

EPA CompTox Chemistry Dashboard: *Data and Tools to Support Chemical and Environmental Risk Assessment*

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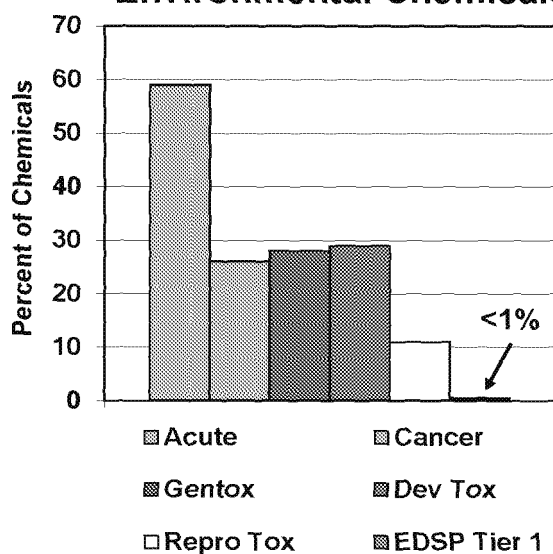
New England State Commissioners' Visit to AED
June 19, 2018

Problem: Too Many Chemicals, Too Little Data

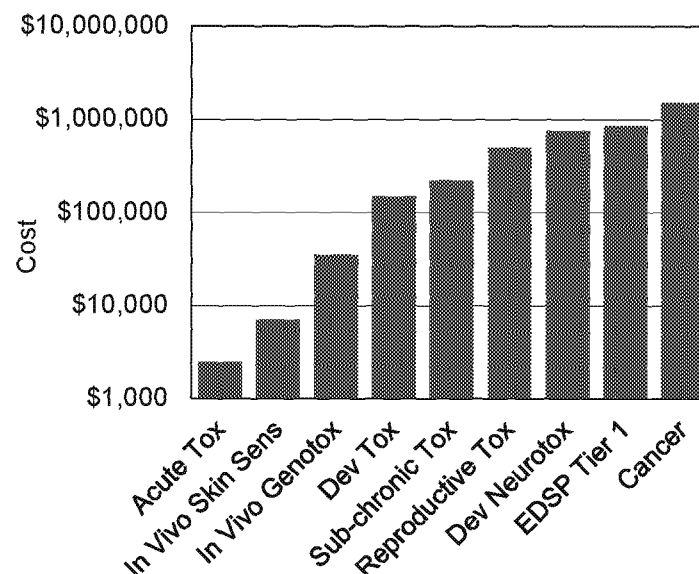


- **Timely characterization of human and ecological risk posed by thousands of existing and emerging chemicals is a critical challenge to protect public health and the environment**
 - Nearly 60% of chemicals on various EPA lists have acute toxicity data, less than 30% have data on other types of toxicity
 - Cost and time associated with traditional animal toxicity testing is significant

