



# Informatics-Based Approaches for Managing and Curating Exposure Data

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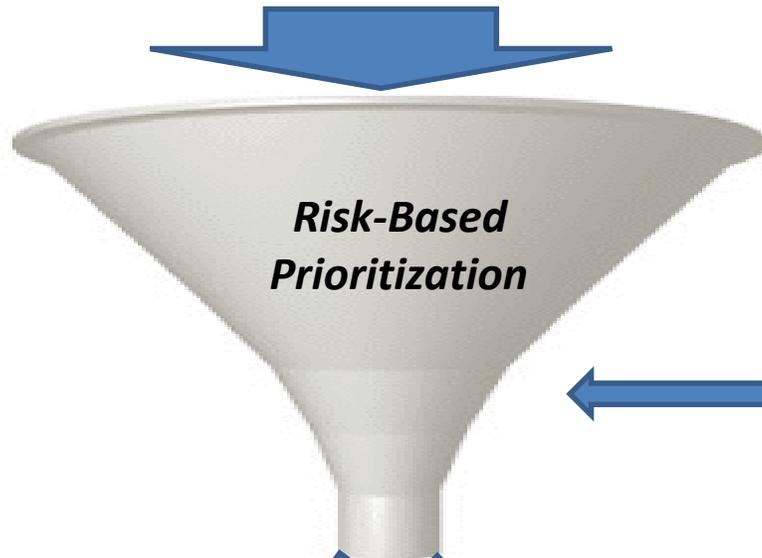
*Computational Toxicology*  
*Communities of Practice Webinar*  
*September 24, 2020*



