Package ‘chem.databases’

September 21, 2023

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>]
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
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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).

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R topics documented:

- atsdr_tsca_ld50_a
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atsdr_tsca_ld50_a Collection of ATSDR, NCI, and TSCA Chemical Databases Combined Focused on ATSDR and TSCA Data

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:

- itemCAS: Chemical Abstracts Service (CAS) Registry Number
- itemSubstance Name: Preferred Chemical Substance Name
- itemRegistry Name: Registry Chemical Name
- itemSMILES: Simplified Molecular-Input Line-Entry System (SMILES) Chemical Structural Notation
Source


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**atsdr_tsca_ld50_b**

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

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**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:

- itemCAS: Chemical Abstracts Service (CAS) Registry Number
- itemSubstanceName: Preferred Chemical Substance Name
- itemRegistryName: Registry Chemical Name
- itemSMILES: Simplified Molecular-Input Line-Entry System (SMILES) Chemical Structural Notation

**Source**


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:
- itemCAS: Chemical Abstracts Service (CAS) Registry Number
- itemSubstanceName: Preferred Chemical Substance Name
- itemIUPACName: IUPAC Chemical Name
- itemMolecularFormula: Chemical Molecular Formula
- itemSMILES: Simplified Molecular-Input Line-Entry System (SMILES) Chemical Structural Notation
- itemInChI: International Chemical Identifier (InChI) Chemical Structural Notation
- itemInChIKey: Hashed Version of the InChI
- itemAverageMass: Average Chemical Molecular Mass
- itemMonoisotopicMass: Single 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.
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