menu **View**. This feature applies to a **phase exclusively**.

Entering phase transition data: C_p coefficients of the liquid phase, III

Compound calculates automatically the values of $\Delta H^\circ_{L, 298.15}$ and $S^\circ_{L, 298.15}$ (these values are the same as those in slide 4.3).

The screenshot shows the FactSage software interface for MgCl2. The 'Formula' field contains 'MgCl2'. The left sidebar shows a tree view with 'MgCl2' selected, and 'L1' and 'Cp 1691' highlighted. The main window displays the 'Cp expression for L1' section. The 'from' temperature is 298.150 K and the 'to' temperature is 1691.000 K. The 'Cp(T)' expression is set to 92.5. The 'T^' column is set to 0.00. The 'Edit' button is visible. A red arrow points from the text below to the 'Cp(T)' field.

Property	Value
ΔH_{298}	-633619.130104762 J/mol
S_{298}	106.211274831458 J/(mol K)
from	298.150 K
to	1691.000 K
$C_p(T)$	92.5
$T^$	0.00
$T^$	

5. Enter the C_p range from 298.15 K to 1691 K and the C_p expression for $MgCl_2$ liquid (slide #6): $C_{P(L)} = 92.5 J/mol \cdot K$

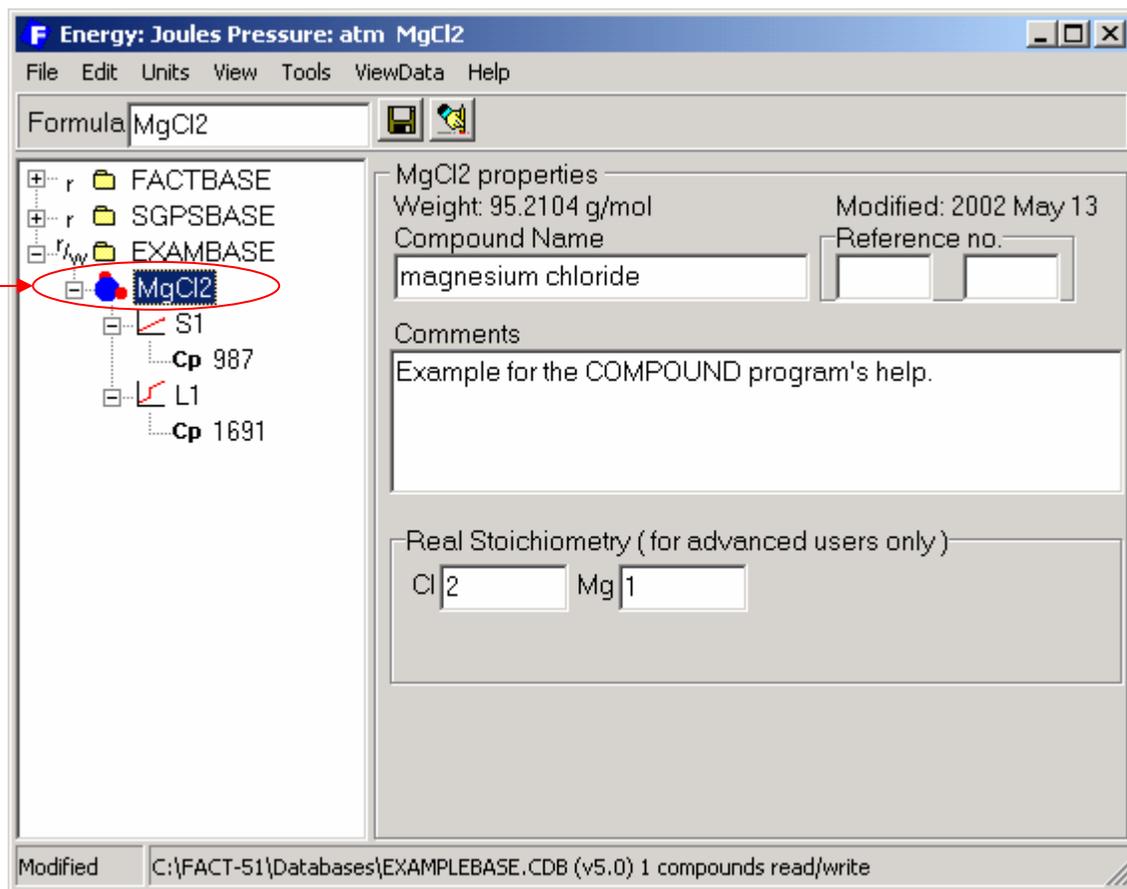
Entering a new phase with H_{298} , S_{298} and C_p : the **gaseous** phase

The following three slides show how an **additional phase** (here the **gas**) is entered for which H_{298} , S_{298} and C_p are known.

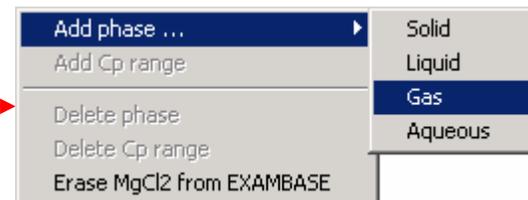
The entry of extended data for the non-ideal behaviour of the gas according to the **Tsonopoulos** method is also shown.

