SUBSTANCES

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A Chemical Database

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English documentation

The SUBSTANCES package allows you to create a database like file that contains data of various chemicals. These data can be retrieved in the document. An index creation of the chemicals used in the document is directly supported.

Contents

1 Licence and Requirements

Permission is granted to copy, distribute and/or modify this software under the terms of the LaTeX Project Public License, version 1.3 or later (http://www.latex-project.org/lppl.txt). The package has the status "maintained."

SUBSTANCES loads and needs the following packages: expl3,[1] xparse,[2] xtemplate[3] and l3keys2e.[4] It also needs the chemistry package chemmacros.[5]

2 About

The SUBSTANCES package allows you to create a database like file that contains data of various chemicals. These data can be retrieved in the document. An index creation of the chemicals used in the document is directly supported.

3 Options

SUBSTANCES has only a few options:

▸ `draft = true|false` Default: `false`
If set to true all warnings will be errors.

▸ `final = true|false` Default: `true`
The opposite of `draft`.

▸ `index = true|false` Default: `false`
Add index entries when `\chem` is called, see section 7.

▸ `style = <style>` Default: `default`
Load specific style, see section 4.3.

▸ `strict = true|false` Default: `false`
If set to true all warnings will be errors. This option overwrites any `draft` or `final` option that is passed on by the document class.

4 The Database

4.1 Declaring the Chemicals

The data about substances are stored via the command

▸ `\DeclareSubstance{<id>}{<list of properties>}`

An entry could look like this:

```
\DeclareSubstance{NaCl}{
  name    = Sodiumchloride ,
  sum     = NaCl ,
  CAS     = 7647-14-5,
  mass    = 58.44 ,
  mp      = 801 ,
  bp      = 1465 ,
```

[1] CTAN: expl3 [2] CTAN: xparse [3] CTAN: xtemplate [4] CTAN: l3keys2e [5] CTAN: chemmacros

```
    phase   = solid ,
    density = 2.17
}
```

Such entries can either be declared in the document preamble or probably more useful in a file with the ending `.sub`. Such a file can be input in the document via

- `\LoadSubstances{<filename>}` ⟶ input the file *without* specifying the file ending.

  Suppose you have the file `mysubstances.sub` then you input it in the document preamble via `\LoadSubstances{mysubstances}`.

4.2 Available Fields

4.2.1 Always Defined Fields

Below all fields defined by SUBSTANCES are listed.[6]

- `name` required
  The IUPAC name of the substance. This is the only field that *has* to be used. The field's input is parsed with chemmacros' command `\iupac`.

- `sort` optional
  If you plan to use the `index` option you should specify this field to get the sorting of the index right. This then creates index entries `\index{<sort field>@<name field>}`.

- `alt` optional
  An alternative name. The field's input is parsed with chemmacros' command `\iupac`.

- `altsort` optional
  This is the same as the `sort` field but for the alternative name.

- `CAS` optional
  The Chemical Abstract Service (CAS) number. The input needs to be input in the form `<num>-<num>-<num>`.

- `PubChem` optional
  The PubChem number.

The `CAS` field processes the number using the macro `\CAS{<number>}` which is defined like this:

```
\def\@CAS#1-#2-#3{\iupac{#1\-#2\-#3}}
\NewDocumentCommand\CAS{m}{\@CAS#1}
```

You're free to redefine it to your needs.

[6] Look in the file `substances-examples.sub` which is part of this package and should be in the same place as this documentation for example uses.

4.2.2 Style-dependend Fields

SUBSTANCES defines the style 'default' which is loaded if no other style has been specified. It defines the following additional fields and loads the packages chemfig[7] and siunitx.[8]

▸ formula optional
The molecular formula of the substance. The field's input is parsed with chemmacros' command \ch.

▸ structure optional
The structural formula of the substance. The field's input is parsed with chemfig's command \chemfig.

▸ mp optional
The boiling point. The field's entry is input into the siunitx command \SI in the following way: \SI{<field>}{\celsius}.

▸ bp optional
The melting point. The field's entry is input into the siunitx command \SI in the following way: \SI{<field>}{\celsius}.

