

Green Ribbon Science Panel Meeting

January 28-29, 2010



Department of Toxic Substances Control
Toxics Information Clearinghouse

Suhasini Patel
January 28, 2010

Presentation Overview



- Green Chemistry Initiative
- Legislation
- Other Databases
 - International
 - National
- Toxics Information Clearinghouse

Green Chemistry Initiative



- April 2007: Green Chemistry Initiative
- December 2008: California Green Chemistry Initiative Final Report
 - Six Recommendations
- Green Ribbon Science Panel

DTSC



- **Recommendation 4 – Toxics Information Clearinghouse**

Create online *database* providing data on chemical toxicity and hazard traits to the market place and public.

- **April 2009: Green Ribbon Science Panel**

Legislation - 2008



Senate Bill 509 (SB 509)

- The Department of Toxic Substances Control to establish a Toxics Information Clearinghouse for the collection, maintenance, and distribution of *specific* chemical hazard traits and environmental and toxicological end-point data...

Legislation – 2008

continued...



- The Office of Environmental Health Hazard Assessment required to evaluate and specify the hazard traits and environmental and toxicological end-points and any other relevant data that are to be included in the clearinghouse by January 1, 2011

Other Databases



- International Databases...
 - eChemPortal, OECD
 - CHRIP, Japan
 - CESAR, Canada
- United States
 - U.S. EPA: ACToR
 - Interstate Chemical Clearinghouse (IC2)

Other Databases: Abbreviations



- **OECD:** Organization for Economic Co-operation and Development
- **CHRIP:** Chemical Risk Information Platform
- **CESAR:** Canada's Existing Substances Assessment Repository
- **ACToR:** Aggregated Computational Toxicology Resource

OECD: Organization for Economic Co-operation and Development



eChemPortal:

- Public access to information on properties of chemicals.
- Allows for simultaneous search of multiple databases (up to 15).
- Provides clearly described sources and quality of data.

[Home](#)[General Information on the Portal](#)[Participating Databases](#)[Roles and Responsibilities](#)[Extension of the Portal](#)[What's new](#)[Contact Us](#)[Disclaimer](#)[Home](#) > [Find Document links](#)

by CAS Number:

by Chemical name or synonym

or

in

Search in:

[Reset](#)

You searched "**Trichloroethene**" which was identified as a synonym or trade name of the chemical substance "**Trichloroethylene**".

CAS number related to the chemical substance: **79-01-6**

Found: 11

Click on "Go to results" to access data. Multiple records may be found.

CESAR	Priority Substance List Assessment Report	Go to results
CHRIP		Go to results
EnviChem		Go to results
ESIS		Go to results
HSDB		Go to results
HSNO CCID		Go to results
INCHEM		Go to results
NICNAS PEC		Go to results
OECD HPV		Go to results
US EPA IRIS		Go to results
US EPA SRS		Go to results

[Go to top](#)

CHRIP: Chemical Risk Information Platform



- Provided by the National Institute of Technology and Evaluation
 - Biodegradation and bioconcentration test results
 - Testing condition of Existing Chemical Substances under the Chemical Substances Control Law
 - Other related information, are provided in a database called “TOTAL SEARCH SYSTEM” in CHRIP.

CHRIP (CHemical Risk Information Platform) - Windows Internet Explorer

http://www.safe.nite.go.jp/english/sougou/view/ComprehensiveInfoDisplay_en.faces

File Edit View Favorites Tools Help

CHRIP (CHemical Risk Information Platform)

nite Incorporated Administrative Agency
National Institute of Technology and Evaluation

Search | Sitemap | Links | Japanese

NITE TOP > Chemical Management Field > CHRIP > Total Search System for Chemical Substances

Chemical Management Field

Collecting and transmitting information required for total risk assessment and management of chemical substance

Chemical Risk Information Platform (CHRIP)

Total Search > Enter Search Condition > Interim Search Results > Comprehensive Information

>>>Help >>>Help >>>Help

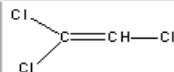
Comprehensive Information

(The only items containing some data are displayed.)

