

## BUILDING YOUR RAW MATERIAL LIBRARY

SDScribe™ is most efficiently used as an authoring tool when your raw materials are in the database as Substance records and if you use either SDS templates or stock phrases. The goal of this procedure is to help you create these Substance records. Many users benefit by purchasing live training sessions with us.

### IS YOUR PRODUCT A PURE CHEMICAL OR A MIXTURE?

Ask yourself this question: Is your product a pure chemical, such as Acetone or a mixture made by combining multiple ingredients, such as Acetone, Toluene, and Xylene.

If your product is a pure chemical, then this procedure does not apply. If your product is a mixture, then this procedure applies.



*Pure chemical*



*Mixture of chemicals*

### FORMULATION VERSUS CHEMICAL INGREDIENT LIST WITH WEIGHT PERCENTAGES

A common conundrum is whether it is best to start with a formulation or chemical ingredient list. There is often a big difference between the two. A formulation lists raw materials with the respective weight percent needed to create the product. A raw material could be a pure chemical or a mixture of chemicals. A chemical ingredient list is just that: a list of each chemical in your product with its respective weight percent. The chemical ingredient list (or some part of it) is ultimately included on the safety data sheet in Section 3.

WT. %	STEP #	RAW MATERIAL DESCRIPTION	POUNDS	CHECK OFF	ADD WEIGHTS
55.698	1	DEIONIZED OR TAP WATER	4817.09	<input type="checkbox"/>	
4.000	2	SURFACTANT 1	345.94	<input type="checkbox"/>	
20.000	4	SOFTENER	1729.72	<input type="checkbox"/>	
7.000	5	SURFACTANT 2	605.40	<input type="checkbox"/>	
5.000	6	SODIUM XYLENBULFONATE 30	432.43	<input type="checkbox"/>	
0.300	7	D-LIMONENE	25.95	<input type="checkbox"/>	
0.002	8	FD&C BLUE DYE #1	0.17	<input type="checkbox"/>	
5.000	9	DEIONIZED OR TAP WATER	432.43	<input type="checkbox"/>	
97.000			8389.12		

Product Name: Laundry Detergent      Product Number: \_\_\_\_\_  
 Batch Size: 1000 Gallons      Batch Number: \_\_\_\_\_  
 Batch Price: 11.50 per 100L      Batch Number: \_\_\_\_\_

**MIXING INSTRUCTIONS:**  
 1. Dissolve in 1000 gallons, 2 minutes.  
 2. Add ingredients in the order in which listed below.  
 3. Stir for 45 minutes.  
 4. Sample in QC.

Special Instructions: PROB TO FILLING BOTTLES SETFORM #3 FROM 1100 to 2000 BPS

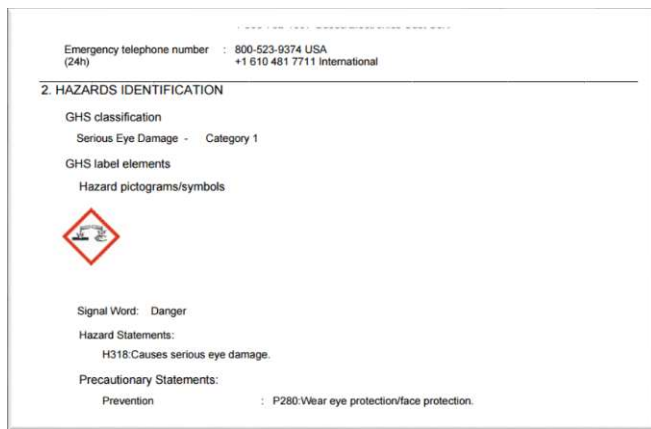
Appearance: <u>Clear slightly thickened liquid</u>	Specific Gravity: <u>1.022</u>	1.022
Color: <u>Light Blue</u>	Pounds per Gallon: <u>8.66</u>	8.66
Odor: <u>Clean</u>	pH: <u>10.5 - 11.0</u>	10.5 - 11.0
Viscosity: <u>70 cP</u>	% Solids: <u>20.4</u>	20.4