Entering a new phase with H_{298} , S_{298} and C_p : the **gaseous** phase, I

1. Right click on «  » to open a **pop-up menu**.



2. Point the arrow to « **Add phase...** » and select « **Gas** » from the sub menu with a click.



Entering a new phase with H_{298} , S_{298} and C_p : the **gaseous** phase, II

3. Enter the values for the **enthalpy of formation** ($\Delta H^\circ_{G,298.15}$) and the **entropy** ($S^\circ_{G,298.15}$). (See [slide 4.3](#))

4. Click on **C_p 6000** to open the box « **C_p expression for L1**»

Energy: Joules Pressure: atm MgCl2

File Edit Units View Tools ViewData Help

Formula MgCl2

FACTBASE
SGPSBASE
EXAMBASE
MgCl2
S1
Cp 987
L1
Cp 1691
G1
Cp 6000

G1 properties
 Heat of form. + Entropy Heat + Temperature of transf.

Form. of G1
ΔH298 (Joules) -481145
S298 (J/(mol K)) 194.1

Phase Name gas Reference no. Density g/cc

Extended properties (optional)
Critical
Temperature Pressure Volume
K bar cc/mol
Omega Dipole moment
Debyes

Modified C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 1 compounds read/write



The **Extended properties** input box appears if you have checked «**Extended properties**» in the menu **View**. This feature applies to a **phase exclusively**.

The truncated virial equation of state is employed to treat real gases:

$$\frac{PV}{RT} = 1 + \frac{BP}{RT}$$

B is estimated for pure gases and mixtures by the Tsonopoulos* method from P_c , T_c , and Ω (omega, the acentric factor) for the pure gases. Gases are treated as non-polar. For **ideal gases**, the value of B is **zero**.

Extended properties (optional)

Critical

Temperature T_c K Pressure P_c bar Volume V_c cc/mol

Omega Ω Dipole moment μ Debyes

* «An Empirical Correlation of Second Virial Coefficients» by C. Tsonopoulos, AIChE Journal, vol. 20, No 2, pp. 263-271, 1974.

Finishing and saving the entry

The next slide shows how the last data item for MgCl_2 , the C_p coefficient of the gas phase, is entered

and

the complete dataset is saved in the private database.

Finishing and saving the entry, I

Energy: Joules Pressure: atm MgCl2

Formula: MgCl2

FACTBASE
SGPSBASE
EXAMBASE

MgCl2

S1
Cp 987
L1
Cp 1691
G1
Cp 6000

Cp expression for G1

ΔH_{298} : -481145 J/mol
 S_{298} : 194.1 J/(mol K)

from 298.150 K to 6000.000 K

Cp(T) = 95 T[^] 0.00

Modified C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 0 compounds read/written

5. Enter the C_p range from 298.15 K to 6000 K and the C_p expression for $MgCl_2$ gas (slide 4.3): $C_{P(G)} = 95 \text{ J/mol}\cdot\text{K}$

Energy: Joules Pressure: atm MgCl2

Formula: MgCl2

FACTBASE
SGPSBASE
EXAMBASE

MgCl2

S1
Cp 987
L1
Cp 1691
G1
Cp 6000

Cp expression for G1

ΔH_{298} : -481145 J/mol
 S_{298} : 194.1 J/(mol K)

from 298.150 K to 6000.000 K

Cp(T) = 95 T[^] 0.00

Modified C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 1 compounds read/written

6. Press on the **Save** button () to complete your entry for this compound (You can also select «**Save MgCl2 to EXAMBASE**» from the menu **Edit**). Now your database contains **1** compound. The fading of the compound **icon** (from  MgCl2 to ) indicates that your data are **saved**.

Viewing data and finding species

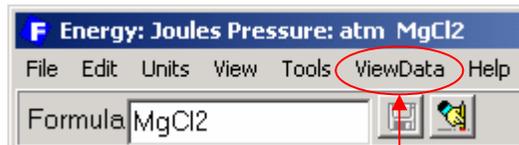
If you wish to inspect data for a compound in the **format** used by the **View Data** module you may do so from **within** the **Compound** module.

You may also inspect **lists of chemical systems** as generated by the **View Data** module from **within** the **Compound** module.

The following three view graphs show how to perform these tasks.

Viewing data and finding species, I

1. Click on «**ViewData**» in the menu bar to open the **ViewData** application at the compound (**MgCl₂**) and the database (**EXAMBASE**) you have selected (or the last you just worked in).



2. Click on the **Cp(T)** and **Phases** tabs to see the **data** you have just entered or the **values** calculated by **Compound** from your data entry.

F MgCl₂ Units: P(atm) Energy(J)
File Edit Units Summary Databases Table Graph Help
3 Phases EXAM - EXAM compound database

Phases **Cp(T)** H(T) G(T) S(T) Volume Magnetic Refs.