▸ density optional
The density. The field's entry is input into the siunitx command \SI in the following way: \SI{<field>}{\gram\per\cmc}.

▸ phase optional
The state of aggregation.

▸ pKa optional
The pK_A value. The field's entry is input into the siunitx command \num.

▸ pKa1 optional
The first of several pK_A values. The field's entry is input into the siunitx command \num.

▸ pKa2 optional
The second of several pK_A values. The field's entry is input into the siunitx command \num.

▸ pKb optional
The pK_B values. The field's entry is input into the siunitx command \num.

▸ pKb1 optional
The first of several pK_B values. The field's entry is input into the siunitx command \num.

▸ pKb2 optional
The second of several pK_B values. The field's entry is input into the siunitx command \num.

▸ pictograms optional
The GHS pictograms. This field takes a list of pictogram names as they're input into chemmacros' command \ghspic.

[7] CTAN: chemfig [8] CTAN: siunitx

▸ H optional

The H statements. This field takes a list of numbers as they're input into chemmacros' command \ghs{h}{<number>}.

▸ P optional

The P statements. This field takes a list of pictogram names as they're input into chemmacros' command \ghs{p}{<number>}.

▸ EUH optional

The EUH statements. This field takes a list of pictogram names as they're input into chemmacros' command \ghs{h}{<number>}.

▸ LD50 optional

The Median Lethal Dose (LD50) in mg kg^{-1}. The field's entry is input into the siunitx command \SI in the following way: \SI{<field>}{\milli\gram\per\kilo\gram}.

4.3 Define Custom Styles

4.3.1 Background

You might have other needs for fields than the ones defined by SUBSTANCES and the 'default' style. You can easily define your own style which means that you save a file with the name substances-<style>.def. In it you save the commands you need and use the command \DeclareSubstanceProperty, which is explained in the next section, to declare your own fields.

Please beware that this style file is loaded by the package when the expl3 namespace is active. This means that all spaces are ignored and you need to use ~ if you need a space. It also means that _ and : are letters (as is @). Should you ever decide to call \ExplSyntaxOff to turn off the expl3 namespace *don't* forget to use \ExplSyntaxOn at the end of the file!

4.3.2 Declare New Fields or Change Existing Fields

You might want other fields or change the definition of the predefined ones. For this there's

▸ \DeclareSubstanceProperty*{<field name>}[<pre code>][<post code>]

This command declares a new property field for a substance. The star makes the property a required one which means an error will be issued if a substance is declared without it. The optional arguments <pre code> and <post code> specify any code that should be input directly before or after the field entry, respectively. The <pre code> may end with a command that takes one mandatory argument. In this case the field entry will be its argument.

The following example would define a field EC which uses a custom command to parse the field entry. The European Commission Number (EC) is assigned to chemical substances for regulatory purposes within the European Union by the regulatory authorities.

```
\makeatletter
\def\@EC#1-#2-#3{#1-#2-#3}
\newcommand*\EC[1]{\@EC#1}
\makeatother
\DeclareSubstanceProperty{EC}[\EC]
```

For further examples of the usage of pre and post code look at the definition of the name and the mp field:

```
\DeclareSubstanceProperty*{name}[\iupac]
\DeclareSubstanceProperty{mp}[\SI][{\celsius}]
```

5 Retrieving the Data

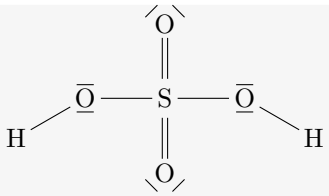
There are two commands defined by SUBSTANCES that allow the retrieving of the data. The command \chem is intended as user command, the command \GetSubstanceProperty can be used to define your own user command (perhaps in your own style file, see section 4.3).

- \chem*[<pre>][<post>]{<id>}[<property>]
- \GetSubstanceProperty{<id>}{<property>}

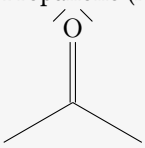
If the command \chem is called without the [<property>] argument the name entry will be called. The starred version calls the alt entry if it is defined and the name entry otherwise. The arguments [<pre>] and [<post>] add arbitrary input before or after the output, respectively.

