

## NEW DATA RESOURCES:

### OECD'S ECHEMPORTAL

25 March 2014, Society for Chemical Hazard Communication Spring Meeting 2014

Sally de Marcellus OECD, Environment Directorate, Health and Safety Division sally.demarcellus@oecd.org





- OECD
- What eChemPortal is
- How to use eChemPortal
- Data sources
- Information classifications according to the GHS
- Conclusion

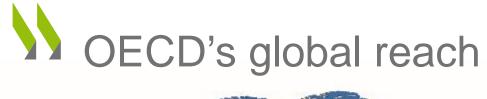


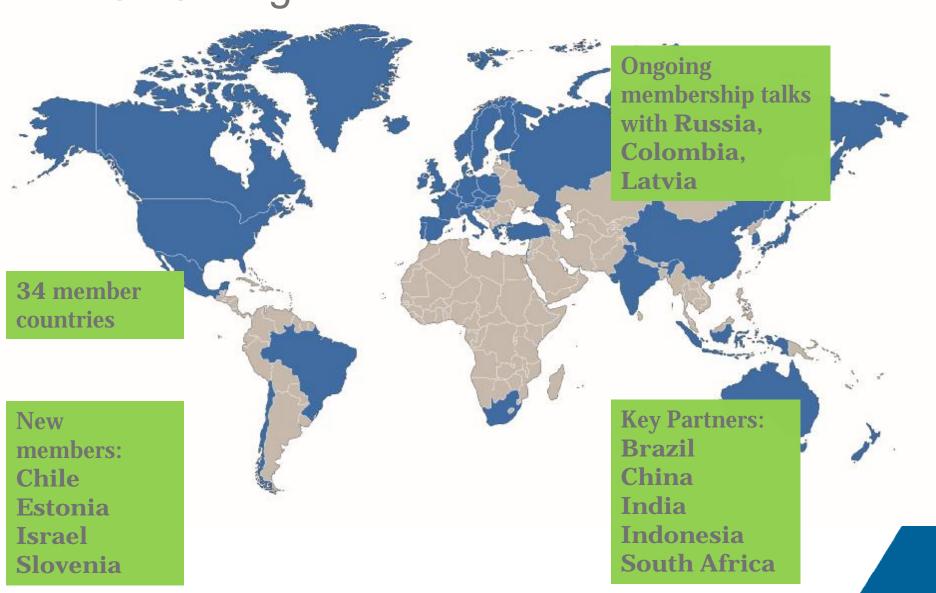
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# Organisation for Economic Co-operation and Development (OECD)

- An intergovernmental organization
- A forum in which governments:
  - work together and with representatives from business and civil society
  - compare and share policy experiences (social, economic, environmental)
  - seek answers to common problems & identify good practices
  - promote decisions and recommendations
- Key words at OECD: dialogue, consensus, peer review & pressure



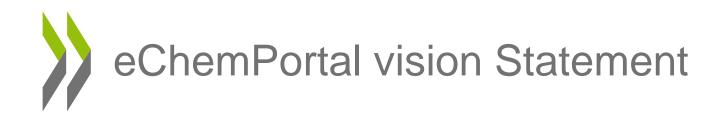




- Step towards achieving international commitments
  - SAICM: "Facilitate public access to appropriate information and knowledge of chemicals throughout their life cycle...".
- OECD Steering Group for development
  - Canada, Japan, United States, EC, ECHA, the OECD Business and Industry Advisory Committee (BIAC), IPCS, UNEP, chemicals and environmental NGOs
- Developed in collaboration with ECHA
- Hosted by ECHA



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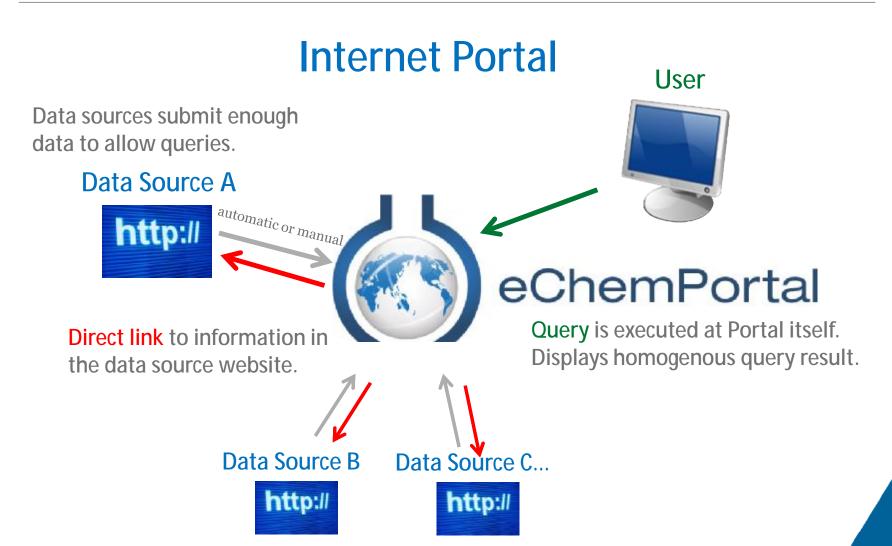


eChemPortal - The Global Portal to Information on Chemical Substances, will be the preferred worldwide source of information about chemicals from authorities and international organisations.



