



EPA Tools and Resources Webinar

CompTox Dashboard:

Data and Tools to Support Chemical and Environmental Risk Assessment

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National Center for Computational Toxicology

US EPA Office of Research and Development

August 22, 2018

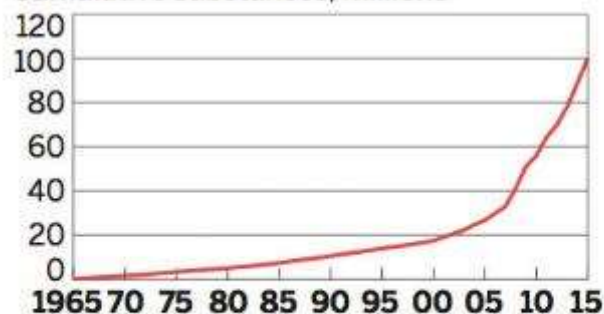
Problem: Too Many Chemicals, too Few Resources

- Timely characterization of human and ecological risk posed by thousands of existing and emerging chemicals is a critical challenge to protect public health and the environment
 - Significant growth in the number of substances and chemicals / and the associated data
 - Nearly 60% of chemicals on various EPA lists have acute toxicity data, 30% have data on other types of toxicity

Chemical & Engineering News 2015 93(32), p14

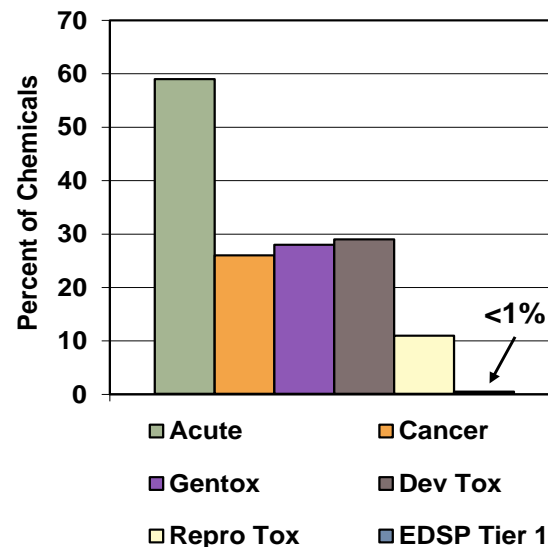
EXPONENTIAL GROWTH In the past 10 years, CAS has added 75 million entries to its registry—triple the number added during the first 40 years.