# Disclaimer

**The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA**

2019: 40,655 chemicals on the active TSCA Inventory



*Risk-Based  
Prioritization*

Low priority

High priority  
Risk  
Evaluation

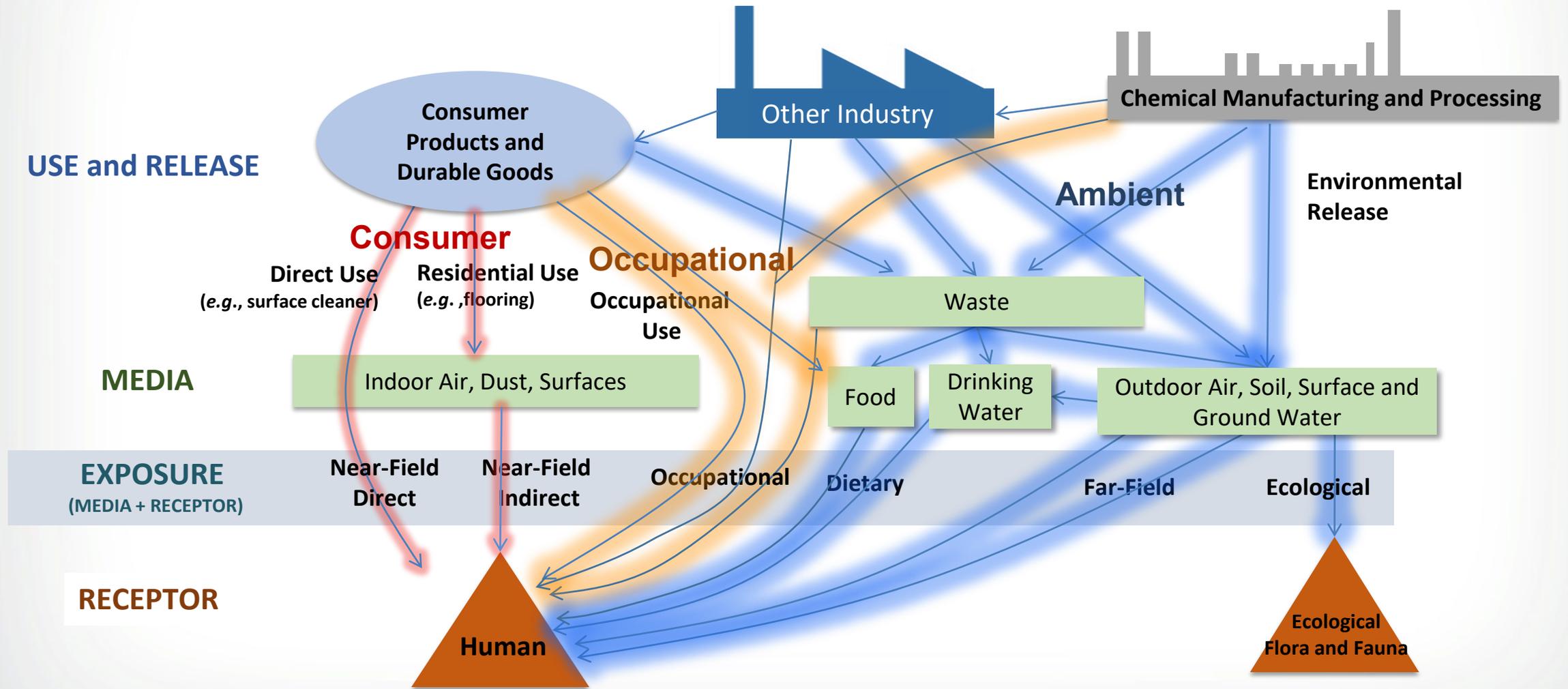
**TSCA section 6(b)(1)(A):**

- Exposure potential of the chemical substance

- *Problem formulation and scoping activities*
- *Exposure assessments*

- “Chemical exposure evaluations require ***information to estimate exposure for a variety of high-priority pathways***, including ...consumer products and materials in the indoor environment, as well as occupational, ambient and ecological pathways.”