www.oecd.org/ehs/echemportal







## Information found through eChemPortal

- Information prepared for government chemical review programmes
  - Property information (e.g. hazard & risk assessments, test data)
  - Exposure and use information
  - National classification results (GHS)
- Existing & new industrial chemicals, pesticides & biocides
- Assessment scheduling information on existing industrial chemicals (not in search)



- All stakeholders for whom such regulatory relevant information is critical
  - Regulators
  - Industry
  - Academics
  - International organisations
  - General public



# eChemPortal's added value

- Searches data from multiple sources simultaneously
- Identifies relevant information
- Provides direct free access to information
- Describes the type of review the data have undergone
- Allows a broad search on substance identification (incl. synonyms, trade names, in different languages)
- Is implemented with the common electronic data formats for reporting chemical test summaries
  - OECD Harmonised Templates for Reporting Chemical Test Summaries (OHTs)
     www.oecd.org/ehs/templates
  - Tests according to OECD Test Guidelines, national guidelines: US EPA, EU methods, ISO...
  - Data sources based on OHT can participate efficiently, e.g. IUCLID 5



- OECD
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- Searches by
  - substance identification
  - property and effects criteria
  - substance and then by property criteria



### Home page (www.oecd.org/ehs/echemportal)



Print
English

### The Global Portal to Information on Chemical Substances



### eChemPortal > Substance Search > Property Search What's new? > General Information Participating Databases > Roles & Responsibilities > Extension of the Portal > Linking to eChemPortal > Schedules of Assessments Structure Search GHS Classifications > Other useful information > FAQ > Help > Contact us > Disclaimer

Chemical Substance Search

Chemical Property Data Search Twenty-eight data sources participate under Chemical Substance Search.

Four databases participate under Chemical Property Data Search.

The list of data sources participating in eChemPortal is continuously expanding.

### Help us to help you. Answer the User Survey

eChemPortal provides free public access to information on properties of chemicals:

- Physical Chemical Properties
- Environmental Fate and Behaviour

Ecotoxicity

Toxicity

eChemPortal allows simultaneous searching of reports and datasets by

#### Latest news

Help us to help you. A new survey is on-line to collect eChemPortal user feedback

21 February 2014

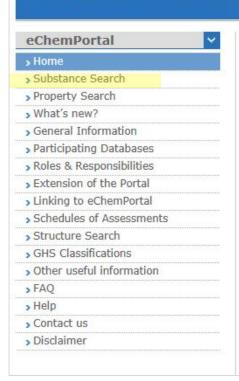
eChemPortal has a new refreshed logo

21 February 2014



### The Global Portal to Information on Chemical Substances





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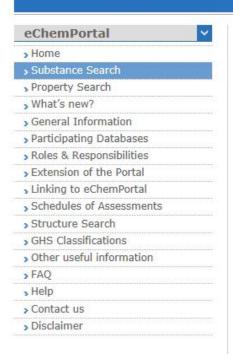
21 February 2014



### Substance Search - criteria entry screen

### The Global Portal to Information on Chemical Substances





#### Substance Search

#### Number:

CAS, EC, IUBMB, MITI, UN or NA Number.

Example: 108-88-3 for a CAS Number. Make sure you include the number separators. Do not search on partial Numbers.

#### Chemical name or synonym:

#### triclosan

Example: Use gluta\* to find Glutamic acid, use \*chloro\* to find dichlorobenzene. To search for \* as character (non wildcard use) use \*\* instead.

#### Databases:

- ✓ ACTOR
- **▼** AGRITOX
- ☑ APVMA-CR
- **V** CCR
- V CESAR
- Combined Exposures
- ▼ ECHA CHEM
- ☑ EnviChem
- FPA HHBP

- FPA OPPALB

V FSIS

V GDI

#### Select All Deselect All

Select one or more of the participating databases for your search.