All of the next examples use the data defined in the file substances-examples.sub that is part of this package, see section 8.

```
\chem{H2SO4}[structure] \newline
\chem{H2SO4} has the boiling point \(\chem[T_b =]{H2SO4}[bp]\) and a
density of \(\chem[\rho =]{H2SO4}[density]\).

Compare the melting points of methane and ethane,
\(\chem[T_m=]{methane}[mp]\) and \(\chem[T_m=]{ethane}[mp]\),
with the boiling points \(\chem[T_b=]{methane}[bp]\) and
\(\chem[T_b=]{ethane}[bp]\).

\chem{NaCl} has the \ac{CAS} number \chem{NaCl}[CAS].

\chem{acetone} (\chem*{acetone}) is the most simple ketone:

\chem{acetone}[structure]
```



Sulfuric Acid has the boiling point $T_b = 279.6\,°C$ and a density of $\rho = 1.8356\,g\,cm^{-3}$.
Compare the melting points of methane and ethane, $T_m = -182\,°C$ and $T_m = -183\,°C$, with the boiling points $T_b = -162\,°C$ and $T_b = -89\,°C$.
Sodiumchloride has the CAS number 7647-14-5.
Propanone (Acetone) is the most simple ketone:



The following code creates table 1.

```
\begin{table}[htp]
\centering\chemsetup[ghsystem]{hide}
\sisetup{scientific-notation=fixed,fixed-exponent=0,per-mode=
  symbol}
\begin{tabular}{l>{\raggedright\arraybackslash}p{.6\linewidth}}
 \toprule
  name               & \chem{methane} \\
  formula            & \chem{methane}[formula] \\
                     & \chem{methane}[structure] \\
 \midrule
  CAS                & \chem{methane}[CAS] \\
  PubChem            & \chem{methane}[PubChem] \\
 \midrule
  boiling point      & \chem{methane}[bp] \\
  melting point      & \chem{methane}[mp] \\
  density            & \chem{methane}[density] \\
  molar mass         & \chem{methane}[mass] \\
 \midrule
                     & \chem{methane}[pictograms] \\
  H statements       & \chem{methane}[H] \\
  P statements       & \chem{methane}[P] \\
 \bottomrule
\end{tabular}
\caption{\label{tab:methane}All properties of \chem{methane} that
  have been
saved in the example database.}
\end{table}
```

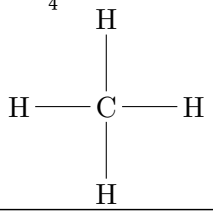
name	Methane
formula	CH_4
	
CAS	74-82-8
PubChem	297
boiling point	−162 °C
melting point	−182 °C
density	0.000 72 g/cm^3
molar mass	16.04 g/mol
	
H statements	H220
P statements	P210, P377, P381, P410 + P403

Table 1: All properties of Methane that have been saved in the example database.

6 Additional Commands

SUBSTANCES provides a few commands that maybe are useful in building custom macros for styles. A field exists if it has been defined with \DeclareSubstanceProperty regardless if it has been used or not. A substance exists if it has been defined with \DeclareSubstance.

- \GetSubstanceProperty{<id>}{<field>} ⟶ You know that already: retrieve the property specified in <field> for a given substance. This command is *not* expandable.
- \RetrieveSubstanceProperty{<id>}{<field>} ⟶ Same as \GetSubstanceProperty but expandable.
- \ForAllSubstancesDo{<code>} ⟶ Loops through all existing substances. Inside <code> #1 may be used to refer to the <id> of the current substance. This command is expandable.
- \AllSubstancesSequence ⟶ A sequence of all substances. This is a sequence of balanced groups each containing the <id> of a substance. This command is expandable.
- \AllSubstancesClist ⟶ A comma separated list of all substances. Every <id> is separated from the next with a comma. This command is expandable.
- \IfSubstancePropertyTF{<id>}{<field>}{<true code>}{<false code>} ⟶ Tests if the property <field> is defined for the substance <id> and returns either <true code> or <false

code>. This command is expandable.

