

# Package ‘chem.databases’

July 22, 2025

**Title** Collection of 3 Chemical Databases from Public Sources

**Version** 1.0.0

**Maintainer** Irucka Embry <iembry@ecoccs.com>

**Depends** R (>= 3.5.0)

**Suggests** data.table (>= 1.10.2), install.load, spelling

**Description** Contains the Multi-Species Acute Toxicity Database (CAS & SMILES columns only) [United States (US) Department of Health and Human Services (DHHS) National Institutes of Health (NIH) National Cancer Institute (NCI), ``Multi-Species Acute Toxicity Database", <<https://cactus.nci.nih.gov/download/acute-toxicity-db/>>] combined with the Toxic Substances Control Act (TSCA) Inventory [United States Environmental Protection Agency (US EPA), ``Toxic Substances Control Act (TSCA) Chemical Substance Inventory", <<https://www.epa.gov/tsca-inventory/how-access-tsca-inventory>] and <<https://cdxapps.epa.gov/oms-substance-registry-services/substance-list-details/169>>] and the Agency for Toxic Substances and Disease Registry (ATSDR) Database [United States (US) Department of Health and Human Services (DHHS) Centers for Disease Control and Prevention (CDC)/Agency for Toxic Substances and Disease Registry (ATSDR), ``Agency for Toxic Substances and Disease Registry (ATSDR) Database", <<https://cdxapps.epa.gov/oms-substance-registry-services/substance-list-details/105>>] in 2 data sets. One data set has a focus on the latter 2 databases and one data set focuses on the former database. Also contains the collection of chemical data from Wikipedia compiled in the US EPA CompTox Chemicals Dashboard [United States Environmental Protection Agency (US EPA) / Wikimedia Foundation, Inc. ``CompTox Chemicals Dashboard v2.2.1", <<https://comptox.epa.gov/dashboard/chemical-lists/WIKIPEDIA>>].

**URL** <https://gitlab.com/iembry/chem.databases>

**BugReports** <https://gitlab.com/iembry/chem.databases/-/issues>

**License** CC0

**Copyright** This software is in the public domain because it contains mostly materials that originally came from the United States (US) Environmental Protection Agency (US EPA), the United States (US) Department of Health and Human Services (DHHS) Centers for Disease Control and Prevention (CDC)/ Agency for Toxic Substances and Disease Registry (ATSDR), or the United States (US) Department of Health and Human Services (DHHS) National Institutes of Health (NIH) National Cancer Institute (NCI).

**Language** en-US

**Encoding** UTF-8

**LazyData** true

**LazyDataCompression** xz

**RoxygenNote** 7.2.3

**NeedsCompilation** no

**Author** Irucka Embry [aut, cre]

**Repository** CRAN

**Date/Publication** 2023-09-21 13:40:05 UTC

## Contents

atsdr_tsca_ld50_a . . . . .	2
atsdr_tsca_ld50_b . . . . .	3
chem_wiki . . . . .	4

<b>Index</b>	<b>5</b>
--------------	----------

---

atsdr_tsca_ld50_a	<i>Collection of ATSDR, NCI, and TSCA Chemical Databases Combined Focused on ATSDR and TSCA Data</i>
-------------------	--

---

## Description

A table containing chemical data from 3 US federal agencies.

## Usage

```
atsdr_tsca_ld50_a
```

## Format

A data.table data frame with 69,557 rows and 4 variables:

itemCASChemical Abstracts Service (CAS) Registry Number itemSubstance NamePreferred  
Chemical Substance Name itemRegistry NameRegistry Chemical Name itemSMILESSimpli-  
fied Molecular-Input Line-Entry System (SMILES) Chemical Structural Notation

**Source**

1. United States (US) Department of Health and Human Services (DHHS) Centers for Disease Control and Prevention (CDC)/Agency for Toxic Substances and Disease Registry (ATSDR), "Agency for Toxic Substances and Disease Registry (ATSDR) Database", <https://cdxapps.epa.gov/oms-substance-registry-services/substance-list-details/105>.
2. United States (US) Department of Health and Human Services (DHHS) National Institutes of Health (NIH) National Cancer Institute (NCI), "Multi-Species Acute Toxicity Database", <https://cactus.nci.nih.gov/download/acute-toxicity-db/>.
3. United States Environmental Protection Agency (US EPA), "Toxic Substances Control Act (TSCA) Chemical Substance Inventory", <https://www.epa.gov/tsca-inventory/how-access-tsca-inventory> and <https://cdxapps.epa.gov/oms-substance-registry-services/substance-list-details/169>.

atsdr\_tsca\_ld50\_b

*Collection of ATSDR, NCI, and TSCA Chemical Databases Combined  
Focused on NCI Data*

**Description**

A table containing chemical data from 3 US federal agencies.

**Usage**

atsdr\_tsca\_ld50\_b

**Format**

A data.table data frame with 80,081 rows and 4 variables:

itemCASChemical Abstracts Service (CAS) Registry Number itemSubstance NamePreferred  
Chemical Substance Name itemRegistry NameRegistry Chemical Name itemSMILESSimpli-  
fied Molecular-Input Line-Entry System (SMILES) Chemical Structural Notation

**Source**

1. United States (US) Department of Health and Human Services (DHHS) Centers for Disease Control and Prevention (CDC)/Agency for Toxic Substances and Disease Registry (ATSDR), "Agency for Toxic Substances and Disease Registry (ATSDR) Database", <https://cdxapps.epa.gov/oms-substance-registry-services/substance-list-details/105>.
2. United States (US) Department of Health and Human Services (DHHS) National Institutes of Health (NIH) National Cancer Institute (NCI), "Multi-Species Acute Toxicity Database", <https://cactus.nci.nih.gov/download/acute-toxicity-db/>.
3. United States Environmental Protection Agency (US EPA), "Toxic Substances Control Act (TSCA) Chemical Substance Inventory", <https://www.epa.gov/tsca-inventory/how-access-tsca-inventory> and <https://cdxapps.epa.gov/oms-substance-registry-services/substance-list-details/169>.

---

chem\_wiki

*CompTox Chemicals Dashboard From Wikipedia*

---

### Description

A table containing chemical data from the CompTox Chemicals Dashboard which is derived from various Wikipedia pages.

### Usage

chem\_wiki

### Format

A data.table data frame with 19,239 rows and 9 variables:

itemCASChemical Abstracts Service (CAS) Registry Number itemSubstance NamePreferred Chemical Substance Name itemIUPAC NameIUPAC Chemical Name itemMolecular FormulaChemical Molecular Formula itemSMILESSimplified Molecular-Input Line-Entry System (SMILES) Chemical Structural Notation itemInChIInternational Chemical Identifier (InChI) Chemical Structural Notation itemInChIKeyHashed Version of the InChI itemAverage MassAverage Chemical Molecular Mass itemMonoisotopic MassSingle Chemical Isotope Mass

### Source

United States Environmental Protection Agency (US EPA) / Wikimedia Foundation, Inc. "CompTox Chemicals Dashboard v2.2.1", <https://comptox.epa.gov/dashboard/chemical-lists/WIKIPEDIA>.

# Index

## \* datasets

atsdr\_tsca\_ld50\_a, 2

atsdr\_tsca\_ld50\_b, 3

chem\_wiki, 4

atsdr\_tsca\_ld50\_a, 2

atsdr\_tsca\_ld50\_b, 3

chem\_wiki, 4