Name: magnesium chloride

$$C_p = \sum_{i=1}^8 C_{(i)} T^{P(i)}$$

Cp range: T(min) - T(max).
When T < T(min), Cp(T) is extrapolated.
When T > T(max), Cp(T) at T(max) is used.

	DH(298.15) (J)	S(298.15) (J/K)	C(i)	P(i)	C(i)	P(i)	Cp (K)
S	-668000.00	79.000000	79.100000	0	5.940000000E-03	1	298 - 987
L	-633619.13	106.211275	92.500000	0			298 - 1691
G	-481145.00	194.100000	95.000000	0			298 - 6000

FactSage 5.1 C:\FACT-51\DATABASES\EXAMPLEBASE.CDB (v

Phases **Phases** Cp(T) H(T) G(T) S(T) Volume Magnetic Refs.

Name: magnesium chloride
Formula Weight: 95.2104
Stoichiometric Compound: MgCl₂

Phase	Cp Range, K	Density, g/ml	Ref.
S	298.15 - 987.00		
L	298.15 - 1691.00		
G	298.15 - 6000.00	ideal	

Viewing data and finding species, II

1. To look at the data of a **compound** found in a **database**, for example **MgSO₄** in **FACTBASE**: **enter MgSO₄** in the Formula input box.

The screenshot shows the FactSage software interface. The title bar reads "Energy: Joules Pressure: atm MgSO4". The menu bar includes "File", "Edit", "Units", "View", "Tools", "ViewData", and "Help". The "Formula" input box contains "MgSO4". On the left, a tree structure shows the expansion of "FACTBASE" into "MgSO4", which is further divided into "S1", "L1", and "Aq1". The "Aq1" branch is selected. The main panel displays "Aq1 properties" with radio buttons for "Heat of form. + Entropy" (selected) and "Heat + Temperature of transf.". Below this is a table for "Form. of Aq1" with columns for ΔH_{298} (Joules) and S_{298} (J/(mol K)). The values are -1355616 and -7.113, respectively. Below the table are fields for "Phase Name" (Aqueous), "Reference no." (14), and "Density g/cc". The status bar at the bottom indicates the file path: "C:\FACT-51\FACTDATA\F550BASE.CDB (v5.0) 4429 compounds read-only".

Move the pointer over the reference text box to view the **detailed bibliography**

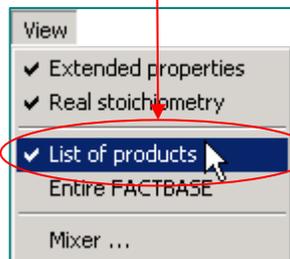
"Thermochemical Properties of Inorganic Substances",
I. Barin, O. Knacke, and O. Kubaschewski,
Springer-Verlag, Berlin, 1977.
(for non-aqueous species)
appended to:
"Handbook of Thermochemical Data for Compounds and Aqueous Species",
H.E. Barner and R.V. Scheuerman,
Wiley-Interscience, New York, 1978.
(for aqueous species)

2. Expand the tree structure for **FACTBASE** and search through the **MgSO₄** branches to list its data. Note that data for **MgCl₂** is also shown.

Viewing data and finding species, III

1. Select «**List of products**» in the **View** menu.

2. Enter a chemical formula of a compound () or the elements () of interest in the Formula input box. For example **O**, **S** and **Mg**.



A screenshot of the FACTSAGE software interface. The title bar reads 'Energy: Joules Pressure: atm Mg'. The menu bar includes 'File', 'Edit', 'Units', 'View', 'Tools', 'ViewData', and 'Help'. The 'Formula' input box contains 'MgSO4'. Below the input box is a tree structure under 'FACTBASE' with the following items: O[-], O, O[+], O2[-], O2, O2[+], O3, Mg (highlighted with a blue selection box), Mg[+], Mg[2+], Mg2, MgO, S[2-], S[-], S, S[+], S2[2-], and S2. To the right of the tree is a panel for 'Mg properties' showing 'Weight: 24.305 g/mol', 'Modified: 1992 Mar 10', 'Compound Name: Magnesium', and 'Reference no.'. Below this is a 'Comments' section with text: 'JNF85(332-3) SEP83. Cp for S1,L1 fitted JUL90. DISK31 JNF85(334) SEP83 (1 bar). Cp for G1 fitted JUL90. DISK31 Cp(S1) above 1200K modified for proper extrapolation APR94.' At the bottom is a 'Real Stoichiometry (for advanced users only)' section with 'Mg' and a value of '1'. The status bar at the bottom reads 'C:\FACT-51\FACTDATA\F550BASE.CDB (v5.0) 4429 compounds read-only'. Red circles and arrows highlight the 'View' menu, the 'Formula' input box, and the 'Mg' entry in the tree structure.

3. Expand the tree structure to see the list of compounds containing **O**, **S** and/or **Mg**.

Transferring data between databases

Data for single compounds can easily be transferred between databases.

This is particularly useful if you want to investigate how data changes for a compound in a read only database affect results in calculations. Simply generate your own private read and write database and copy the desired compound(s) from the read only database over to your private database.

There are two ways how to do that which will be described in the following to view graphs.