To convert pounds to grams multiply pounds by 453.59  
 Example: 0.07 pounds x 453.59 = 31.75 grams

*Formulation or recipe or batch sheet*

## SDSs OF RAW MATERIALS

Collect the SDS of each raw material, preferably in an electronic format. Make sure the SDS is the latest version, which should also be in the new GHS format. If you see the GHS pictograms with red borders (see below), this is a good indication that the SDS is in the GHS format. You should also verify the date is recent, preferably 2014 or later. This is a good time to also inspect Section 3 of the SDSs to see if the raw material is a pure chemical or a mixture. This will make more sense as you proceed.



## ASSEMBLING A MASTER INGREDIENT LIST

Next, create a list or spreadsheet with columns labeled **Raw Material**, **components (chemical name and CAS)**, and **concentration** and **Status**. This is an important step which will save you time since it will help you keep track of which specific chemical component records have already been completed. In the example below, you will note that the Substance records for Dowicil TM 75 with CAS: 4080-31-3 and Hexamethylenetetramine with CAS: 100-97-0 have been marked done.

	A	B	C	D	E
	Raw Material	Components (chemical name)	Components (CAS#)	Concentration	Status
1	Super Cleaner XYZ	DowicilTM 75	4080-31-3	10	done
2	Super Cleaner XYZ	Hexamethylenetetramine	100-97-0	4	done
3	Super Cleaner XYZ	1,3-Dichloropropene	542-75-6	4	
4	Super Cleaner XYZ	Propylene glycol	57-55-6	2	
5	Boric Acid	Boric acid	10043-35-3	100	
6	Acme Cleaner A	Propylene glycol	57-55-6	80	
7	Acme Cleaner A	Ethyl alcohol	64-17-5	2	
8					
9					
10					
11					

You will also note that CAS: 57-55-6 appears in both Super Cleaner XYZ and Acme Cleaner A. So once you have completed the CAS: 57-55-6 and marked it done, you will not need to revisit this record (see below).

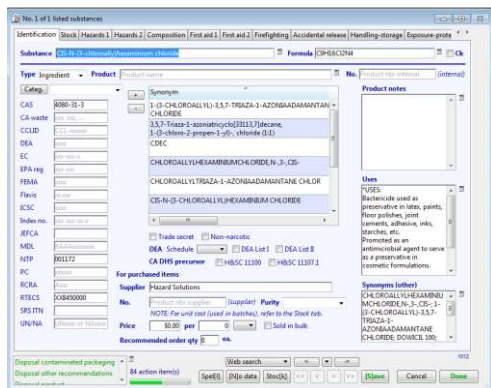
Raw Material	Components (chemical name)	Components (CAS#)	Concentration	Status
Super Cleaner XYZ	Dowicil™ 75	4080-31-3	10	done
Super Cleaner XYZ	Hexamethylenetetramine	100-97-0	4	done
Super Cleaner XYZ	1,3-Dichloropropene	542-75-6	4	done
Super Cleaner XYZ	Propylene glycol	57-55-6	2	done
Boric Acid	Boric acid	10043-35-3	100	
Acme Cleaner A	Propylene glycol	57-55-6	80	done
Acme Cleaner A	Ethyl alcohol	64-17-5	2	

## SDS RECORDS OF COMPONENTS

Once you have identified all the chemical components, you will want to obtain the SDS of each of these as well, preferably in an electronic format. If your raw materials were pure chemicals, then you may be able to use these SDSs. You may consider using online resources of possibly large chemical suppliers of pure chemical, such as Sigma Aldrich.

## OVERALL STRATEGY: COMPONENTS (of raw materials) FIRST AND THEN RAW MATERIALS

The strategy for building a raw material library is 1) to ensure Substance records are built for components of the raw materials; and then 2) ensure Substance records are built for each Raw Material. You will find that the amount of data needed for a Substance record of a raw material is less than its components. You will need to add the completed component record as a component in the Composition tab of its Raw Material.