Lack of Data for Environmental Chemicals



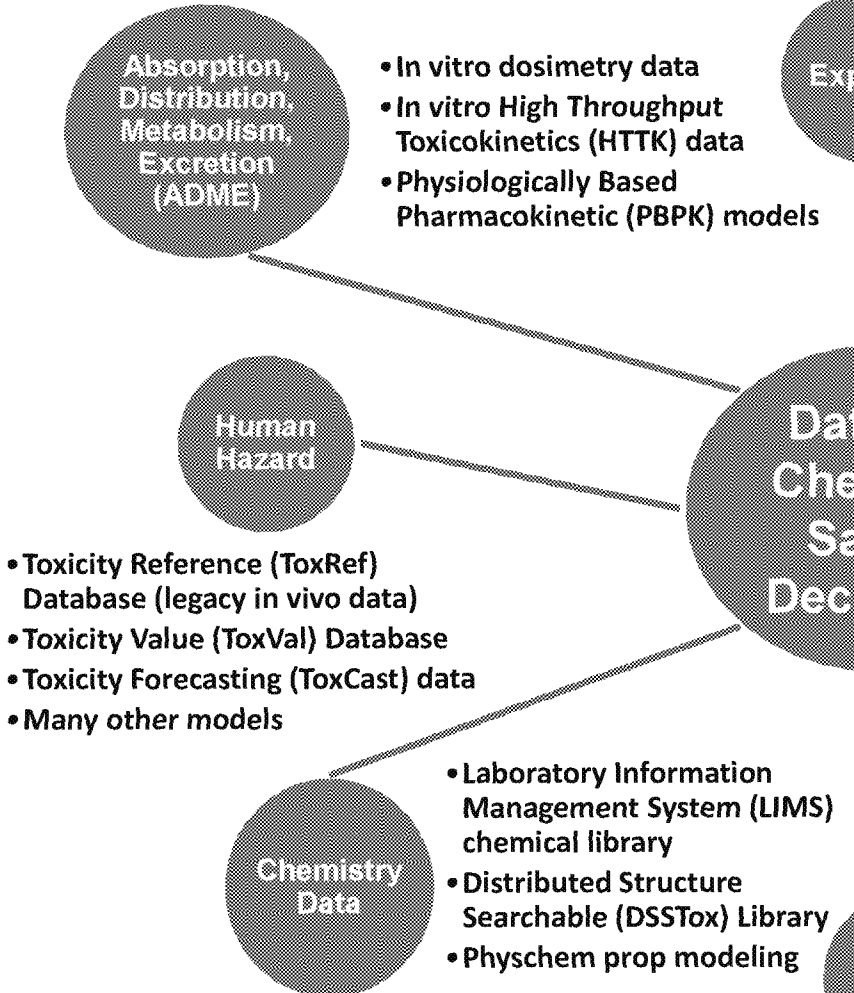
Economics



Modified from Judson *et al.*, EHP 2010

- 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



Exposure

- National Health and Nutrition Examination Survey (NHANES) biomonitoring
- Functional Use Categories
- Non-targeted Screening
- Models

Data for
Chemical
Safety
Assessments

Other
Data
Sources

- European Chemicals Agency (ECHA)
- US EPA Office of Pollution Prevention and Toxics (OPPT)
- Health Canada (HC)

Results: EPA CompTox Chemistry Dashboard



- **A publicly accessible website** delivering:
 - ~760,000 chemicals with related property data
 - Experimental and predicted physicochemical property data
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding consumer products containing chemicals
 - 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 Chemistry Dashboard Live Demo Time



Chemistry Dashboard

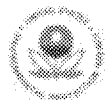


PFOS

Identifier searching search

A YouTube video regarding using the Dashboard
March 28, 2012 at 4:43:26 AM

- A YouTube video describing the application of the CompTox Dashboard and the advantages of the dashboard in terms of data query and follow-up



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781 Thousand Chemicals

What other people are saying: read the dashboard comments



Latest News

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Dashboard for Non-Targeted Analysis

This Dashboard is suited for non-targeted analysis by trade, specificity or location. This dashboard connects you to the best tool for environmental non-targeted analysis. [View a tour of the tool.](#)

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CompTox Chemistry Dashboard

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



[Home](#) [Advanced Search](#) [Basic Search](#) [Links](#) [Feedback](#) [Downloads](#)

Chemistry Dashboard

Go



761 Thousand Chemicals

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

Identifier subsetting search

See what people are saying, read the dashboard comment!

Latest News

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

March 28th, 2017 at 7:55:41 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 499, Issue 1, pp 1726-1735. A movie explaining the paper in full annotated detail has been put on YouTube. Enjoy the movie [interlude here](#).



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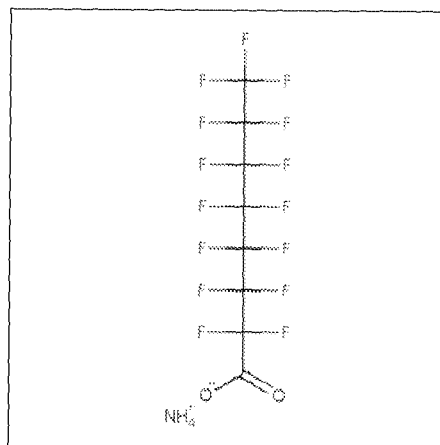
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Ammonium perfluorooctanoate



3825-26-1 | DTXSID8037708


Searched by DSSTox Substance Id.