Transferring data between databases, I

1. **Select** the **compound** of interest in its **database**.
For example, **click** on **MgSO₄** in **FACTBASE**.

2. Select «**Copy**» from the **Edit** menu.

Energy: Joules Pressure: atm MgSO4

File Edit Units View Tools ViewData Help

Formula MgSO4

FACTBASE

MgSO4

MgCl2

SGPSBASE

ELEMBASE

SGSLBASE

EXAMBASE

MgSO4 properties

Weight: 120.3686 g/mol Modified: 1992 Mar 10

Compound Name Reference no.

Magnesium Sulfate

Comments

JNF85(339-40) MAR66. Cp for S1,L1 fitted JUL90. DISK32

Real Stoichiometry (for advanced users only)

S 1 Mg 1 O 4

C:\FACT-51\FACTDATA\F550BASE.CDB (v5.0) 4429 compounds read-only

3. **Select** the destination **database**.
Here, **EXAMBASE**.

Compound

File Edit Units View Tools ViewData Help

Formula MgSO4

FACTBASE

MgSO4

MgCl2

SGPSBASE

ELEMBASE

SGSLBASE

EXAMBASE

Information on EXAMBASE

Nickname (4 chars)

EXAM

Edit

Add MgSO4 to EXAMBASE

Remove from list

Clear list of compounds

Erase

Save

Copy Ctrl+C

Paste MgSO4 Ctrl+V

4. Select «**Paste MgSO₄**» from the **Edit** menu.

Transferring data between databases, II

Note that the MgSO_4 data retrieved from the **read only (r) FACTBASE** database are shown in gray color and you **can not** edit them.

Simply **drag-and-drop** MgSO_4 from **FACTBASE** to **EXAMBASE**.

Note that the MgSO_4 data retrieved from the **read and write (r/w) EXAMBASE** database are shown in **black** color and you **can edit** them.

The image displays two screenshots of the FactSage software interface, illustrating the transfer of data between databases. Both windows show the 'Energy: Joules Pressure: atm MgSO4' window with the 'Formula' field set to 'MgSO4'. The left pane shows a tree view of databases: FACTBASE, SGPSBASE, ELEMBASE, SGSLBASE, and EXAMBASE. The right pane shows the 'MgSO4 properties' for Magnesium Sulfate, including weight (120.3686 g/mol), compound name, and comments.

In the top screenshot, the 'MgSO4' entry under 'FACTBASE' is highlighted in gray, indicating it is read-only. A red circle highlights this entry, and a red arrow points to it. The 'EXAMBASE' database is also visible in the tree view.

In the bottom screenshot, the 'MgSO4' entry under 'EXAMBASE' is highlighted in black, indicating it is read and writeable. A red circle highlights this entry, and a blue arrow points to it from the top screenshot. The 'FACTBASE' database is also visible in the tree view.

The status bar at the bottom of the top window shows 'C:\FACT-51\FACTDATA\F550BASE.CDB (v5.0) 4429 compounds r', while the bottom window shows 'C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 2 compounds read/write'.

Editing a read and write (r/w) database

Data in a read and write database may be **added**, **removed** or **modified**.

In the example the C_p range for the **solid** (S1) phase of **MgSO₄** in the r/w **EXAMBASE database** is **edited**.

The **Erase**, **Remove** and **Clear** commands

The **Erase**, **Remove** and **Clear** commands permit

- to **erase** (delete) single compounds from a particular database,
- to **remove** single compounds from an edit list
and
- to **clear** complete edit lists.

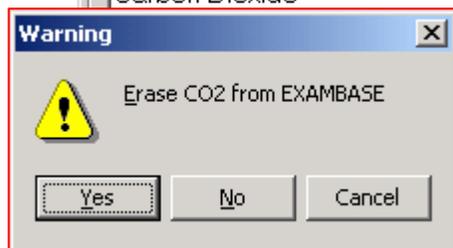
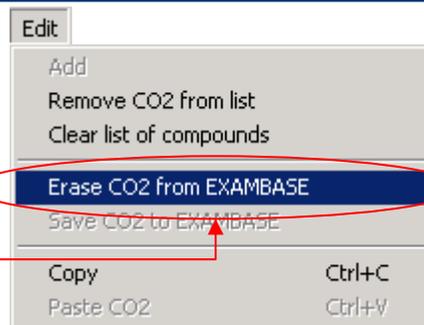
NOTE: The latter two commands do NOT interfere with the contents of databases. They are therefore applicable with all types of databases. The **Erase** command only works for read/write databases.

The Erase, Remove and Clear commands, I

1. **Select** the compound you want to **delete** (say, CO₂) from the **r/w database**.

2. **Go to the Edit menu** and select **Erase CO2 from EXAMBASE**.

3. **Confirm** your intention to **erase** data



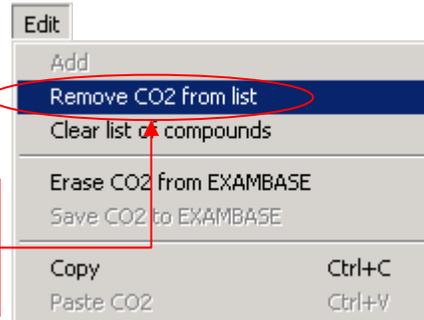
Now the database **EXAMBASE** contains only **2** (= **3** - **1**) compounds.