Search

Reset

### Search by

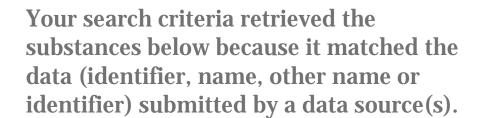
- Reference Number
- Chemical name or synonym
- Query URLs, e.g.

http://www.echemportal.org/eche mportal/substancesearch/substa ncesearch execute.action?numb erType=CAS&number=95-63-6&allParticipants=true



# Substance Search - results

Query results, level 1



Indirect query results, level 2



These tables contain results that do not directly match your search criteria but that may be of interest to you.

Indirect query results, level 3



# Substance search - intermediate results

#### Overall query results

Click the following link to see details for all query results.

. 17 Line(s) with 24 Hit(s) found as overall query results (including indirect query results)

### Query results, level 1



Your search criteria retrieved the substance(s) below or the same substance(s) identified by another identifier. Click on the column headers to sort the results in the table.

Hit(s)	Number	Name
4	3380-34-5 (CAS Number)	Triclosan (Unknown)
2	3380-34-5 (CAS Number)	triclosan (EC Name)
1	3380-34-5 (CAS Number)	2,4,4'-Trichloro-2'hydroxydiphenyl ether (Unknown)
1	3380-34-5 (CAS Number)	TRICLOSAN (Unknown)
1	64111-81-5 (CAS Number)	Triclosan (Unknown)
1	88032-08-0 (CAS Number)	TRICLOSAN (Unknown)
1		Triclosan (Unknown)

### Indirect query results, level 2

The table below contains the results of a subsequent search on numbers, names or synonyms based on the query results. Click on the column headers to sort the results in the table.

Hit(s)	Number	Name	
3	3380-34-5 (CAS Number)	Phenol, 5-chlora-2-(2,4-dichlorophenoxy)- (Unknown)	
2	64111-81-5 (CAS Number)	Phenol, 2-phenoxy-, trichloro deriv.	

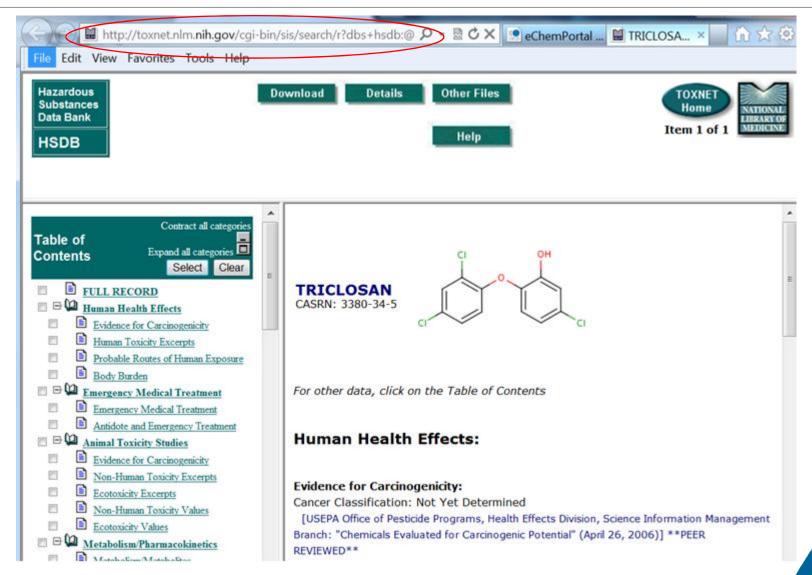


# Substance search - final results

Check	Number	Name	Remark	Level	Result	Source
	3380-34-5 (CAS Number)	5-Chloro-2-(2,4- dichlorophenoxy) phenol (Unknown)			<b>&amp;</b>	EnviChem
	3380-34-5 (CAS Number)	Triclosan (Unknown)		8	<b>₽</b>	HSNO CCID
	3380-34-5 (CAS Number)	Triclosan (Unknown)		<b>b</b>	函	ACToR
	3380-34-5 (CAS Number)	5-chloro-2-(2,4- dichlorophenoxy) phenol (IUPAC Name)	triclosan	<b>&amp;</b>	KP	ECHA CHEM
	3380-34-5 (CAS Number)	triclosan (EC Name)	ESIS: LPVCs (Low Production Volume Chemicals)	<b>&amp;</b>	₩	ESIS
	3380-34-5 (CAS Number)	TRICLOSAN (Unknown)		•	图	HSDB
	3380-34-5 (CAS Number)	triclosan (Unknown)	Priority Existing Chemical Assessment Report No. 30: Triclosan	<b>&amp;</b>	<b>₹</b>	NICNAS PEC
	3380-34-5 (CAS Number)	Triclosan (Unknown)		•	图	EPA HHBI
	3380-34-5 (CAS Number)	triclosan (EC Name)	ESIS: CLP/GHS (Classification, Labelling and Packaging of substances and mixtures), CLP implements the Globally harmonised System (GHS),	<b>&amp;</b>	장	ESIS