DETAILS
EXECUTIVE SUMMARY
PROPERTIES
ENV. FATE/TRANSPORT
HAZARD
ACME
▶ EXPOSURE
▶ BIOACTIVITY
GENRA
SMILAP COMPOUNDS
RELATED SUBSTANCES
SYNONYMS
▶ LITERATURE
LINKS
COMMENTS





Intrinsic Properties

 Molecular Formula: $C_8H_4F_{16}NO_2$  [Mol File](#)

 [Find All Chemicals](#)

 Average Mass: 434.104 g/mol

 [Isotope Mass Distribution](#)

 Monoisotopic Mass: 431.003291 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Citation

U.S. Environmental Protection Agency, Chemistry Dashboard. <https://complex.epa.gov/dashboard/DTXSID0021206> (accessed March 29, 2018).

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

Properties, Fate and Transport



Ammonium perfluorooctanoate

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Searched by DSSTox Substance Id.

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

Property

Summary

Download

Columns

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Melting Point	184 (2)	78.477	184	65.8648	184	3.82 to 194.247	°C
LogP, Octanol-Water	-	5.5296	-	5.2847	-	3.78814 to 7.748	
Vapor Pressure	-	0.1817	-	0.21623	-	0.0223908 to 0.274	mmHg
Water Solubility	-	0.28444	-	0.80012	-	0.02020473151 to 0.853195	mg/L
Boiling Point	-	189.58135	-	199.042	-	187.969 to 192.241	°C
Flash Point	-	65.5365	-	65.5365	-	62.109 to 68.17	°C
Surface Tension	-	18.819	-	-	-	18.819	dyne/cm
Index of Refraction	-	1.289	-	-	-	1.289	
Molar Refractivity	-	42.863	-	-	-	42.863	cm³
Polarizability	-	17.004	-	-	-	17.004	Å³
Density	-	1.731	-	1.731	-	1.717 to 1.748	g/cm³
Molar Volume	-	237.268	-	-	-	237.268	cm³
Thermal Conductivity	-	65.258	-	-	-	65.258	mW/mK
Henry's Law	-	2.02278e-10	-	-	-	0.02278e-10	atm-m³/mole
LogKow, Octanol-AW	-	4.15593	-	-	-	4.15593	

Ammonium perfluorooctanoate

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Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD**
- ACUTE
- ▶ EXPOSURE
- ▶ BIOACTIVITY
- GENRA
- SIMILAR COMPOUNDS
- RELATED SUBSTANCES
- SYNONYMS
- ▶ LITERATURE
- LINKS
- DOCUMENTS

Data type

Point of Departure
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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	15.1	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 - 8days	short-term	30	mg/kg-day	short-term	oral	mouse	Toxicol. Sci. 2008; 105 (1):85-95	HAAC
	3	LOEL	Recovery study - 8days	short-term	30	mg/kg-day	short-term	oral	mouse	Toxicol. Sci. 2008; 105 (1):89-99	HAAC
	3	LOEL	Recovery study - 8days	short-term	30	mg/kg-day	short-term	oral	mouse	Toxicol. Sci. 2008; 105 (1):88-98	HAAC
	3	LOEL	Recovery study - 8days	short-term	30	mg/kg-day	short-term	oral	rat	Toxicol. Sci. 2008; 105 (1):85-95	HAAC
	3	LOEL	Recovery study - 8days	short-term	30	mg/kg-day	short-term	oral	mouse	Toxicol. Sci. 2008; 105 (1):85-95	HAAC

https://epa.gov

In Vitro Bioassay Screening

ToxCast and Tox21



United States
Environmental Protection
Agency

Home Advanced Search Batch Search Lists Predictions Downloads

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Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADMS
- EXPOSURE
- BIOACTIVITY
- TOXCAST SUMMARY
- TOXCAST DATA**
- PLUGCHEM
- GENRA
- SIMILAR COMPOUNDS
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LRMS
- COMMENTS

QC Data ID	Shade
Tox21_200908	Not determined

Assay Selection 4 Selected A Single Assay Can Have Multiple

Active Inactive All
Filter

Filter: 33 of 35

Assay Set: ER (3 of 10 Selected)