Cumulative substances, millions



SOURCE: CAS

Data for
Environmental Chemicals

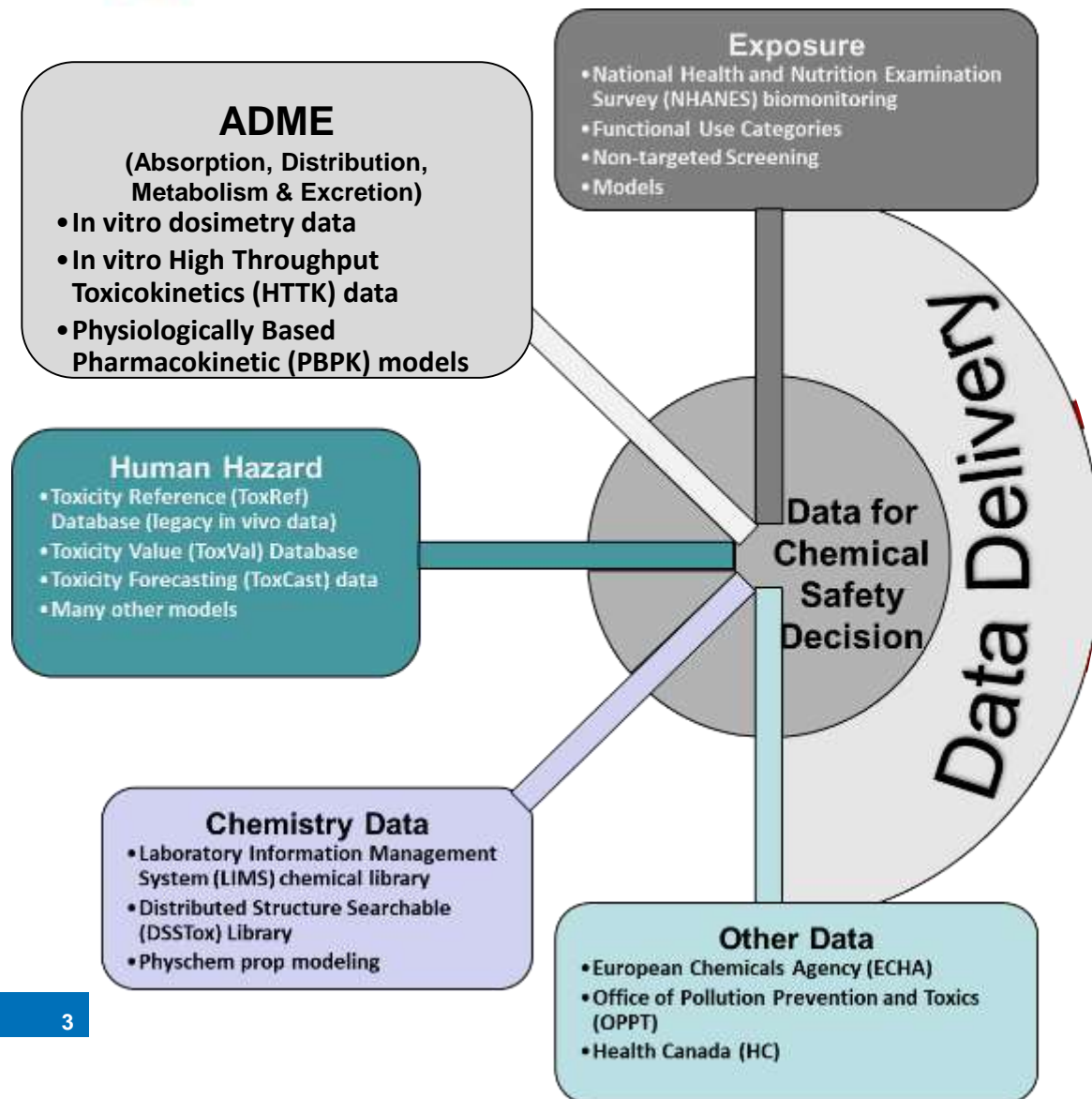


Modified from Judson *et al.*, EHP 2010

Approach

- **Develop a “one-stop-shop” for data as an integration node for environmental chemical data to support EPA and partner decision making:**
 - Centralized location for relevant chemical safety data:
 - Chemistry, exposure, hazard, dosimetry
 - Combination of existing data and predictive models
 - Publicly accessible, periodically updated, curated
- **Ease of access to data results in efficiency and accelerates chemical risk assessment**


Approach



A publicly accessible website delivering:


- ~760,000 chemicals with related property data
- Experimental and predicted physicochemical property data
- Integration to “biological assay data” for 1000’s of chemicals
- Information regarding consumer products containing chemicals
- Generalized Read-Across (GenRA) module
- Links to other agency websites and public data resources
- “Literature” searches for chemicals using public resources
- “Batch searching” for thousands of chemicals
- Downloadable Open Data for reuse and repurposing
- Many features (only highlighting a few)
- Access to multiple tools (direct data interpolation and predictive) for multiple disciplines

EPA CompTox Dashboard: Live Demo

 United States Environmental Protection Agency

HomeAdvanced SearchBatch SearchListsPredictionsDownloads

AaAaAa

761 Thousand Chemicals

☐ Identifier substring search

[See what people are saying: read the dashboard commercial](#)


Latest News

[Read more news](#)

A YouTube video regarding using the Dashboard for Non-Targeted Analysis

March 7th, 2018 at 9:43:35 AM

◀ A YouTube video discussing the application of the CompTox Chemistry Dashboard to support non-targeted analysis by mass spectrometry is available. This short video summarizes the advantages of the dashboard in terms of data quality and focused data set for environmental non-targeted analysis. [View it here on Youtube.](#) ▶