Display all items Partial Display Printable Page

[General Information](#) [Exposure Information](#) [Laws and Regulations in Japan](#) [Inventories, Regulations, etc](#)
[Hazard Assessments](#) [Physical Chemical Properties](#) [Environmental Toxicity](#) [Toxicity to Humans](#)

I. General Information [\(Return to TOP\)](#)

General Information	Data Description
CAS Registry No.	79-01-6
Chemical Substance Name	Ethene, trichloro-
Molecular Formula	C2HCl3
Structure	

II. Exposure Information [\(Return to TOP\)](#)

Internet 100%

CESAR: Canada's Existing Substances Assessment Repository



- Risk and Regulatory Assessment Reports on existing chemicals produced or imported in Canada or released into the Canadian environment.
- Chemicals include:
 - individual substances,
 - groups or classes of chemicals, or
 - effluents or wastes

Canadian Environmental Protection Act

Priority Substances List
Assessment Report

Trichloroethylene

Government of Canada
Environment Canada
Health Canada

Aussi disponible en français sous le titre de :
Loi canadienne sur la protection de l'environnement
Liste des substances d'intérêt prioritaire
Rapport d'évaluation : Trichloroéthylène

U.S.EPA: ACToR



Collection of databases, collated by the US EPA National Center for Computational Toxicology

- > 200 sources data on environmental chemicals
- Searchable by chemical name and by chemical structure.
- Data includes chemical structure, physico-chemical values, in vitro assay data and in vivo toxicology data.

U.S.EPA: ACToR



Chemicals include, but are not limited to,

- Industrial chemicals
- Pesticides
- Potential ground and drinking water contaminants

Home | ACToR | US EPA - Windows Internet Explorer

http://actor.epa.gov/actor/faces/ACToRHome.jsp

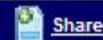
File Edit View Favorites Tools Help

Home | ACToR | US EPA

Home RSS Print Page

U.S. ENVIRONMENTAL PROTECTION AGENCY

ACToR: Aggregated Computational Toxicology Resource



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You are here: [EPA Home](#) » [National Center for Computational Toxicology](#) » [ACToR](#)

ACToR (Aggregated Computational Toxicology Resource) is a collection of databases collated or developed by the US EPA National Center for Computational Toxicology (NCCT). More than 200 sources of publicly available data on environmental chemicals have been brought together and made searchable by chemical name and other identifiers, and by chemical structure. Data includes chemical structure, physico-chemical values, in vitro assay data and in vivo toxicology data. Chemicals include, but are not limited to, high and medium production volume industrial chemicals, pesticides (active and inert ingredients), and potential ground and drinking water contaminants.

Chemical Name Parameters

- Search on Chemical Names
- Search on CAS Numbers

Match by

- Exact
- Any

Enter Chemical Name:

TCE

Chemical Name Parameters

Match by

- Search on Chemical Names
- Search on CAS Numbers

- Exact
- Any

Enter Chemical Name:

TCE

Search

Search Results

Details

Image

CASRN

Preferred Name

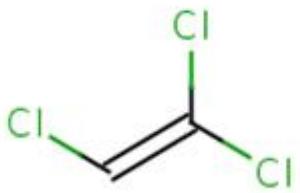
Hazard

Chronic

Carcinogenicity

Genotoxicity

Developmental



Ha	Cr	Ca	G	D
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ACToR: Aggregated Computational Toxicology Resource

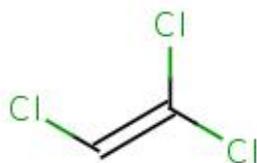

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 Search: All EPA This Area

Go

 You are here: [EPA Home](#) » [National Center for Computational Toxicology](#) » [ACToR](#) » Chemical Summary :

Chemical Summary : Trichloroethylene (TCE)



GCID

324183

A highly volatile inhalation anesthetic used mainly in short surgical procedures where light anesthesia with good analgesia is required. It is also used as an industrial solvent. Prolonged exposure to high concentrations of the vapor can lead to cardiotoxicity and neurological impairment. : Anesthetics, Inhalation : Solvents

MESH DESCRIPTION

CASRN

79-01-6

FORMULA

C₂HCl₃

MW

131.38834

SMILES

C(=C(Cl)Cl)Cl

Toxics Information Clearinghouse



Phase 1:

- Physical and Chemical Characteristics
- Ecological Impact
- Environmental Hazard
- Human Health Hazard
- ...