- \IfSubstancePropertyT{<id>}{<field>}{<true code>} → Tests if the property <field> is defined for the substance <id> and returns <true code> if it is. This command is expandable.
- \IfSubstancePropertyF{<id>}{<field>}{<false code>} → Tests if the property <field> is defined for the substance <id> and returns <false code> if it isn't. This command is expandable.
- \IfSubstanceFieldTF{<field>}{<true code>}{<false code>} → Tests if the property <field> exists and returns either <true code> or <false code>. This command is expandable.
- \IfSubstanceFieldT{<field>}{<true code>} → Tests if the property <field> exists and returns <true code> if it does. This command is expandable.
- \IfSubstanceFieldF{<field>}{<false code>} → Tests if the property <field> exists and returns <false code> if it doesn't. This command is expandable.
- \IfSubstanceExistTF{<id>}{<true code>}{<false code>} → Tests if the property <field> exists and returns either <true code> or <false code>. This command is expandable.
- \IfSubstanceExistT{<id>}{<true code>} → Tests if the substance <id> exists and returns <true code> if it does. This command is expandable.
- \IfSubstanceExistF{<id>}{<false code>} → Tests if the substance <id> exists and returns <false code> if it doesn't. This command is expandable.

```
Just to demonstrate how these commands can be used. And to get
our demonstration index filled.\par
\newcounter{substances}
\ForAllSubstancesDo{%
  \ifnum0=\value{substances}\relax
  \else, \fi
  \stepcounter{substances}%
  \chem{#1}%
  \IfSubstancePropertyT{#1}{alt}{
    (\chem*{#1})}}
```

Just to demonstrate how these commands can be used. And to get our demonstration index filled.
Sodiumchloride, Hydrochloric Acid, Nitric Acid, Sulfuric Acid, Methane, Ethane, Propane, Butane (*n*-Butane), Pentane (*n*-Pentane), Hexane (*n*-Hexane), Heptane (*n*-Heptane), Octane (*n*-Octane), Nonane (*n*-Nonane), Decane (*n*-Decane), Propanone (Acetone)

7 Create an Index

When SUBSTANCES is called with index = true the command \chem will add index entries each time it is used. In this case the entries of the fields name, sort, alt and altsort will be expanded during the process. You should keep that in mind if some error arises. It might be due to a \textbf or similar in your database. In this case you either need to replace it with some robust command or put a \noexpand in front of it.

Alternative names as specified in the alt also get an index entry with a reference to the one of the corresponding name field. The entry of the name field in this case gets the alt name appended in braces.

This behaviour is not customizable for the time being. It is planned for future versions of this package, though.

As a demonstration an index for all chemicals used in this documentation is created with the help of the package imakeidx.[9]

7.1 Formatting Commands

The index entries are formatted with the following commands. You can redefine them to your needs. If you do make sure they have the same number of required arguments and are expandable!

- \SubstanceIndexNameEntry#1#2{#1@#2} ⟶ Formats the name if no alt field is given. #1 refers to the sort field entry and #2 refers to the name field entry.
- \SubstanceIndexNameAltEntry#1#2#3{#1@#2 (#3)} ⟶ Formats the name if also the alt field is given. #1 refers to the sort field entry, #2 refers to the name field entry, and #3 to the alt field entry.
- \SubstanceIndexAltEntry#1#2#3{#1@#3|see#2} ⟶ Formats the entry for the alt field. #1 refers to the altsort field entry, #2 refers to the name field entry, and #3 to the alt field entry.