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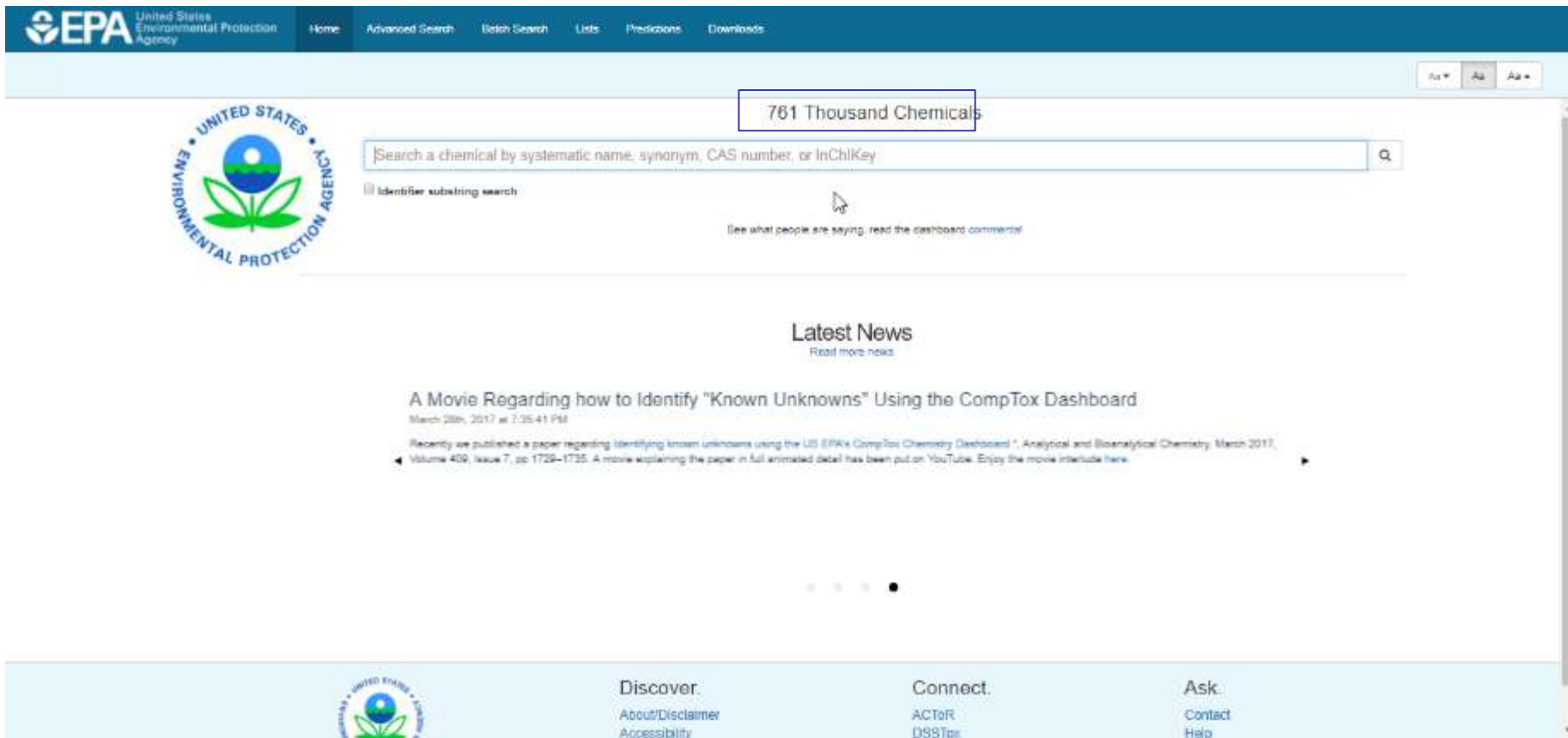
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CompTox Dashboard

<https://comptox.epa.gov/dashboard>



The screenshot shows the CompTox Dashboard interface. At the top is the EPA logo and navigation links: Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. Below this is a search bar with the text "761 Thousand Chemicals" and a search button. To the left of the search bar is the EPA seal. Below the search bar is a section titled "Latest News" with a link to "Read more news". The news section features a headline "A Movie Regarding how to Identify 'Known Unknowns' Using the CompTox Dashboard" dated March 28th, 2017. Below the headline is a paragraph of text about a paper published in Analytical and Bioanalytical Chemistry. At the bottom of the page is a footer with the EPA logo and three columns of links: Discover (About/Disclaimer, Accessibility), Connect (ACToR, DSSTox), and Ask (Contact, Help).