Substance record of a component

No.	Description	CAS	Type	Categ	GHS	Expos	Regs	Act %	Min %	Max %	Batch amt	Units	Cor
1	CIS-N-(3-chlorallyl)hexaminium chloride	4080-31-3	Ingredient		Avail	2	10.00	10.00	10.00	10.00	0.00		
2	Hexamethylenetetramine	100-97-0	Ingredient		Avail	7	4.00	4.00	4.00	4.00	0.00		
3	1,3-Dichloropropene	542-73-6	Ingredient		Avail	4	7	4.00	4.00	4.00	0.00		
4	Propylene glycol	57-55-6	Ingredient		No	1	7	2.00	2.00	2.00	0.00		
								20.00	20.00	20.00			

4 component(s)

Substance record of a Raw Material with components added in Composition tab

## PROCEDURE FOR CREATING A SUBSTANCE RECORDS OF A COMPONENT and RAW MATERIAL

(Note: Yellow highlighted steps are not required for Raw Materials)

- 1) Select the **Identification** tab.
  - a) Select the **Type** and **Ingredient** if a raw material or **Product** if you produce it
  - b) Select the **Category**, such as surfactant, detergent or fragrance
  - c) Enter the **CAS**, such as 107-41-5
  - d) Enter the **EC**, such as 203-489-0
  - e) Enter **Synonyms**
  - f) Make sure they correspond to actual SDS
  - g) Supplier
    - i) Enter **Hazard Solutions** if we created the library or if you want it displayed in blue text

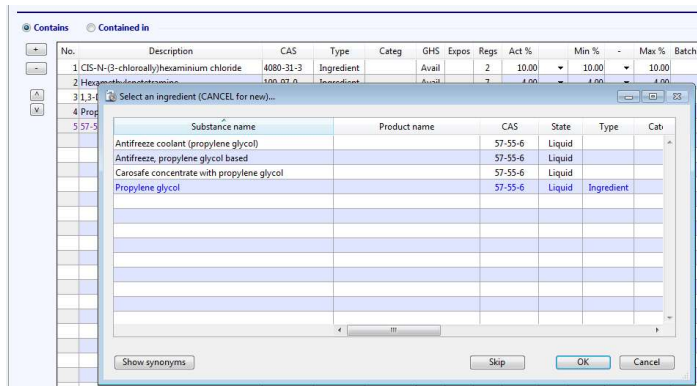
The screenshot shows the 'Identification' tab of a software interface. The substance is 'Glycine glycol'. The 'Type' is 'Ingredient' and the 'Product' is 'Product'. The 'Category' is 'Surfactant'. The 'CAS' is 107-41-5 and the 'EC' is 203-489-0. The 'Synonyms' list includes '2-METHYLPENTANE-2,4-DIOL' and '2,4-Pentanediol, 2-methyl-'. The 'Supplier' is 'Hazard Solutions'. The 'Price' is \$0.00 per unit. The 'Recommended order qty' is 100. The 'Web search' button is visible at the bottom.

- 2) Select the **Hazards 1** tab.
  - a) Enter **GHS Hazard Classification(s)** for the substance
    - i) If **non-hazardous**, check off the **"This Substance has no GHS classifications"**
    - ii) Click on **"Multi"** button and select the applicable GHS hazards. Use Ctrl on your keyboard to select multiple.
    - iii) Click on **"P"** Button to the left of the Hazards table to populate H-Statements, P-Statements, Signal Word and Hazard Pictograms

The screenshot shows the 'Hazards 1' tab of the software interface. The 'GHS only' section is checked. The 'Multi' button is selected. The 'GHS classification 01' is 'Eye damage/irritation (chapter 3.3), Cat. 2A'. The 'GHS classification 02' is 'Skin corrosion/irritation (chapter 3.2), Cat. 2'. The 'GHS hazard 01' is 'H314'. The 'GHS hazard 02' is 'H315'. The 'GHS precaution 01' is 'P284'. The 'GHS precaution 02' is 'P280'. The 'GHS precaution 03' is 'P303+P361+P353'. The 'GHS precaution 04' is 'P337+P313'. The 'Signal word' is 'Warning'. The 'Hazard pictogram' is 'GHS07'. The 'Other hazards (not otherwise classified)' section is empty.