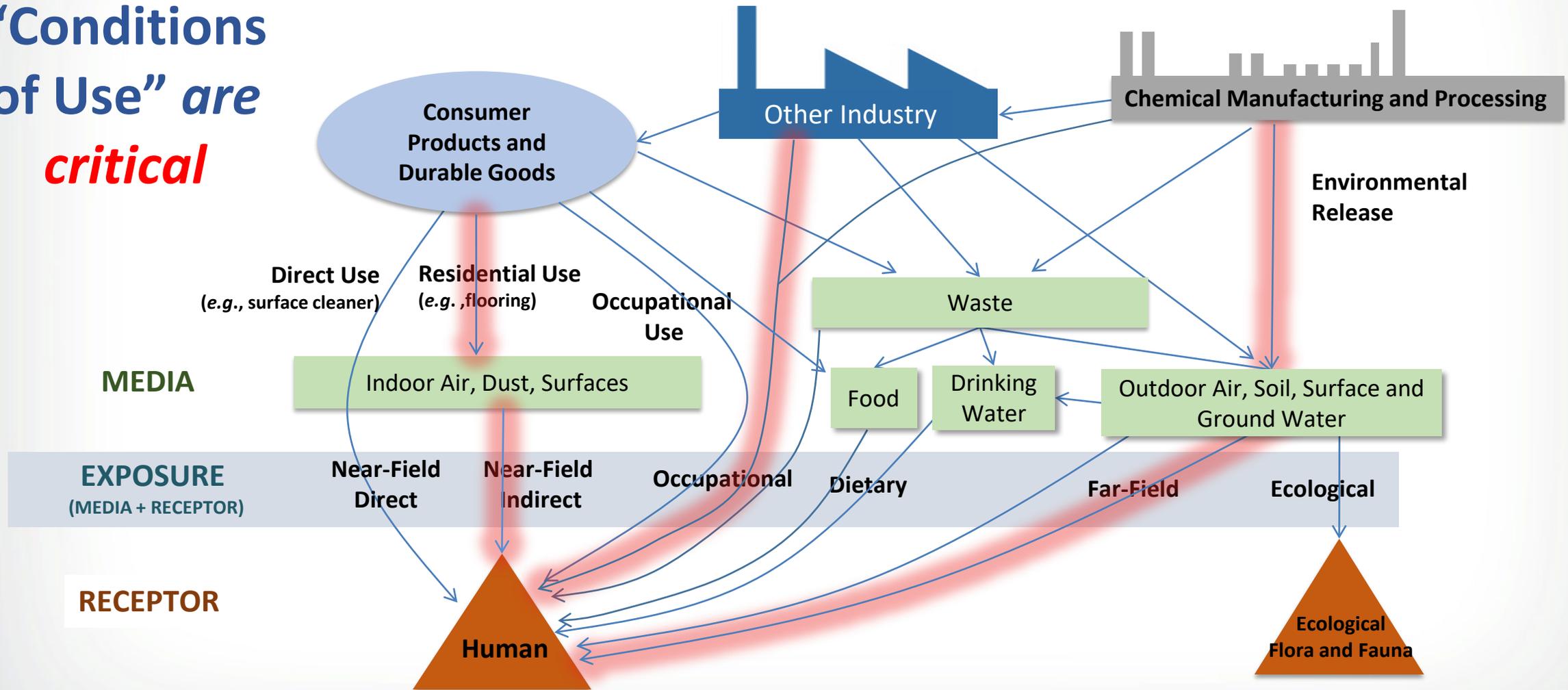
# Exposure Pathways





# Identification of Relevant Pathways for a Chemical

“Conditions of Use” are *critical*





# Developing the Required Chemical Use Data to Support TSCA

- “Conditions of use” under TSCA means “the circumstances, as determined by the Administrator, under which a chemical substance is intended, known, or reasonably foreseen to be manufactured, processed, distributed in commerce, used or disposed of”.
- CCTE is collecting, curating, and storing large amounts of publicly available chemical use information
  - **500,000+** documents
  - **3.9 million** chemical records
  - Qualitative and quantitative information
- Developing tools and data infrastructure to directly support risk-based decision making
  - Seamless and timely delivery of data to EPA partners and the public
  - Quality assurance and data provenance





# Chemical Use Types and Data Sources

- Specific consumer use
  - Use in particular products or product types



Page 1 of 5  
The Procter & Gamble Company  
P & G Household Care  
Fabric & Home Care Innovation Center  
5299 Spring Grove Avenue  
Cincinnati, OH 45217-1087