Toxics Information Clearinghouse



Phase 1:

- All publicly available Data Sources to be included in the Clearinghouse
- January 2011: Include all of the specific Data on hazard traits, and toxicological endpoints as identified by OEHHA

GREEN CHEMISTRY TOXICS INFORMATION CLEARINGHOUSE PORTAL

Green Ribbon Science Panel Discussions
January 28 & 29, 2010



By Donn Diebert, PE
Department of Toxic Substances Control
Team Leader

Objectives of Health and Safety Code 25256

➤ **Toxics Information Clearinghouse:**

- Decentralized,
- Web-based system for collection, maintenance, and distribution of **specific** chemical hazard trait and environmental and toxicological end-point data,
- Accessible to the public through a single Internet Web portal,
- Operate Clearinghouse at the least possible cost to the state,
- On or before January 1, 2011 Office of Environmental Health and Hazard Assessment provides environmental and toxicological end-points and any other relevant data



TOXICS INFORMATION CLEARINGHOUSE SCHEDULE

- Control Agency approvals for the Feasibility Study for the Toxics Information Clearinghouse (Should be completed)
- Request for Proposal document in Spring 2010
- Contractor Working On System late Summer 2010
- Beta System in Winter 2010/11
- Full Operation Spring 2011



Sources of Data

- Government Information
 - International Governments
 - Federal Government Agencies
 - Other State Governments
 - California State Agencies
- Non-Government Agencies/Organizations
- Manufacturers
- University Research
- Independent Research Facilities / Think Tanks / Consultants



INFORMATION ON SOME DATABASE SOURCES

- US EPA ACToR - Generic Chemicals ~542,206
- ECHA - ~2,249 Chemicals
- EU Reach - ~143,834 Chemicals
- Danish EPA - ~82,055 Chemicals
- Canada - ~22,017 Substances
- Prop 65 - ~823 Chemicals
- NIOSH - ~652 chemicals
- Sigma Aldrich - ~90,000 Chemicals
- Fisher Scientific - ~61,000 Chemicals
- NLM Toxnet - ~70,760 Chemicals





Chemical Search

Search by chemical name or CAS number. Use partial name or number.

Search



Endpoint Search

Search by chemical endpoint such as 'rash' or 'asthma'.

Select an Endpoint...



Alphabetical Search

Search for chemicals by an Alphabetical index.

A B C D E F G H I J K L M
N O P Q R S T U V W X Y Z

Double click a letter to get a chemical listing that starts with that letter.

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! Top Chemical Searches - click a chemical to get the information.

[acid](#) [sodium thiosulfate](#) [benzene](#) [perchlorate](#) [methane](#) [ethylene glycol](#) [butyl nitrol](#)
[methyl alcohol](#) [nitric acid](#) [ammonia](#) [arsenic](#) [petn](#) [chromium](#) [more...](#)

As part of the Department of Toxic Control's Green Chemistry implementation we are providing a chemical clearinghouse for finding information about products that are used for manufacturing as well as other commercial and private purposes. Please note that while it is our intent to provide accurate information, we do gather this information for several sources and therefore cannot guarantee 100% accuracy.

What is the source of our data?

>> [click here to find out](#)

Have Questions or Comments?

>> [click here](#)



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The Department of Toxic Substances Control

Toxic Information Clearinghouse



The Green Chemistry Initiative



Chemical Search

Search by chemical name or CAS number. Use partial name or number.

Search



Endpoint Search

Search by chemical endpoint such as 'rash' or 'asthma'.

Select an Endpoint... v

Carcinogenicity

Developmental toxicity

Reproductive toxicity

Endocrine disruption

Neurotoxicity

Respiratory toxicity

Respiratory sensitization/asthma

Organ toxicity

Ecotoxicity

Persistence/bioaccumulation



Alphabetical Search

Search for chemicals by an Alphabetical index.

A B C D E F G H I J K L M
N O P Q R S T U V W X Y Z

Double click a letter to get a chemical listing that starts with that letter.