- ACER_T47D_Bhr_Puative
- ATG_ERE_Cis_up
- ATG_ERA_TRANS_up
- MVE_NR_DER
- MVE_NR_HER
- MVE_NR_ERA
- OT_ER_ERaERa_3480
- OT_ER_GRaERa_3480
- OT_ER_ERaERb_3480
- OT_ER_ERaERb_1446
- OT_ER_ERbERb_3480
- OT_ER_ERaERb_1446
- OT_TRA_EREGFP_3180

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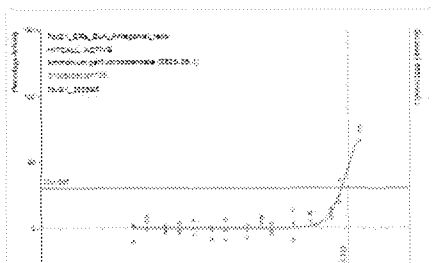
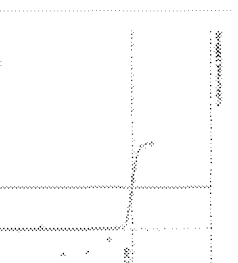
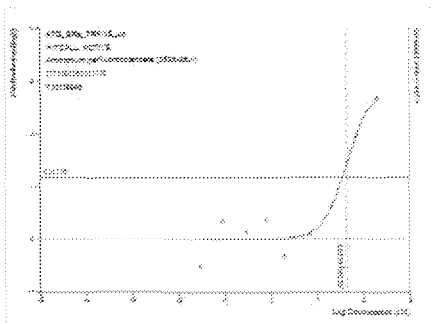
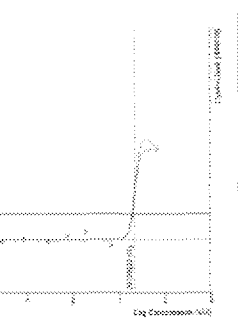
Search for Data

Description

Analysis in progress

Multiple Charts

Number of Charts: 4



Sources of Exposure to Chemicals



Ammonium⁺perfluorooctanoate

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Searched by DSSTox Substance Id

- DETAILS
- EXECUTIVE SUMMARY
- 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
- BIOACTIVITY
- GENRA
- SIMILAR COMPOUNDS
- RELATED SUBSTANCES
- SYNONYMS