7.2 Using makeidx

Using the option index = true with the standard way to create an index will add the entries \index{<name>} to the index. This means you would mix them with other entries if you have any. Below a sample document is shown that needs to be compiled with pdflatex, makeindex and again with pdflatex.

```
\documentclass{article}
\usepackage[T1]{fontenc}
\usepackage[index]{substances}
\LoadSubstances{substances-examples}

\usepackage{makeidx}
\makeindex
\begin{document}
```

[9] CTAN: imakeidx

```
\newcounter{substances}
\ForAllSubstancesDo{%
  \ifnum0=\value{substances}\relax
  \else, \fi
  \stepcounter{substances}\chem{#1}}

\printindex
\end{document}
```

7.3 Using splitidx

Maybe a seperate index for the chemicals will make more sense. In this case you could use the package splitidx.[10] SUBSTANCES will recognize this and create `\sindex[\jobname-chem]{<name>}` entries each time `\chem` is used. The sample document below needs to be compiled with `pdflatex`, `splitindex` and again with `pdflatex`.

```
\documentclass{article}
\usepackage[T1]{fontenc}
\usepackage[index]{substances}
\LoadSubstances{substances-examples}

\usepackage{splitidx}
\makeindex
\newindex[Chemicals]{\jobname-chem}
\begin{document}

\newcounter{substances}
\ForAllSubstancesDo{%
  \ifnum0=\value{substances}\relax
  \else, \fi
  \stepcounter{substances}\chem{#1}}

\printindex[\jobname-chem]
\end{document}
```

7.4 Using imakeidx

Another way to create multiple indexes is the package imakeidx. SUBSTANCES recognizes its usage and creates index entries `\index[\jobname-chem]{<name>}`. The sample document below needs to be compiled with `pdflatex --shell-escape`.

```
\documentclass{article}
\usepackage[T1]{fontenc}
\usepackage[index]{substances}
```

[10] CTAN: splitidx

```
\LoadSubstances{substances-examples}

\usepackage{imakeidx}
\makeindex[name=\jobname-chem,title=Chemicals]
\begin{document}

\newcounter{substances}
\ForAllSubstancesDo{%
  \ifnum0=\value{substances}\relax
  \else, \fi
  \stepcounter{substances}\chem{#1}}

\printindex[\jobname-chem]
\end{document}
```