## MATERIAL SAFETY DATA SHEET

MSDS: RQ1305623  
RQ1400356

Issue Date: 02/05/2014

### SECTION I - PRODUCT IDENTIFICATION

Identity: **Liquid Laundry Detergent\***

**This MSDS applies to the following Liquid Tide Detergent Brands:**

**Tide Simply Fresh Refreshing Breeze  
Tide Simply Fresh Daybreak Fresh**

Emergency Telephone Number: 24hr P&G Operator – 1-800-879-8433

**\* This MSDS applies to all uses/handling of these products in a retail package for consumer home use.**

### SECTION II - HAZARDS IDENTIFICATION

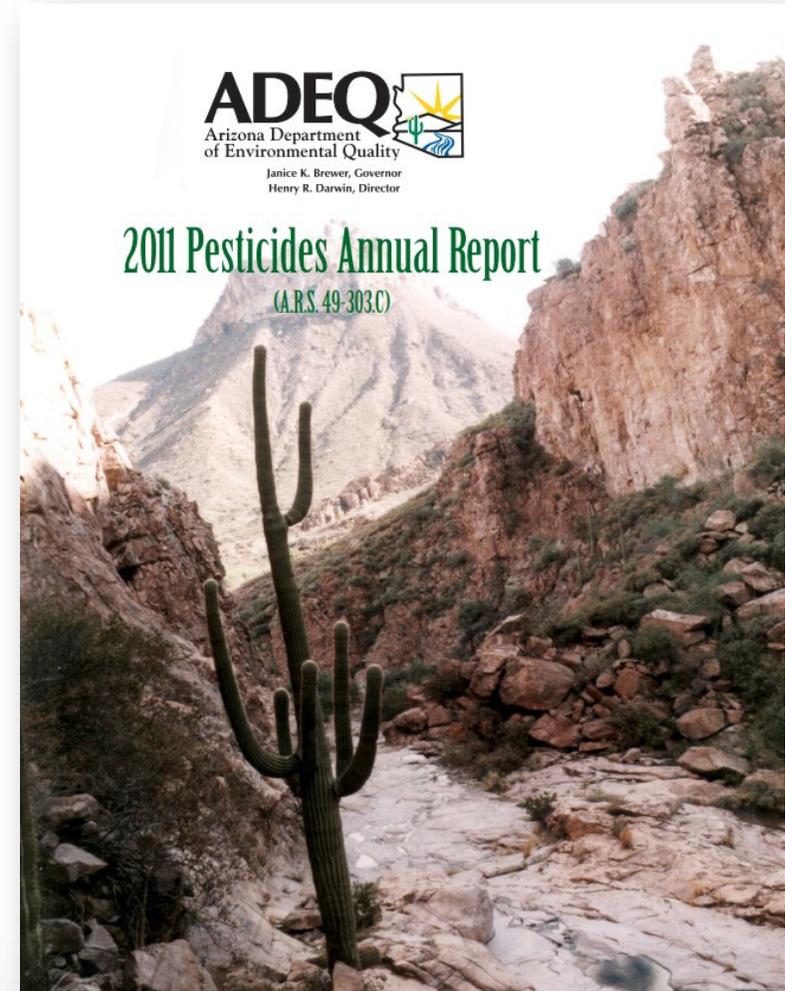
#### Health Hazards (Acute and Chronic):

Ingestion: May cause transient gastrointestinal irritation.  
Eye Contact: May cause mild, transient irritation.  
Inhalation: Transient irritation with prolonged exposure to concentrated material.

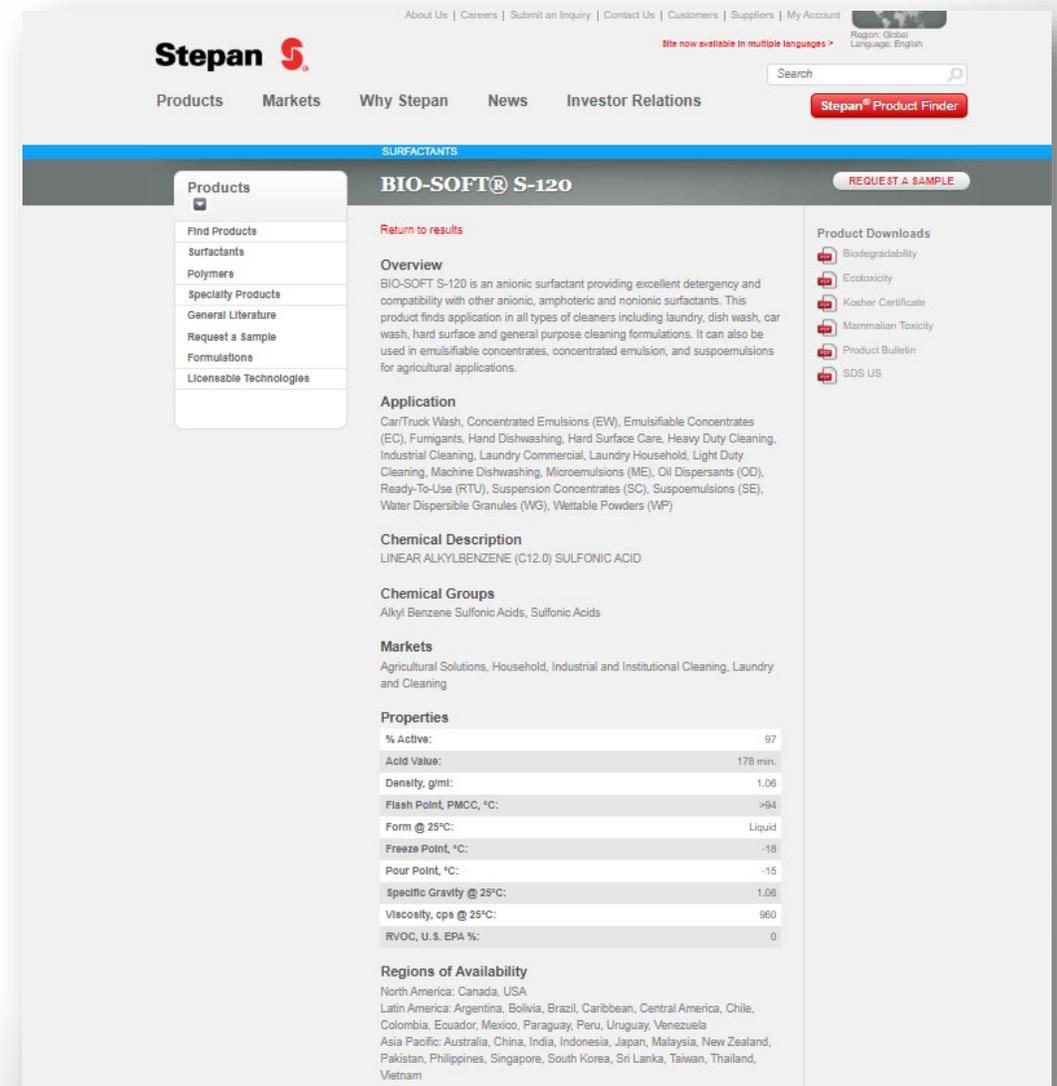
#### Signs and Symptoms of Exposure:

Ingestion: May result in nausea, vomiting, and/or diarrhea.  
Eye Contact: May cause stinging, tearing, itching, swelling, and/or redness.  
Skin: Prolonged contact with concentrated material may be drying or transiently irritating to skin.

- Specific consumer use
  - Use in particular products or product types
- General use
  - Use in particular commercial or industrial sectors



- Specific consumer use
  - Use in particular products or product types
- General use
  - Use in particular commercial or industrial sectors
- Functional use
  - Role the chemical plays in different consumer products or industrial processes



The screenshot shows the Stepan website product page for BIO-SOFT® S-120. The page includes a navigation menu with 'Products', 'Markets', 'Why Stepan', 'News', and 'Investor Relations'. A search bar and a 'Stepan® Product Finder' button are also visible. The main content area is titled 'SURFACTANTS' and features a 'REQUEST A SAMPLE' button. The product details are organized into sections: Overview, Application, Chemical Description, Chemical Groups, Markets, Properties, and Regions of Availability. The Properties section contains a table with various chemical and physical characteristics.

Property	Value
% Active:	97
Acid Value:	178 min.
Density, g/ml:	1.08
Flash Point, PMCC, °C:	>94
Form @ 25°C:	Liquid
Freeze Point, °C:	-18
Pour Point, °C:	-15
Specific Gravity @ 25°C:	1.08
Viscosity, cps @ 25°C:	960
RVOC, U.S. EPA %:	0



## Chemicals and Products Database (CPDat) and ChemExpoDB

Integrated family of exposure databases, linking data across multiple exposure data streams

- Different types of chemical use data (“CPDat”, Dionisio et al. *Scientific Data*, 2018)
- Other exposure data (e.g., measured concentrations of chemicals in biological and environmental media)



## Factotum

Internal application for the extraction, management, and curation of exposure factor data into ChemExpoDB

- Facilitates loading of large quantities of data into ChemExpoDB (raw documents and curated data)
- Allows for tracking of data provenance
- Provides tools for curating data
- Disseminates data to other EPA users (e.g., program offices)



ChemExpoDB



Factotum



Cleaned,  
curated,  
harmonized  
data set



Web services



CompTox Chemicals Dashboard