Product and Use Categories (PUCs) ⓘ

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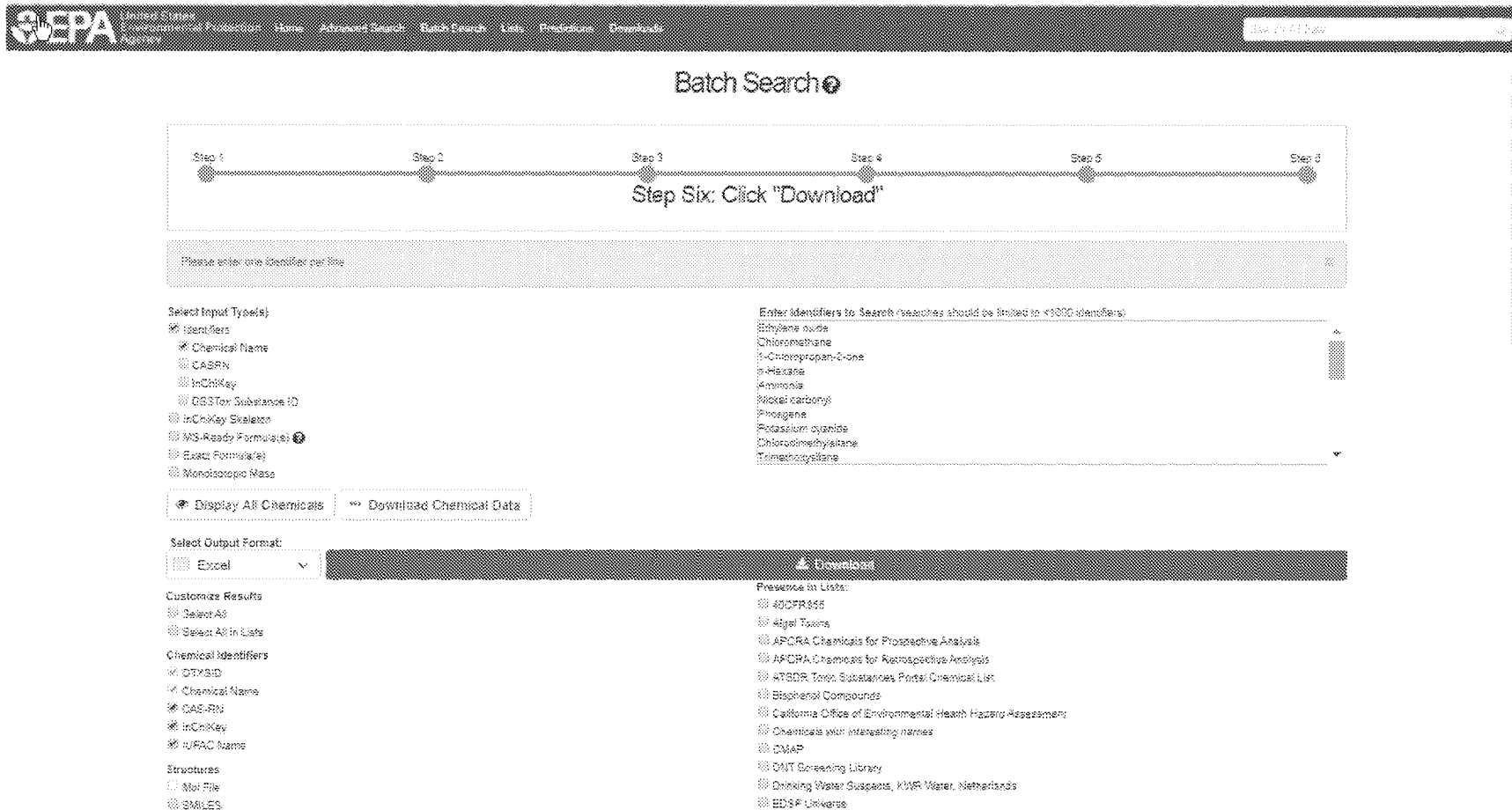
Columns

See history

Product or Use Categorization	Categorization Area	Number of Unique Products
automotive	CPCat Cassette	4
consumer_use_A07toR03a08	CPCat Cassette	1
food_consum_03a09	CPCat Cassette	1
impregnation_consumer_use_03a09	CPCat Cassette	1
industrial_manufacturing_407toR03a08	CPCat Cassette	1
manufacturing_03a09	CPCat Cassette	1
manufacturing_plastics	CPCat Cassette	1
process_regulator	CPCat Cassette	1

3 records

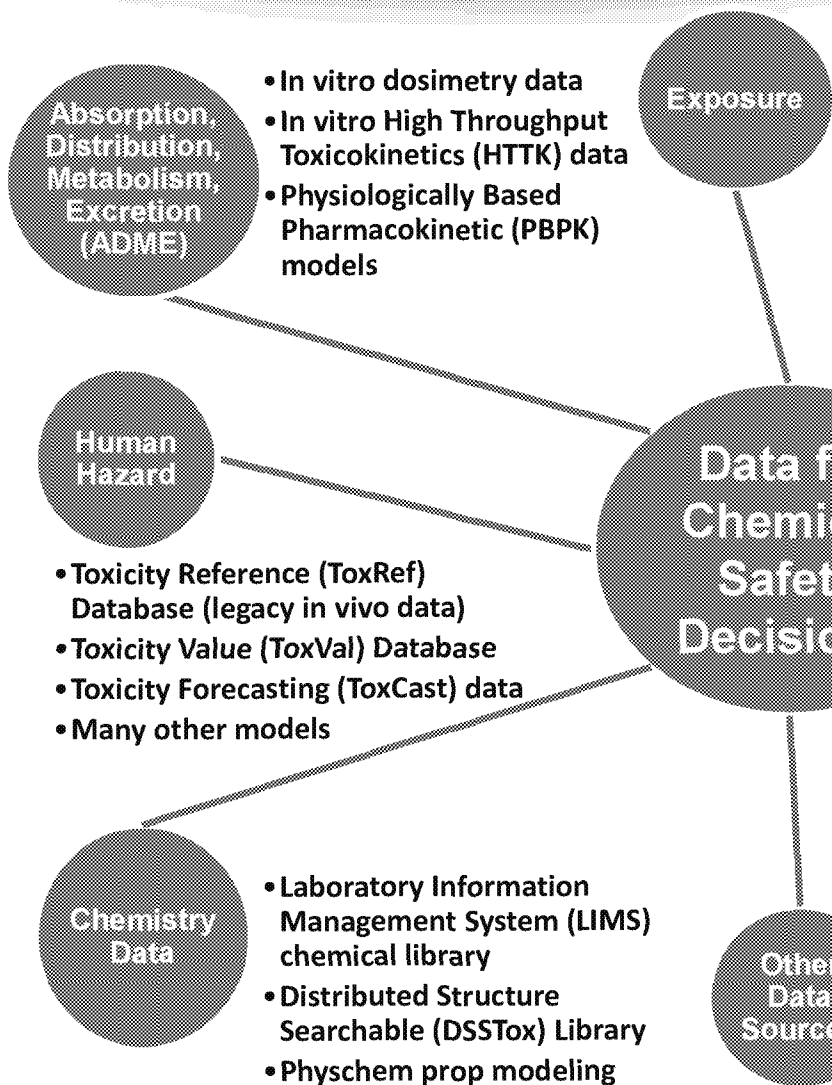
Searching For More Than One Chemical – Batch Searching