C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 2 compounds read/write

The Erase, Remove and Clear commands, II

1. **Select** the compound you want to **remove** (say, CO_2) from the tree view list.

2. **Go to the Edit menu and **select Remove CO2 from list.****



The screenshot displays two windows from the software. The top window, titled 'Energy: Joules Pressure: atm CO2', shows the 'EXAMBASE' database with 'CO2' selected in the tree view. The bottom window, titled 'Energy: Joules Pressure: atm MgSO4', shows the same 'EXAMBASE' database but with 'MgSO4' selected. The status bar at the bottom of both windows indicates '3 compounds'. A red box on the right contains the text: 'The compound CO_2 is **not shown** in the tree view **but** the database **EXAMBASE** still contains **3** compounds.' Red arrows point from this text to the 'CO2' entry in the top window's tree view and to the '3 compounds' status bar in the bottom window.

The Erase, Remove and Clear commands, III

To **remove** all the compounds from **all** the **lists** (you are **not** removing the compounds from the **databases**) in the **treeview** (i.e. to **clear** the **treeview**):

Go to the **Edit** menu and **select** «**Clear list of compounds**». You can also **press** the button «**Clear list of compounds**» in the **toolbar**.

The screenshot displays the FactSage Compound 13.3 interface. The main window is titled 'Energy: Joules Pressure: atm CO2'. The 'Edit' menu is open, showing options: 'Add', 'Remove CO2 from list', 'Clear list of compounds' (highlighted with a red circle), 'Erase CO2 from EXAMBASE', 'Save CO2 to EXAMBASE', 'Copy' (Ctrl+C), and 'Paste CO2' (Ctrl+V). The 'tree view' on the left shows a hierarchy of databases: FACTBASE, SGPSBASE, ELEMBASE, SGSLBASE, and EXAMBASE. The 'EXAMBASE' folder is selected and highlighted with a red circle. The 'tree view' also shows a list of compounds: CO2, MgSO4, MgCl2, CO2, MgO4S, Cl2Mg, CO2, MgSO4, MgCl2, and CO2. The 'CO2' compound is selected and highlighted with a red circle. The 'Properties' panel on the right shows 'CO2 properties' with 'Weight: 44.0098 g/mol' and 'Compound Name: Carbon Dioxide'. The 'Comments' panel is empty. The 'Real Stoichiometry' panel shows 'O 2' and 'C 1'. The status bar at the bottom indicates 'C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 3 compounds' and 'C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 3 compounds read/write'. A red box with text is overlaid on the 'tree view' area.

The compounds are **not shown** in the **tree view** but the database **EXAMBASE** still contains **3** compounds.

The «Mixer» feature

The «Mixer » feature permits the generation of new compound data using «simple algebra» on the data of already stored compounds.

The first example shows how the known data for Na_2O and Al_2O_3 are used in a Neumann-Kopp type sum to generate data for the unknown compound NaAlO_4 . The scale down command is used to come to the desired formula.

Alternatively, the use of the scale up command is shown for the formula $\text{Na}_3\text{Al}_3\text{O}_6$.

The second example shows how the known data for Li_3N , Li and Na are used to generate data for the unknown compound Na_3N using $\text{Li}_3\text{N} + 3\text{Na} - 3\text{Li} = \text{Na}_3\text{N}$.

The «Mixer» feature: Example 1, I

The «Mixer» option enables you to create and store compound data on a new (possibly hypothetical) species by mixing data of existing species. For example, new data on NaAlO_2 via the reaction: $\frac{1}{2} \text{Na}_2\text{O}(\text{s1}) + \frac{1}{2} \text{Al}_2\text{O}_3(\text{s1}) \rightarrow \text{NaAlO}_2(\text{s1})$.

1. Open the database containing the data on Na_2O and Al_2O_3 and expand the treeview to list phases.

2. Click on View > Mixer...

Energy: calories Pressure: atm Na2O

File Edit Units View Fools ViewData Help

Formula Al2O3

FACTBASE

- Na2O
 - S1
 - S2
 - S3
 - L1
- Al2O3
 - S1
 - S2
 - S3
 - S4
 - L1
- SGPSBASE
- ELEMBASE
- SGSLBASE
- EXAMBASE

S1 properties

Heat of form. + Entropy Heat + Temperature of transf.

Form. of S1

ΔH298 (calories)	S298 (cal/(mol K))
-99900.096	17.940009

Phase Name	Reference no.	Density g/cc
Solid-A	133	2.27

C:\FACT-51\FACTDATA\F550BASE.CDB (v5.0) 4429 compounds read-only

View

- Extended properties
- Real stoichiometry
- List of products
- Entire FACTBASE
- Mixer ...