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Home Advanced Search Batch Search Lists Predictions Downloads

761 Thousand Chemicals

Search a chemical by systematic name, synonym, CAS number, or InChIKey

Identifier substring search

See what people are saying, read the dashboard commentary

Latest News

Read more news

A Movie Regarding how to Identify "Known Unknowns" Using the CompTox Dashboard

March 28th, 2017 at 7:35:41 PM

Recently we published a paper regarding identifying known unknowns using the US EPA's CompTox Chemistry Dashboard. Analytical and Bioanalytical Chemistry, March 2017, Volume 409, Issue 7, pp 1729-1735. A movie explaining the paper in full animated detail has been put on YouTube. Enjoy the movie interlude here.

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Detailed Chemical Pages

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Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search All Data

Ammonium perfluorooctanoate

3825-26-1 | DTXSID8037708
Searched by DSSTox Substance Id

DETAILS

- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- GENRA
- SIMILAR COMPOUNDS
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Intrinsic Properties

- Molecular Formula: $C_8H_7F_{17}NO_2$ [View File](#) [Find All Chemicals](#)
- Average Mass: 431.101 g/mol
- Isotope Mass Distribution
- Monoisotopic Mass: 431.000251 g/mol

Structural Identifiers


Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Data Quality


United States Environmental Protection Agency

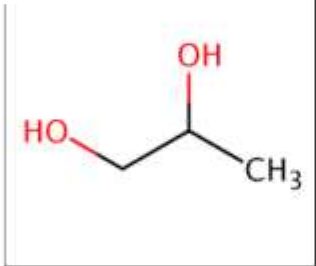
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[Aa](#)

1,2-Propylene glycol

57-55-6 | DTXSID0021206

Searched by Approved Name: Found 1 result for '1,2-propylene glycol'



Wikipedia

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Citation

U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID0021206> (accessed March 29, 2018). 1,2-Propylene glycol

Data Quality

Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers

Level 2: Expert curated, unique chemical identifiers using multiple sources

Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem

Level 4: Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem

Level 5: Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source

Quality Control Notes

[Executive Summary \(Beta\)](#)
[Chemical Properties](#)
[Env. Fate/Transport](#)
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[ADME \(Beta\)](#)
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Properties, Fate and Transport

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Search All Data

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Ammonium perfluorooctanoate

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Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

► EXPOSURE

► BIOACTIVITY

GENRA

SIMILAR COMPOUNDS

RELATED SUBSTANCES

SYNONYMS

► LITERATURE

LINKS

COMMENTS

Property

Summary

Summary

Download

Columns

Search query

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Melting Point	164 (2)	79.477	164	65.6548	164	8.53 to 164.247	°C
LogP: Octanol-Water	-	5.5266		5.2847	-	3.78814 to 7.749	
Vapor Pressure	-	0.1817		0.21528	-	0.0223936 to 0.274	mmHg
Water Solubility	-	0.28444		0.00012	-	0.00000473151 to 0.853196	mol/L
Boiling Point	-	189.58125		189.042	-	187.999 to 192.241	°C
Flash Point	-	65.6365		65.6365	-	62.103 to 69.17	°C
Surface Tension	-	16.819			-	16.819	dyn/cm
Index of Refraction	-	1.289			-	1.289	
Molar Refractivity	-	42.893			-	42.893	cm³
Polarizability	-	17.004			-	17.004	Å³
Density	-	1.731		1.731	-	1.717 to 1.745	g/cm³
Molar Volume	-	237.268			-	237.268	cm³
Thermal Conductivity	-	65.258			-	65.258	mW/(m²K)
Henry's Law	-	2.02276e-10			-	2.02276e-10	atm-m³/mole
LogK _{ow} : Octanol-Air	-	4.15596			-	4.15596	

Chemical Hazard Data

United States Environmental Protection Agency

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Ammonium perfluorooctanoate

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Searched by DSSTox Substance Id.

DETAILS
EXECUTIVE SUMMARY
PROPERTIES
ENV. FATE/TRANSPORT
HAZARD
ACMI
EXPOSURE
BIOACTIVITY
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SIMILAR COMPOUNDS
RELATED SUBSTANCES
SYNONYMS
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COMMENTS