The screenshot shows the EPA Batch Search web application interface. At the top, there is a navigation bar with the EPA logo and links for Home, Advanced Search, Batch Search, Lists, Publications, and Downloads. A search box on the right contains the text "Batch Search". Below the navigation bar is a progress indicator with six steps, where Step 6 is highlighted and labeled "Step Six: Click 'Download'". The main content area is divided into several sections:

- Input Section:** A text input field with the placeholder "Please enter one identifier per line".
- Select Input Type(s):** A list of checkboxes for input types: Identifiers (checked), Chemical Name, CASRN, InChIKey, CASTox Substance ID, InChIKey Skeleton, MS-Ready Formulae (checked), Exact Formulae, and Molecular Mass.
- Enter Identifiers to Search:** A text area containing a list of chemical names: Ethylene oxide, Chloroethane, 1-Chloropropan-2-one, p-Halothane, 4-monois, Methyl carbonyl, Propylene, Potassium cyanide, Chlorodimethylsilane, and Trimethylsilane.
- Buttons:** "Display All Chemicals" and "Download Chemical Data".
- Select Output Format:** A dropdown menu with "Excel" selected and "Download" as an option.
- Customize Results:** Checkboxes for "Select All" and "Select All in Lists".
- Chemical Identifiers:** Checkboxes for CASID, Chemical Name, CAS-RN, InChIKey, and IUPAC Name.
- Structures:** Checkboxes for Mol File and SMILES.
- Presence in Lists:** A list of checkboxes for various databases: 40DFR55, 40DFR56, Atrgl Toxins, APCRA Chemicals for Prospective Analysis, APCRA Chemicals for Retrospective Analysis, ATSDR Toxic Substances Portal Chemical List, Bisphenol Compounds, California Office of Environmental Health Hazard Assessment, Chemicals with interesting names, CMAP, CNT Screening Library, Drinking Water Suspects, KWR Water, Netherlands, and EDSF Universe.

Impact



- National Health and Nutrition Examination Survey (NHANES) biomonitoring
- Functional Use Categories
- Non-targeted Screening
- Models

Dashboards / Portals

- Chemistry Dashboard
- Endocrine Disruptors Screening Program (EDSP21) Dashboard
- Toxicity Forecasting (ToxCast) Dashboard

Data Delivery

RapidTox Workflows

- European Chemicals Agency (ECHA)
- US EPA Office of Pollution Prevention and Toxics (OPPT)
- Health Canada (HC)

- Screening level risk assessments
- Chemical Prioritization

- 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
- Chemistry 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)

- EPA's CompTox Chemistry 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 CompTox Chemistry Dashboard in August 2018
 - Endocrine Disrupting Compounds (EDCs)
 - Per- and Polyfluoroalkyl Substances (PFAS)

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