8 The Example Database

The following code shows the example database `substances-examples.sub` that is part of this package.

```
% ------------------------------------------------------------------------
% the SUBSTANCES package
%
%   A Chemical Database
%
% ------------------------------------------------------------------------
% Clemens Niederberger
% Web:    https://bitbucket.org/cgnieder/substances/
% E-Mail: contact@mychemistry.eu
% ------------------------------------------------------------------------
% Copyright 2012 Clemens Niederberger
%
% This work may be distributed and/or modified under the
% conditions of the LaTeX Project Public License, either version 1.3
% of this license or (at your option) any later version.
% The latest version of this license is in
%   http://www.latex-project.org/lppl.txt
% and version 1.3 or later is part of all distributions of LaTeX
% version 2005/12/01 or later.
%
% This work has the LPPL maintenance status ‘maintained’.
%
% The Current Maintainer of this work is Clemens Niederberger.
% ------------------------------------------------------------------------
% The substances package consists of the files
%  - substances.sty, substances-default.def, substances-examples.sub,
%    substances_en.tex, substances_en.pdf, README
% ------------------------------------------------------------------------
% If you have any ideas, questions, suggestions or bugs to report, please
% feel free to contact me.
% ------------------------------------------------------------------------
%
```

```
% example database to the package ‘substances’
%
\DeclareChemIUPAC\normal{\textit{n}}
\DeclareSubstance{NaCl}{
  name       = Sodium\|chloride ,
  sort       = Sodiumchloride ,
  formula    = NaCl ,
  CAS        = 7647-14-5,
  mass       = 58.44 ,
  mp         = 801 ,
  bp         = 1465 ,
  phase      = solid ,
  density    = 2.17
}

\DeclareSubstance{HCl}{
  name       = Hydro\|chloric Acid ,
  formula    = HCl ,
  CAS        = 7647-01-0 ,
  pictograms = {acid,exclam} ,
  H          = {314,335} ,
  P          = {260,301+330+331,303+361+353,305+351+338,405,501} ,
  mass       = 36.46 ,
  density    = 1.19 ,
  mp         = -30
}

\DeclareSubstance{HNO3}{
  name       = Nitric Acid ,
  sort       = Nitric Acid ,
  formula    = HNO3 ,
  CAS        = 7697-37-2 ,
  PubChem    = 944 ,
  mass       = 63.01 ,
  density    = 1.51 ,
  mp         = -42 ,
  bp         = 86 ,
  pKa        = -1.37 ,
  pictograms = {flame-O,acid} ,
  H          = {272,314} ,
  P          = {220,280,305+351+338,310}
}

\DeclareSubstance{H2SO4}{
  name       = Sulfuric Acid ,
  sort       = Sulfuric Acid ,
  formula    = H2SO4 ,
  structure  = {H-[:30]\Lewis{26,O}-S(=[2]\Lewis{13,O})(=[6]\Lewis{57,O})-\Lewis{26,
  O}-[:-30]H} ,
  CAS        = 7664-93-9 ,
  PubChem    = 1118 ,
  mass       = 98.08 ,
  density    = 1.8356 ,
  mp         = 10.38 ,
```

```
  bp          = 279.6 ,
  phase       = liquid ,
  pKa         = -3.0 ,
  pKa1        = -3.0 ,
  pKa2        = 1.9 ,
  pictograms  = acid ,
  H           = 314 ,
  P           = {280,301+330+331,309,310,305+351+338} ,
  LD50        = 510
}

\DeclareSubstance{methane}{
  name        = Methane ,
  sort        = Methane ,
  formula     = CH4 ,
  structure   = H-C(-[2]H)(-[6]H)-H ,
  CAS         = 74-82-8 ,
  PubChem     = 297 ,
  pictograms  = {flame,bottle} ,
  H           = 220 ,
  P           = {210,377,381,410+403} ,
  mass        = 16.04 ,
  density     = 0.72e-3 ,
  mp          = -182 ,
  bp          = -162 ,
  phase       = gaseous
}

\DeclareSubstance{ethane}{
  name        = Ethane ,
  sort        = Ethane ,
  formula     = C2H6 ,
  structure   = H-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-H ,
  CAS         = 74-84-0 ,
  PubChem     = 6324 ,
  pictograms  = {flame,bottle} ,
  H           = 220 ,
  P           = {210,377,381,403} ,
  mass        = 30.07 ,
  density     = 0.72e-3 ,
  mp          = -183 ,
  bp          = -89 ,
  phase       = gaseous
}

\DeclareSubstance{propane}{
  name        = Propane ,
  sort        = Propane ,
  formula     = C3H8 ,
  structure   = H-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-H ,
  CAS         = 74-98-6 ,
  pictograms  = {flame,bottle} ,
  H           = 220 ,
  P           = {201,377,381,403} ,
```

```
  mass       = 44.10 ,
  density    = 2.01e-3 ,
  mp         = -188 ,