Point of Departure
Download

Human
Eco

Columns: 10

More	Priority	Toxval type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	NOAEL	systemic	chronic	10.1	mg/kg-day	chronic	oral	rat	unpublished_submission	ToxRefDB
	7	NOAEL	systemic	chronic	15	mg/kg-day	chronic	oral	rat	open_lit	ToxRefDB
	7	NOAEL	systemic	chronic	15	mg/kg-day	chronic	oral	rat	open_lit	ToxRefDB
	7	NOAEL	systemic	chronic	14.2	mg/kg-day	chronic	oral	rat	unpublished_submission	ToxRefDB
	7	NOAEL	systemic	chronic	15	mg/kg-day	chronic	oral	rat	open_lit	ToxRefDB
	3	LOEL	Recovery study - 6days	short-term	30	mg/kg-day	short-term	oral	mouse	Toxicol. Sci. 2008; 105 (1):88-95	HWAC
	3	LOEL	Recovery study - 6days	short-term	30	mg/kg-day	short-term	oral	mouse	Toxicol. Sci. 2008; 105 (1):88-95	HWAC
	3	LOEL	Recovery study - 6days	short-term	30	mg/kg-day	short-term	oral	mouse	Toxicol. Sci. 2008; 105 (1):88-95	HWAC
	3	LOEL	Recovery study - 6days	short-term	30	mg/kg-day	short-term	oral	rat	Toxicol. Sci. 2008; 105 (1):88-95	HWAC
	3	LOEL	Recovery study - 6days	short-term	30	mg/kg-day	short-term	oral	mouse	Toxicol. Sci. 2008; 105 (1):88-95	HWAC

<https://epa.gov>

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Last

In Vitro Bioassay Screening

ToxCast and Tox21

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Ammonium perfluorooctanoate

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DETAILS

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HAZARD

ACME

EXPOSURE

BIOACTIVITY

TOXCAST SUMMARY

TOXCAST DATA

FLUORENCE

GENRA

SIMILAR COMPOUNDS

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

QC Data ID	Grade	Description
Tox21_3000096	Not determined	Analysis in progress

Assay Selection 4 Selected

A Single Assay Can Have Multiple Charts

Number of Charts: 4

☒ Active ☐ Inactive ☐ All

Filter

Filter assays

Assay Set: ER (3 of 18 Selected)

- ☐ ACEA_T47D_ER_Positive
- ☒ ATO_ER_CIS_up
- ☒ ATG_ERa_TRANS_up
- ☐ NVS_NR_ER
- ☐ NVS_NR_ERa
- ☐ QT_ER_ERaERa_6480
- ☐ QT_ER_ERaERa_1440
- ☐ QT_ER_ERaERb_6480
- ☐ QT_ER_ERaERb_1440
- ☐ QT_ER_ERaERb_0480
- ☐ QT_ER_ERaERb_1440
- ☐ QT_ERa_EREGFP_0120

Sources of Exposure to Chemicals

United States
Environmental Protection
Agency

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DETAILS
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PROPERTIES
ENV. FATE/TRANSPORT
HAZARD
ADME
EXPOSURE
PRODUCT & USE CATEGORIES
CHEMICAL WEIGHT FRACTION
CHEMICAL FUNCTIONAL USE
TOXICS RELEASE INVENTORY
MONITORING DATA
EXPOSURE PREDICTIONS
PRODUCTION VOLUME
BIODIVERSITY
GENRA
SIMILAR COMPOUNDS
RELATED SUBSTANCES
SYNONYMS

Ammonium⁺perfluorooctanoate

3825-26-1 | DTXSID8037708

Searched by DSSTox Substance Id.

Product and Use Categories (PUCs) ⓘ

Download
Columns

Product or Use Categorization	Categorization Type	Number of Unique Products
automotive	OPCat Cassette	4
consumer_use_ACToRUseDB	OPCat Cassette	1
food_contact_plastics	OPCat Cassette	1
impregnation_consumer_use_deleted	OPCat Cassette	1
industrial_manufacturing_ACToRUseDB	OPCat Cassette	1
manufacturing_chemical	OPCat Cassette	1
manufacturing_plastics	OPCat Cassette	1
process_regulator	OPCat Cassette	1

3 records

Searching for more than one Chemical: Batch Searching

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Home Advanced Search Batch Search Labs Predictions Downloads

Search All Data

Batch Search

Step 1 Step 2 Step 3 Step 4 Step 5 Step 6

Step Six: Click "Download"

Please enter one identifier per line.