! Top Chemical Searches - click here

[acid sodium thiosulfate benzen](#)

[methyl alcohol nitric acid amm](#)

As part of the Department of Toxic Substances Control's chemical clearinghouse for finding information on chemicals used in commerce as well as other commercial and consumer products, we provide accurate information, we do not guarantee 100% accuracy.

What is the source of our data?

>> click here to find out

Have Questions or Comments?

>> click here

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Chemical Name	CASRN	Toxicity Endpoint data available
---------------	-------	----------------------------------

Closest match

Benzene

71-43-2



Other matches

1,2-Benzenedicarboxaldehyde

643-79-8



1,2-Dichlorobenzene

95-50-1



1,2,4-Trimethylbenzene

95-63-6



1,3-Dichlorobenzene

541-73-1



1,3-Dinitrobenzene

99-65-0



1,4-Dichlorobenzene

106-46-7



Chlorobenzene

108-90-7



Diethylbenzene

25340-17-4



Dodecylbenzenesulfonic acid,
Na salt

25155-30-0



Ethylbenzene

100-41-4



Hexachlorobenzene

118-74-1



12 of 932 results. Click here for next 12 results:



Summary	United States Governments	Governments in other countries	Non-Government Organizations	Others
---------	---------------------------	--------------------------------	------------------------------	--------

Chemical Name:

Benzene

CAS #:

71-43-2

Chemical Formula:

(C₆H₆)

This chemical is known to the State of California to cause cancer and birth defects or other reproductive harm¹

Synonyms²:

Bensol, Benzen, Benzol, Benzolene, Coal naphtha, Cyclohexatriene, Fenzen, Mineral naphtha, Motor benzol, Nitration benzene, Phenyl hydride, Pyrobenzol, Annulene

Chemical summary³:

Benzene is a colorless liquid with a sweet odor. It evaporates into the air very quickly and dissolves slightly in water. It is highly flammable and is formed from both natural processes and human activities.

Benzene is widely used in the United States; it ranks in the top 20 chemicals for production volume. Some industries use benzene to make other chemicals which are used to make plastics, resins, and nylon and synthetic fibers. Benzene is also used to make some types of rubbers, lubricants, dyes, detergents, drugs, and pesticides. Natural sources of benzene include volcanoes and forest fires. Benzene is also a natural part of crude oil, gasoline, and cigarette smoke.

Physical & Chemical Properties⁴:

Physical state and appearance: Liquid.

Odor: Aromatic. Gasoline-like, rather pleasant

Taste: Not available.

Color: Clear Colorless. Colorless to light yellow

pH (1% soln/water): Not available

Odor Threshold: 4.68 ppm

Specific Gravity: 0.8787 @ 15 C (Water = 1)

Molecular Weight: 78.11 g/mole

Boiling Point: 80.1 (176.2°F)

Melting Point: 5.5°C (41.9°F)

Critical Temperature: 288.9°C (552°F)

Vapor Pressure: 10 kPa (@ 20°C)

Vapor Density: 2.8 (Air = 1)

Octinol Water Partition Coefficient: The product is more soluble in oil; log(oil/water) = 2.1

Solubility: Miscible in alcohol, chloroform, carbon disulfide oils, carbon tetrachloride, glacial acetic acid, diethyl ether, acetone. Very slightly soluble in cold water

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether, acetone.

Potential Health Effects⁵

Potential Acute Health Effects: Very hazardous in case of eye contact (irritant), or inhalation. Hazardous in case of skin contact (irritant, permeator), or ingestion. Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:

CARCINOGENIC: Classified A1 (Confirmed for human) by ACGIH, 1 (Proven for human.) by IARC.

MUTAGENIC: Classified possible for human, Mutagenic for mammalian somatic cells, Mutagenic for bacteria and/or yeast.

New search by Chemical Name or CAS #

Search

Toxicity Endpoints

- * **Carcinogenicity**
- * **Developmental toxicity**
- * Reproductive Toxicity
- * Endocrine Disruption
- * Neurotoxicity
- * **Respiratory Toxicity**
- * Respiratory sensitization / asthma
- * Organ toxicity
- * Ecotoxicity
- * Persistence/ Bioaccumulation

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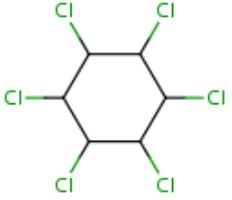
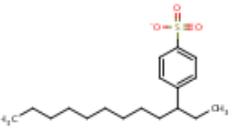
Question:

- What suggestions do you have for the design of a web site that can be easily used by consumers, manufacturers and scientific community; and will encourage them to return to the Clearinghouse?