  bp         = -42 ,
  phase      = gaseous
}

\DeclareSubstance{butane}{
  name       = Butane ,
  sort       = Butane ,
  alt        = \normal\-Butane ,
  altsort    = n-Butane ,
  formula    = C4H10 ,
  structure  = H-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-H ,
  CAS        = 106-97-8 ,
  PubChem    = 7843 ,
  pictograms = {flame,bottle} ,
  H          = {220,280} ,
  P          = {201,377,381,403} ,
  mass       = 58.12 ,
  density    = 2.71e-3 ,
  mp         = -138.3 ,
  bp         = -0.5 ,
  phase      = gaseous
}

\DeclareSubstance{pentane}{
  name       = Pentane ,
  sort       = Pentane ,
  alt        = \normal\-Pentane ,
  altsort    = n-Pentane ,
  formula    = C5H12 ,
  structure  = H-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-C(-[2]H)(-[6]H)-C
  (-[2]H)(-[6]H)-H ,
  CAS        = 109-66-0 ,
  PubChem    = 8003 ,
  pictograms = {flame,health,exclam,aqpol} ,
  H          = {225,304,336,411} ,
  EUH        = 066 ,
  P          = {273,301+310,331,403+235} ,
  mass       = 72.15 ,
  density    = 0.63 ,
  mp         = -130 ,
  bp         = 36 ,
  phase      = liquid
}

\DeclareSubstance{hexane}{
  name       = Hexane ,
  sort       = Hexane ,
  alt        = \normal\-Hexane ,
  altsort    = n-Hexane ,
  formula    = C6H14 ,
  structure  = -[:30]-[:-30]-[:30]-[:-30]-[:30] ,
```

```
  CAS        = 110-54-3 ,
  PubChem    = 8058 ,
  pictograms = {flame,health,exclam,aqpol} ,
  H          = {225,361f,304,373,315,336,411} ,
  P          = {210,240,273,301+310,331,302+352,403+235} ,
  mass       = 86.18 ,
  density    = 0.66 ,
  mp         = -95 ,
  bp         = 69 ,
  phase      = liquid
}

\DeclareSubstance{heptane}{
  name       = Heptane ,
  sort       = Heptane ,
  alt        = \normal\-Heptane ,
  altsort    = n-Heptane ,
  formula    = C7H16 ,
  structure  = -[:30]-[:-30]-[:30]-[:-30]-[:30]-[:-30] ,
  CAS        = 142-82-5 ,
  PubChem    = 8900 ,
  pictograms = {flame,health,exclam,aqpol} ,
  H          = {225,304,315,336,410} ,
  P          = {210,273,301+310,331,302+352,403+235} ,
  mass       = 100.21 ,
  density    = 0.68 ,
  mp         = -91 ,
  bp         = 98 ,
  phase      = liquid
}

\DeclareSubstance{octane}{
  name       = Octane ,
  sort       = Octane ,
  alt        = \normal\-Octane ,
  altsort    = n-Octane ,
  formula    = C8H18 ,
  structure  = -[:30]-[:-30]-[:30]-[:-30]-[:30]-[:-30]-[:30] ,
  CAS        = 111-65-9 ,
  PubChem    = 356 ,
  pictograms = {flame,health,exclam,aqpol} ,
  H          = {225,304,315,336,410} ,
  P          = {210,273,301+330+331,302+352} ,
  mass       = 114.23 ,
  density    = 0.70 ,
  mp         = -56.8 ,
  bp         = 126 ,
  phase      = liquid
}

\DeclareSubstance{nonane}{
  name       = Nonane ,
  sort       = Nonane ,
  alt        = \normal\-Nonane ,
```

```
    altsort    = n-Nonane ,
    formula    = C9H20 ,
    structure  = -[:30]-[:-30]-[:30]-[:-30]-[:30]-[:-30]-[:30]-[:-30] ,
    CAS        = 111-84-2 ,
    PubChem    = 8141 ,
    pictograms = {flame,exclam,health} ,
    H          = {226,304,315,319,332,336,413} ,
    P          = {261,301+310,305+351+338,331} ,
    mass       = 128.26 ,
    density    = 0.72 ,
    mp         = -54 ,
    bp         = 151 ,
    phase      = liquid
  }

  \DeclareSubstance{decane}{
    name       = Decane ,
    sort       = Decane ,
    alt        = \normal\-Decane ,
    altsort    = n-Decane ,
    formula    = C10H22 ,
    structure  = -[:30]-[:-30]-[:30]-[:-30]-[:30]-[:-30]-[:30]-[:-30]-[:30] ,
    CAS        = 124-18-5 ,
    PubChem    = 15600 ,
    pictograms = {flame,health} ,
    H          = {226,304} ,
    P          = {210,260,262,301+310,331} ,
    mass       = 142.29 ,
    density    = 0.73 ,
    mp         = -29.7 ,
    bp         = 174 ,
    phase      = liquid
  }

  \DeclareSubstance{acetone}{
    name       = Propanone ,
    sort       = Propanone ,
    alt        = Acetone ,
    altsort    = Acetone ,
    formula    = C3H6O ,
    structure  = {-[:30](=[2]\Lewis{13,O})-[:-30]} ,
    CAS        = 67-64-1 ,
    PubChem    = 180 ,
    mass       = 58.08 ,
    density    = 0.79 ,
    mp         = -95 ,
    bp         = 56 ,
    pictograms = {flame,exclam} ,
    H          = {225,319,336} ,
    EUH        = {066} ,
    P          = {210,233,305+351+338} ,
    LD50       = 5800
  }
```

```
301 \endinput
```

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