Select Input Type(s)

- ☒ Identifiers
 - ☒ Chemical Name
 - ☐ CASRN
 - ☐ InChIKey
 - ☐ DSSTox Substance ID
 - ☐ InChIKey Skeleton
 - ☐ MS-Ready Formula(s)
 - ☐ Exact Formula(s)
 - ☐ Monoisotopic Mass

Select Output Format:

Excel

Customize Results

- ☐ Select All
- ☐ Select All in List

Chemical Identifiers

- ☒ DTXSID
- ☒ Chemical Name
- ☒ CAS RN
- ☒ InChIKey
- ☒ IUPAC Name

Structures

- ☐ Mol File
- ☐ SMILES

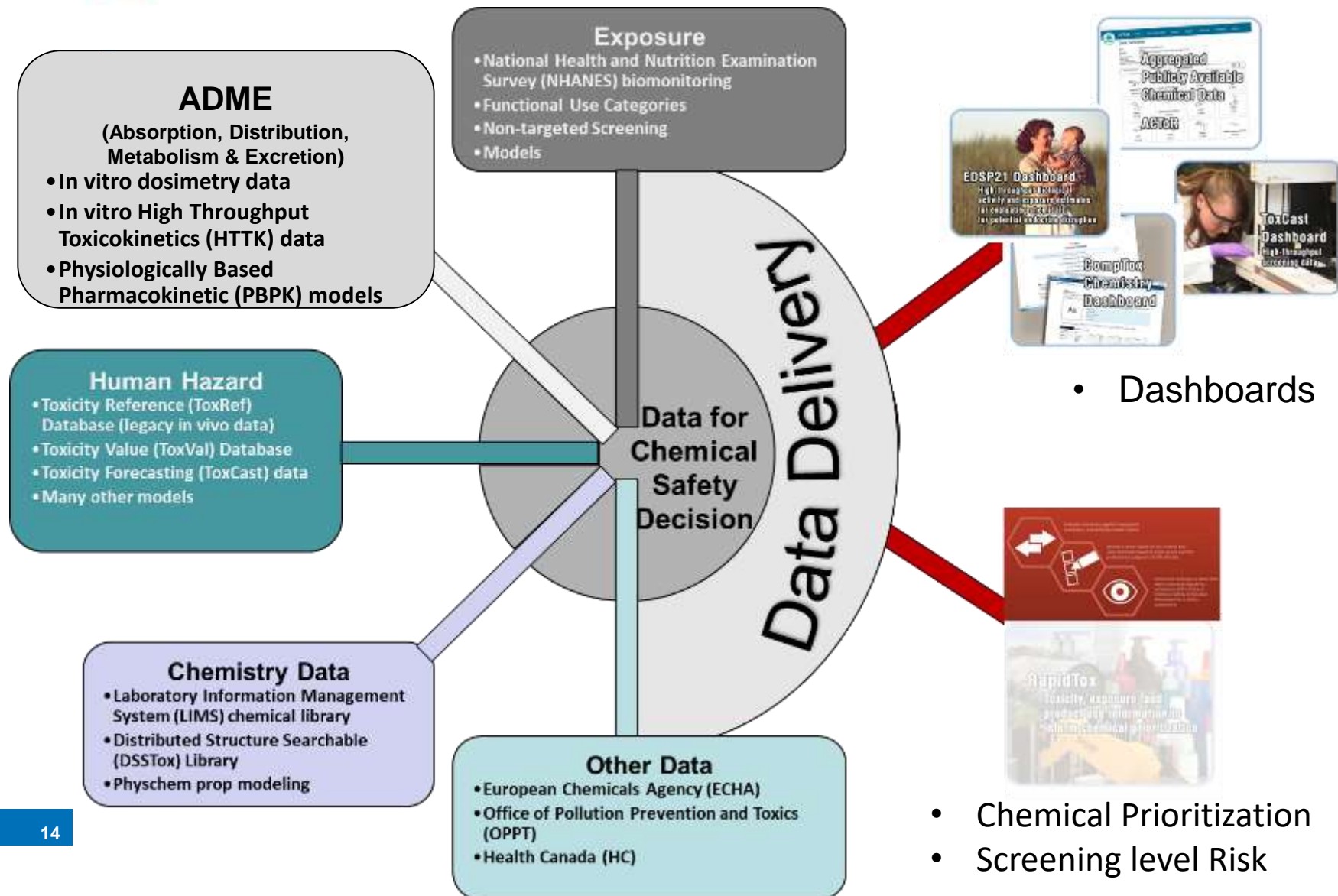
Enter Identifiers to Search (searches should be limited to <1000 identifiers)