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Search Results

Details	Image	CASRN	Preferred Name	Hazard	Chronic	Carcinogenicity	Genotoxicity	Developmental	Reproductive	Food Safety	Exposure
225734		608-73-1	Hexachlorocyclohexane	Ha	Cr	Ca	G	D	R	FS	Ex
10797		106-46-7	1,4-Dichlorobenzene	Ha	Cr	Ca	G	D	R	FS	Ex
110125		25155-30-0	Dodecylbenzenesulfonic acid, Na salt	Ha	Cr	Ca	G	D	R	FS	Ex

[ACToR Home](#)[Basic Information](#)[Data Collections](#)[Search By Name](#)[Search By CASRN](#)[Search By Structure](#)[Browse Toxicity Assays](#)[External Links](#)[Help](#)[Download](#)

Chemical Summary : Benzene



GCID

291723

Toxic, volatile, flammable liquid hydrocarbon byproduct of coal distillation. It is used as an industrial solvent in paints, varnishes, lacquer thinners, gasoline, etc. Benzene causes central nervous system damage acutely and bone marrow damage chronically and is carcinogenic. It was formerly used as parasiticide.

MESH DESCRIPTION

CASRN

71-43-2

FORMULA

C6H6

MW

78.11184

SMILES

c1ccccc1

Substances

Previous [1-10 of 276](#) [Next 10](#)

Name	Data Collection
BENZENE	ATSDR CEP 2007
Benzene	ATSDR HSEES 2006
Benzene	ATSDR Interactions
Benzene	ATSDR HSEES 2006
Benzene	ATSDR Interactions
Benzene	ATSDR MMG
Benzene	ATSDR PDN Status
Benzene	ATSDR PHS
Benzene	ATSDR ToxFaq
Benzene	ATSDR ToxGuides
Benzene	ATSDR ToxProfile
Benzene	AU NPI

Synonyms

(6)ANNULENE

71-43-2

A13-00808

E-Chem Portal for Information Identification



The Global Portal to Information on Chemical Substances

[Home](#) > [Find Chemical Substance](#) > Find Document links

by CAS Number: or by Chemical name or synonym: in Search in: [Reset](#)

Benzene

CAS number related to the chemical substance: **71-43-2**

Found: 12

Click on "Go to results" to access data. Multiple records may be found.

CESAR	Priority Substance List Assessment Report	Go to results
CHRIP		Go to results
EnviChem		Go to results
ESIS		Go to results
HPVIS		Go to results
HSDB		Go to results
HSNO.CCID		Go to results
INCHEM		Go to results
NICNAS PEC		Go to results
OECD.HPV		Go to results
US EPA IRIS		Go to results
US EPA SRS		Go to results

[Go to top](#)

Questions:

- Recognizing that for some chemicals there are vast amounts of information available how do you want to group the various sources of information?

Potential Grouping of sources:

- Regulators, University / Scientific Institutions, Special Interest and Consumer Groups;
or
- US Authorities, Authorities in other Countries, Non-government organizations, Other;
or
- Other Ideas



Search on CAS Numbers

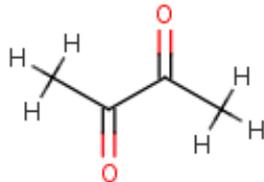
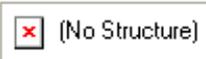
Any

Enter Chemical Name:

625-34-3

Search

Search Results

Details	Image	CASRN	Preferred Name	Hazard	Chronic	Carcinogenicity	Genotoxicity	Developmental	Reproductive	Food Safety	Exposure
233041		625-34-3	acetoacetaldehyde								
338302		84625-34-3	Eupatorium cannabinum, ext.								

ACToR News

Date

Item

24-Sept-2009

ACToR V2 is now online. Improvements include an always-open generic chemical page, a more robust structure search tool and an increased number of data sources, including many with environmental exposure information.