Compound Mixer

Reactants	Phase	Database
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Product State

Solid

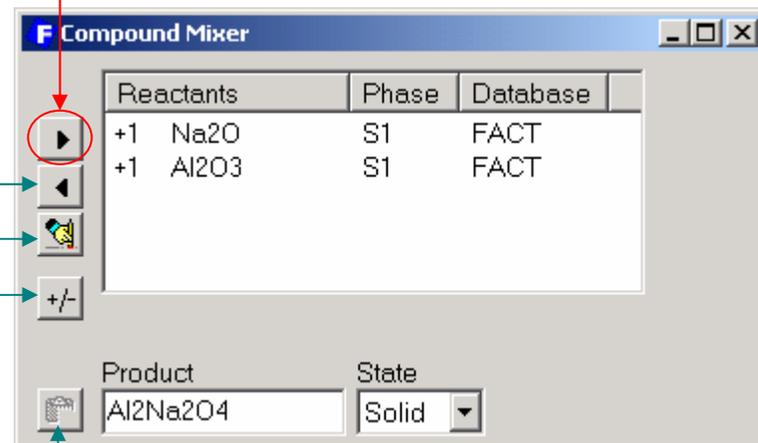
The «Mixer» feature: Example 1, II

3. Drag and drop the phases to the **Compound Mixer** window or use the **Add Phase** button.

Remove the selected phase

Remove all phases

Add or subtract the selected phase



Paste the new compound to a read and write database.

This stores the new compound $\text{Al}_2\text{Na}_2\text{O}_4$ in the database. To store NaAlO_2 you need to use the «**Scale Down**» command in the **Tools** menu.

The «Mixer» feature: Example 1, III

To **scale down** a compound:

1. Save your compound in a r/w database:

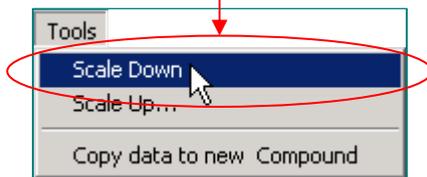
- Select a r/w database.
- Paste your compound.

2. Go to the **Tools** menu and select «**Scale Down**».

The screenshot shows the FactSage software interface. The main window is titled "Energy: calories Pressure: atm Al2Na2O4". The "Formula" field contains "Al2O3". The left pane shows a tree view of databases: FACTBASE, SGPSBASE, ELEMBASE, SGSLBASE, and EXAMBASE. The EXAMBASE database is selected, and the compound Al2Na2O4 is listed under it. The right pane shows the "Al2Na2O4 properties" window, including "Weight: 163.940214 g/mol" and "Modified: 1899 Dec 30". The "Compound Mixer" window is open, showing a table of reactants:

Reactants	Phase	Database
+1 Na2O	S1	FACT
+1 Al2O3	S1	FACT

Below the table, the "Product" is set to "Al2Na2O4" and the "State" is "Solid". The status bar at the bottom indicates "C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 1 compounds read/write".



Now you have the **scaled down** compound AlNaO_2 in your r/w database.

The screenshot shows the EXAMBASE database tree view. The compound AlNaO_2 is highlighted in blue, and $\text{Al}_2\text{Na}_2\text{O}_4$ is listed below it.

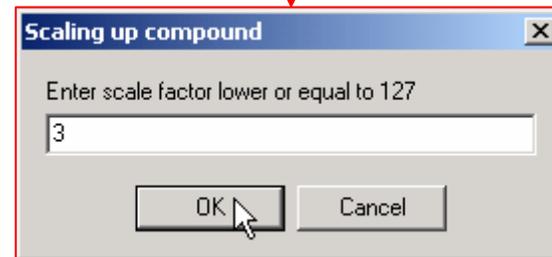
The «Mixer» feature: Example 1, IV

On the other hand, if you want the thermodynamic properties of $\text{Na}_3\text{Al}_3\text{O}_6$, which is 3 times AlNaO_2 , use the **Scale Up** command.

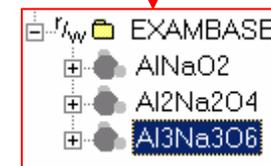
1. Select the compound you want to **scale up**

2. Go to the **Tools** menu and select **Scale Up...**

3. Enter the **scale factor** in the **Scaling up compound** dialog box and press «OK».



Now you have the compound $\text{Al}_3\text{Na}_3\text{O}_6$ in your r/w database



The «Mixer» feature: Example 2

This example shows how to create new data on Li_3N via the synthesis of:
 $\text{Li}_3\text{N} + 3\text{Na} - 3\text{Li}$.

1. Drag and drop the Li_3N , Na and Li phases to **Compound Mixer**.

2. Click on the **Add Phase** button to add 3 Na and 3 Li.

3. Press the **Add and Subtract** button to **subtract 3 Li** from the reactants. This create **Na_3N** as product.

Energy: calories Pressure: atm Li

Formula Li_3N

S1 properties
Heat of form. + Entropy Heat + Temperature of transf.