Ethylene oxide
Chloromethane
1-Chloropropan-2-ol
n-Heptane
Ammonia
N-ethyl carbonyl
Phosgene
Potassium cyanide
Chlorodimethylsilane
Trimethylsilane

Presence in Lists:

- ☐ 40CFR335
- ☐ Aqueous Toxics
- ☐ APCA Chemicals for Prospective Analysis
- ☐ APCA Chemicals for Retrospective Analysis
- ☐ ATSDR Toxic Substances Portal Chemical List
- ☐ Bisphenol Compounds
- ☐ California Office of Environmental Health Hazard Assessment
- ☐ Chemicals with interesting names
- ☐ CMAP
- ☐ DNT Screening Library
- ☐ Drinking Water Suspects, KWR, Vitor, Netherlands
- ☐ EDCP Universe

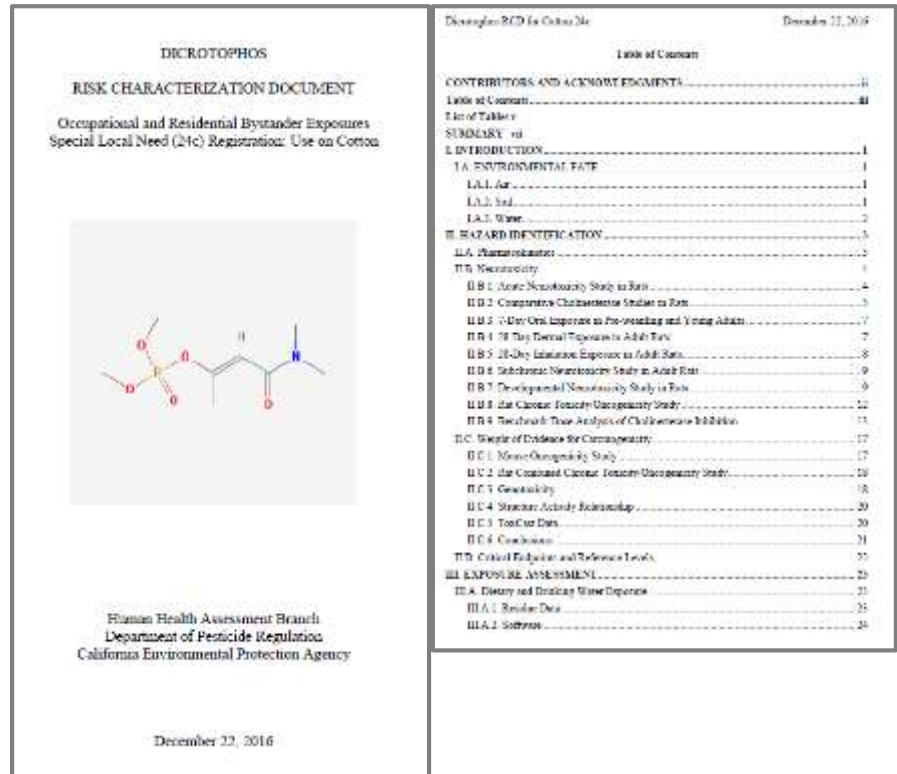
Impact



Impact

- An integration hub for multiple “modules”
 - Experimental and predicted properties
 - Human and Ecological Hazard data
 - Exposure data – products, data in the environment
 - *In vitro* bioassay data – ToxCast/Tox21
 - Literature searching – Google Scholar and PubMed
 - Specialized searches – mass/formula for analytical support
 - Batch searching and Real Time Predictions
- CompTox Dashboard integrates chemical data
- Used by EPA and others to support chemical safety decisions
 - EPA examples: Endocrine Disruptor Screening Program in the 21st Century (EDSP21), Future (RapidTox)

CalEPA Pesticide Assessments



- ToxCast data used for weight of evidence decisions regarding health effects for pesticides

*Not a comprehensive list

16

- Data surfaced through the EPA CompTox Dashboard utilized to prioritize biomonitoring for of emerging contaminants

Conclusion

- EPA's CompTox Dashboard provides access to data for ~760,000 chemicals
- High quality data from ongoing curation efforts
- An integration hub for multiple “modules” and tools to support multiple environmental applications
- Major Update to EPA CompTox Dashboard released in August 2018
 - Endocrine Disrupting Compounds (EDCs)
 - Per- and Polyfluoroalkyl Substances (PFAS)
 - Generalized **Read-Across** (GenRA) module



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