24-Sept-2009

Known Issue: Many assays have multiple phenotypes, which may only apply to a subset of chemicals. A subsequent data release will improve this.

24-Sept-2009

Known Issue: The back button does not behave properly when going from a generic chemical page back to a list. Select Search by ... from the left hand menu to get back to the previous list



ESIS EINECS ELINCS NLP BPD PBT C & L HPV-LPV IUCLID DS ORATS

- CAS#

Result for CAS#: 84852-53-9

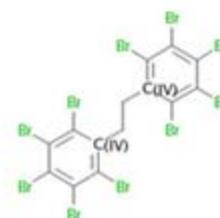
[Expand All \(+\)](#) [Collapse All \(-\)](#)



CAS# found in EINECS (European Inventory of Existing Commercial chemical Substances).

General Information:

EC# : 284-366-9
 CAS# : 84852-53-9
 Substance Name : 1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]
 De : 1,1'-(Ethan-1,2-diyl)bis[pentabromobenzol]
 Es : 1,1'-(etano-1,2-diil)bis[pentabromobenceno]
 Fr : 1,1'-(éthane-1,2-diyl)bis[pentabromobenzène]
 Molecular Formula : C14H4Br10
 Description : Not available



[Enlarge Structure](#)

Biocidal Products Directive (Directive 98/8/EC) Information:

There is no information in ESIS for this substance with respect to the BPD.

Classification and Labelling Information:

This substance is not classified in the Annex I of Directive 67/548/EEC as such, but it may be included in one of the group entries. An example of a group entry is 033-002-00-5 'arsenic compounds with the exception of those specified elsewhere in this Annex'. Substances not listed either individually or in group entries must be self classified..

Export and Import of Dangerous Chemicals (Regulation (EC) No 689/2008) Information:

This substance is not listed in the Annex I of Regulation (EC) No 689/2008.

HPV-LPV (High and Low Production Volume) Information:

LPV Chemical : + [List of Producers/Importers](#)

IUCLID & OECD Chemical Data Sheets and Export Files Information:

Not available for this substance.

European Priority Lists and Risk Assessment (Council Regulation (EEC) No 793/93) Information:

This substance is not listed in a priority list (as foreseen under Council Regulation (EEC) No 793/93 on the evaluation and control of the risks of existing substances.).

Summary	US Governments	Governments in other countries	Non-Government Organizations	Others
---------	----------------	--------------------------------	------------------------------	--------

Chemical Name: Benzene	CAS #: 71-43-2	Chemical Formula: (C ₆ H ₆)
---	--------------------------	--

This chemical is known to the State of California to cause cancer and birth defects or other reproductive harm¹

[Synonyms²:](#)

[Chemical summary³:](#)

[Physical & Chemical Properties⁴:](#)

[Potential Health Effects⁵](#)

Summary of toxicity endpoints by data source

Data Source	Endpoint information available								
	Carcinogenicity	Developmental	Reproductive	Endocrine	Neurotoxicity	Respiratory	Organ toxicity	Ecotoxicity	Persistence
US Governments	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>			
EPA IRIS	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>			
California prop 65	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>			
Foreign Governments	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>			
ECHA	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>			
Non-Governmental Organizations									
IARC	<input checked="" type="checkbox"/>								

New search by Chemical Name or CAS #

Search

- Toxicity Endpoints**
- * **Carcinogenicity**
 - * **Developmental toxicity**
 - * Reproductive Toxicity
 - * Endocrine Disruption
 - * Neurotoxicity
 - * **Respiratory Toxicity**
 - * Respiratory sensitization / asthma
 - * Organ toxicity
 - * Ecotoxicity
 - * Persistence/ Bioaccumulation

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Questions:

- Recognizing there may not be information for some chemicals, how could we best present this lack of information?



Questions Summary

- What suggestions do you have for the design of a web site that can be easily used by consumers, manufacturers and scientific community; and will encourage them to return to the Clearinghouse?
- Recognizing that for some chemicals there are vast amounts of information available how do you want to group the various sources of information?
- Recognizing there may not be information for some chemicals, how could we best present this lack of information?



QUESTIONS / DISCUSSIONS