Form. of S1
 ΔH_{298} (calories) S_{298} (cal/(mol K))
0 6.95148183556405

Phase Name Reference no. Density g/cc
Solid-1 128 0.534

Compound Mixer

Reactants	Phase	Database
+1 Li_3N	S1	FACT
+3 Na	S1	FACT
+3 Li	S1	FACT

Product State
Na3NLI6 Solid

C:\FACT-S1\FACTDATA\F550BASE.CDB (v5.0) 4429 compounds read-only

Compound Mixer

Reactants	Phase	Database
+1 Li_3N	S1	FACT
+3 Na	S1	FACT
-3 Li	S1	FACT

Product State
Na3N Solid

Using known data as **template**

In order to enter data for a **new compound** you may use the data of an **already stored** compound as a **template**.

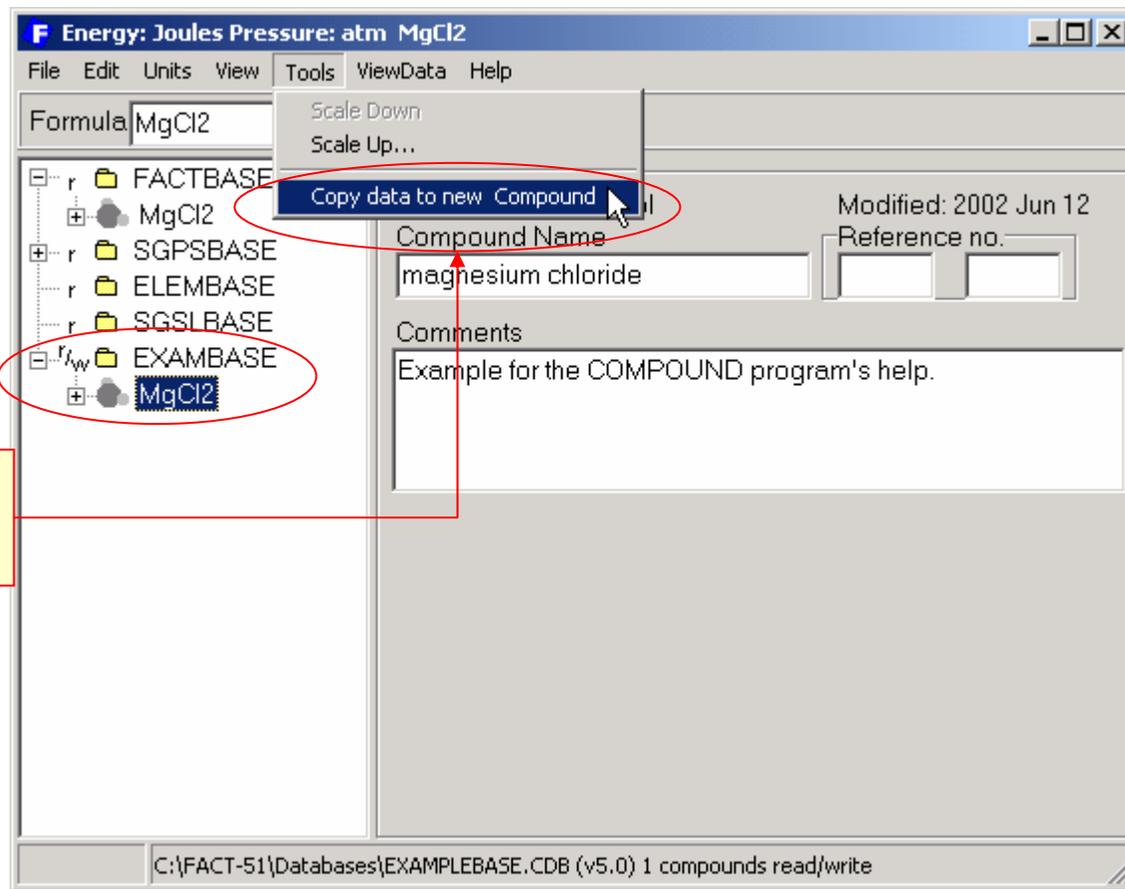
The following two view graphs give an example how to use the **known data for MgCl₂** in order to generate **new data for CaCl₂**.

Using know data as **template**: «**Copy data to new Compound**» option, I

Suppose you do not want to enter the data of a new compound from scratch and that you already have the data of a similar compound in your r/w database. You can use the latter compound's data as a template for the new one by using the **Copy data to new Compound** option in the Tools menu. For example, you have entered data on $MgCl_2$ in EXAMBASE previously and you want to enter data for $CaCl_2$ that is a similar compound:

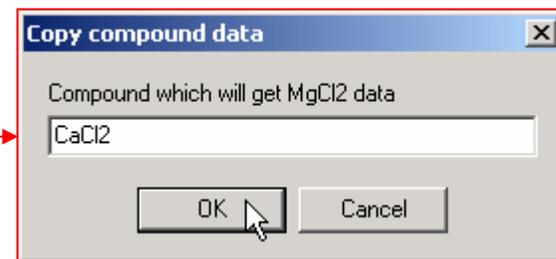
1. Select $MgCl_2$ in EXAMBASE.