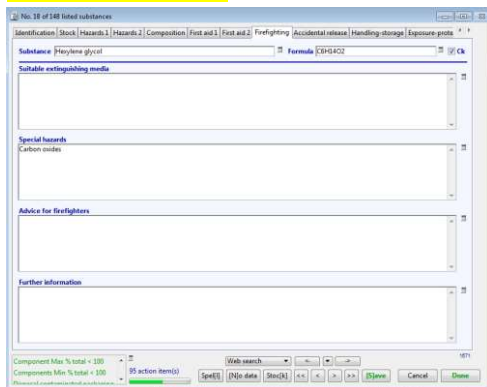
- 3) (For Raw Material Only) Select the **Composition** tab.

- a) Enter the CAS for each component and then select the component record (see image below which includes the word **Ingredient** in the type)
- b) Enter the concentration of the component



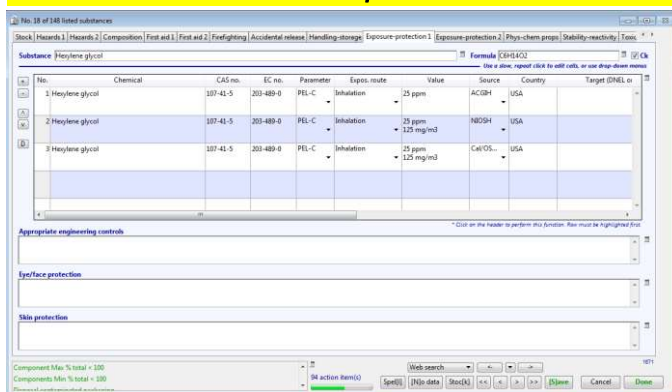
#### 4) Select **Firefighting** tab

- a) Enter **Special hazards**. These are combustion products, which are often carbon oxides, for **organic chemicals**.



#### 5) Select **Exposure-Protection 1** tab.

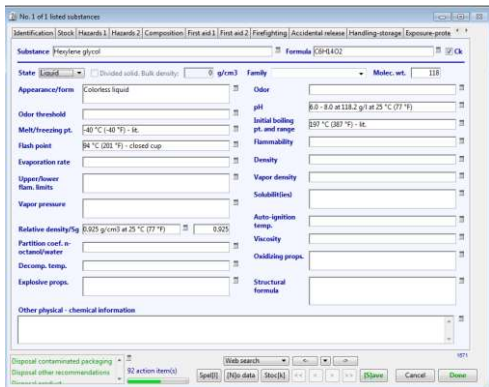
- a) Enter the **OSHA** and **ACGIH exposure limits** in the table if there are any



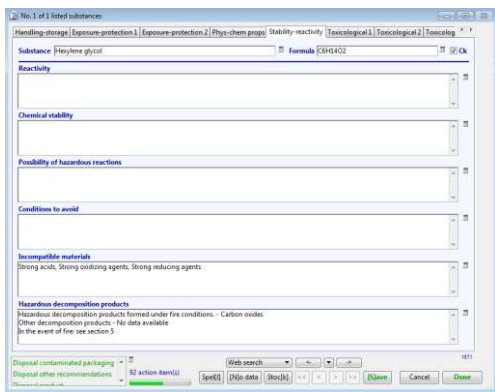
#### 6) Select **Phys-Chem Properties** tab.

- a) Enter **State**
- b) Enter **Appearance/form**
- c) Enter **pH**
- d) Enter **Molecular Weight**.
- e) Enter **Melting, Boiling and Flash Point**

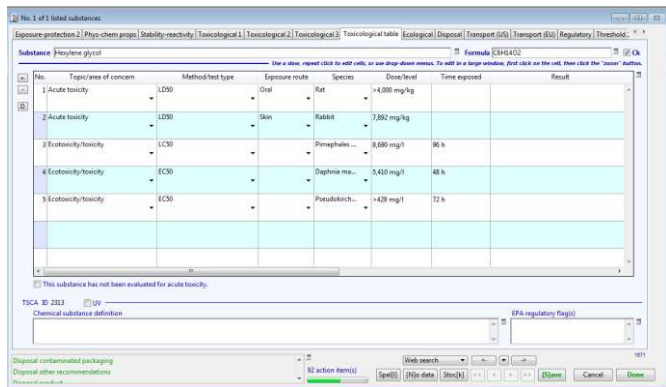
- f) Enter **Relative density/Sg.** Type into first cell. The cell to the right will automatically fill in
- g) Click **Save**



- 7) Select **Stability-Reactivity** tab.
  - a) Enter **Incompatible materials**
  - b) Enter **Hazardous decomposition products.**
  - c) Click **Save**



- 8) Select **Toxicological Table** tab.
  - a) Enter **Oral/dermal/inhalation LD50s/LC50s.**
  - b) Enter **Carcinogenicity.**
  - c) Enter **Ecotoxicity, Etc . . .**
  - d) Click **Save**



- 9) Select **Regulatory** tab.
  - a) Enter **Federal and state regulations/lists.**

b) Make sure format is consistent with CAS-No. first before CAS (e.g., CAS-No. 60-00-4).

1 Massachusetts Right To Know Components	Edetic acid CAS-No. 60-00-4	6/4/20
2 New Jersey Right To Know Components	Edetic acid	6/4/20

c)

d) Put in preferred sort order by right clicking on Regulation.

e) Click Save

No.	Regulation (click to reorder)	Applicability	Created	Modified
1	SARA 302 Components	No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.	2/8/2007 14:58:00 Default user	2/8/2007 14:57:56 Default Expression
2	SARA 303 Components	This material does not contain any items of components with known CAS numbers that exceed the threshold (Or Mixes) reporting levels established by SARA Title III, Section 303.	2/8/2007 14:58:00 Default user	2/8/2007 14:57:56
3	SARA 311/312 Hazards	Acute Health Hazard, Chronic Health Hazard	2/8/2007 14:58:00 Default user	2/8/2007 14:57:52
4	Massachusetts Right To Know Components	Phosgene glycol CAS number: 337-41-9	2/8/2007 14:58:00 Default user	2/8/2007 14:57:52
5	Pennsylvania Right To Know Components	Phosgene glycol CAS number: 337-41-9	6/4/2005 16:54:48 Default user	2/8/2007 14:57:52
6	New Jersey Right To Know Components	Phosgene glycol CAS number: 337-41-9	6/4/2005 16:54:38 Default user	2/8/2007 14:57:51
7	California Prop 65 Components	This product does not contain any chemical listed by State of California as being known to cause cancer, birth defects, or any other reproductive harm.	2/8/2007 14:58:00 Default user	2/8/2007 14:58:00

Select the applicable regulations from the drop down

No. 2 of 3 listed substances

Substance: Sodium hydroxide    Formula: NaOH

No.	Regulation (click to reorder)	Chemical name: Sodium hydroxide CAS number: 1310-73-2	6/9/2015
1	Massachusetts Right To Know Components	Chemical name: Sodium hydroxide CAS number: 1310-73-2	6/9/2015
2	New Jersey Right To Know Components	Common name: SODIUM HYDROXIDE CAS number: 1310-73-2	6/4/2015
3	Pennsylvania Right To Know Components	Chemical name: Sodium hydroxide CAS number: 1310-73-2	6/4/2015
4	Massachusetts Right To Know Components	Chemical name: Sodium hydroxide CAS number: 1310-73-2	6/4/2015
5	New Jersey Right To Know Components	Common name: SODIUM HYDROXIDE CAS number: 1310-73-2	6/4/2015

Disposal contaminated packaging  
Disposal other recommendations: 89 action item(s)

Web search    [N]o data    [S]ave    Cancel    Done

You can create preferred order by right clicking on "Regulatory" heading