2. In the Tools menu, select **Copy data to new Compound**

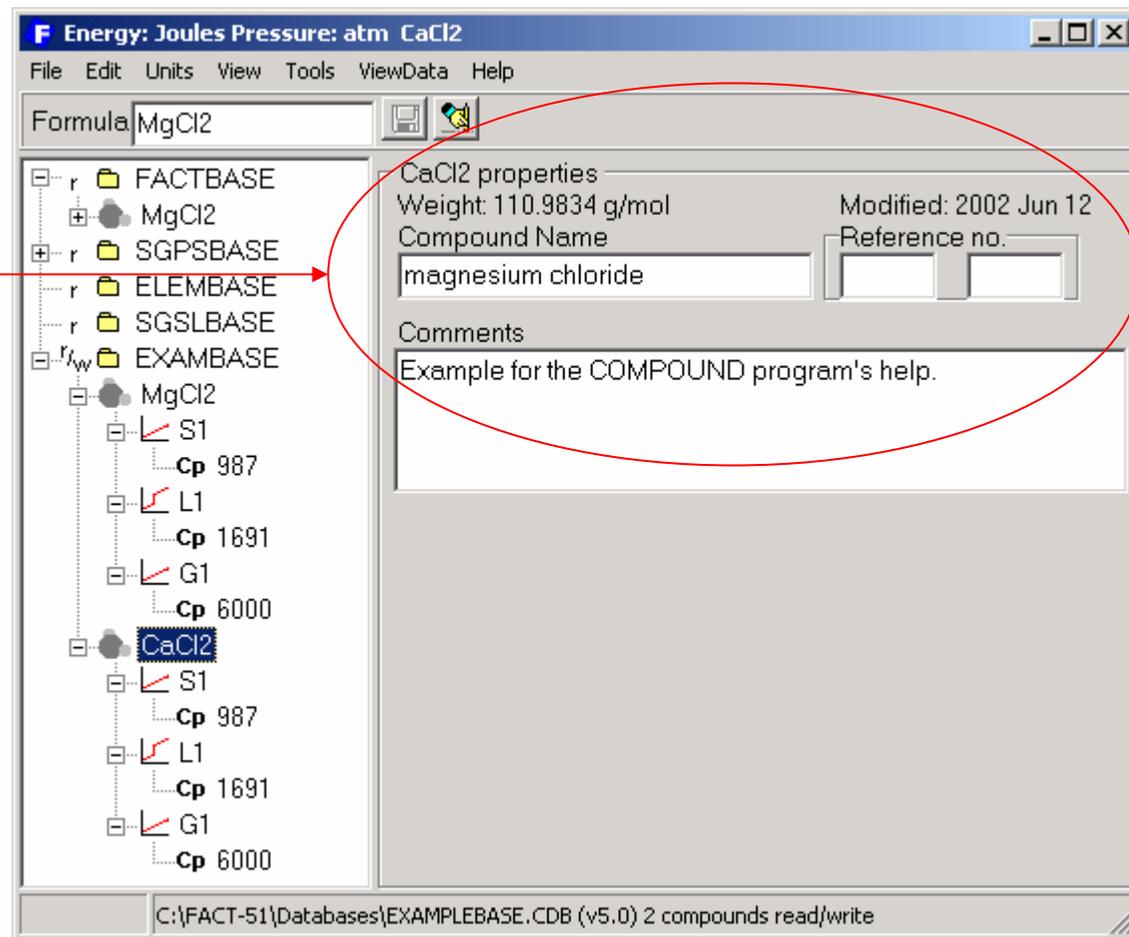


Using know data as **template**, II

3. In the dialog box, enter the new compound **CaCl₂** and press «OK».



4. You now have the **CaCl₂** template.



Changing **Units** of **Energy** or **Pressure**

Compound permits the change of the **units of energy and pressure** both for input and output of the data of a compound.

NOTE: Changing the **energy units** will affect **H, S and C_p** as well as **H, S and G** functions.

Changing the **pressure units** will **ONLY** influence the value of **S_{298}** of gas species, the **first coefficient** of the **S** function, and the **second coefficient** of the **G** function.

Changing Units of Energy or Pressure

Select the new unit from the cascade menu Units.

The screenshot shows the FactSage software interface. The title bar reads "Energy: Joules Pressure: atm MgCl2". The menu bar includes "File", "Edit", "Units", "View", "Tools", "ViewData", and "Help". The "Units" menu is open, showing "Energy" and "Pressure" options. The "Form. of G1" table is visible, showing the current units for ΔH_{298} (Joules) and S_{298} (J/(mol K)).

Form. of G1	ΔH_{298} (Joules)	S_{298} (J/(mol K))
gas	-481145	194.1

Changing Pressure units from atmosphere to bar.

The 'Units' menu is shown with 'Pressure' selected. The 'bar' option is highlighted, indicating the change from atmosphere to bar.

Form. of G1	ΔH_{298} (Joules)	S_{298} (J/(mol K))
gas	-481145	194.209443783103

Changing Energy units from Joules to calories.

The 'Units' menu is shown with 'Energy' selected. The 'calories' option is highlighted, indicating the change from Joules to calories.

Form. of G1	ΔH_{298} (calories)	S_{298} (cal/(mol K))
gas	-114996.414913958	46.3910133843212