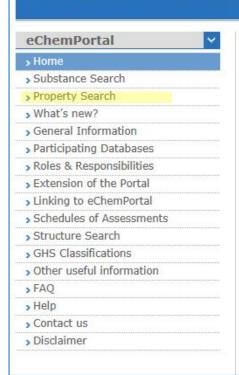
### Result in local data source





### The Global Portal to Information on Chemical Substances





Chemical Substance Search

Chemical Property Data Search

Ecotoxicity

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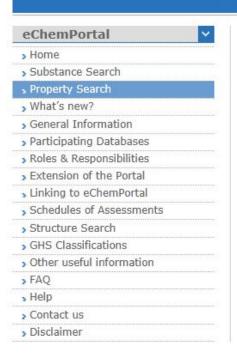
21 February 2014



## Property search - data point tree

### The Global Portal to Information on Chemical Substances





### **Property Search**

### Select Query Block Type

Select a section for which to define query criteria.



- + Physical and chemical properties
- + Environmental fate and pathways
- + Ecotoxicological Information
- + Toxicological information

^



### Property search: <Short-term toxicity to fish>

### **Property Search**

### Select Query Block Type

Select a section for which to define query criteria.



- + Physical and chemical properties
- + Environmental fate and pathways
- Ecotoxicological Information
- Aquatic toxicity

Short-term toxicity to fish

Long-term toxicity to fish

Short-term toxicity to aquatic invertebrates

Long-term toxicity to aquatic invertebrates

Toxicity to aquatic algae and cyanobacteria

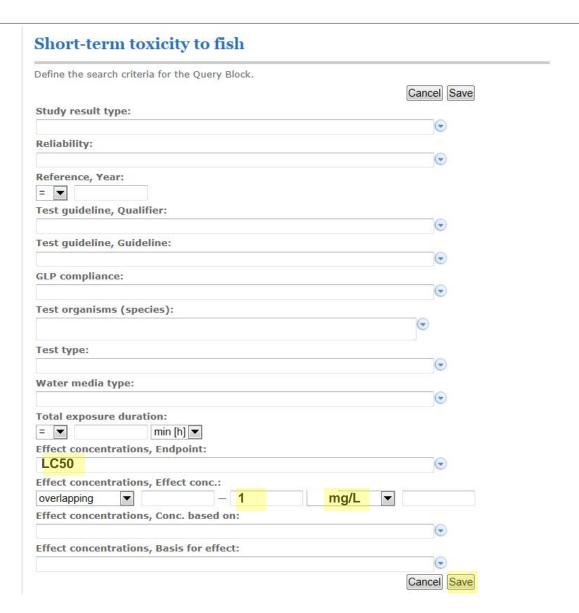
Toxicity to aquatic plants other than algae

Toxicity to microorganisms

Toyicity to other aquatic organisms



### Property search - criteria entry screen





## Property search - criteria

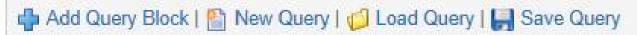
### **Property Search**

Property Search

Property Search

Define the query criteria.

Search is not restricted to a selected source. Select source.



X Short-term toxicity to fish

Effect concentrations, Endpoint = LC50
Effect concentrations, Effect conc. overlapping: < 1 mg/L



Partition coefficient

Partition coefficient, Partition coefficient overlapping: < 3

Execute Query



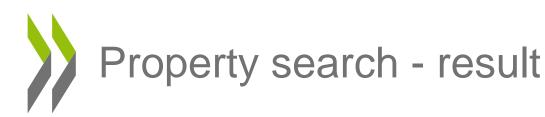
## Property search - result

Back to Property Search

CSV Excel Results 1 - 10 of 3462(limited result)

#### 1 2 3 4 5 6 7 8 9 10 Next

Substance	Results	Source
(RS)-4-hydroxy-3-(3-oxo-1-phenylbutyl)coumarin (IUPAC Name) 81-81-2 (CAS Number) Member of Category: no View Dataset	Partition coefficient Partition coefficient: 0.6	ECHA CHEM 🛂
(RS)-4-hydroxy-3-(3-oxo-1-phenylbutyl)coumarin (IUPAC Name) 81-81-2 (CAS Number) Member of Category: no View Dataset	Partition coefficient  Partition coefficient; 0.7	ECHA CHEM 🔂
(RS)-4-hydroxy-3-(3-oxo-1-phenylbutyl)coumarin (IUPAC Name) 81-81-2 (CAS Number) Member of Category: no View Dataset	Partition coefficient Partition coefficient: 2.9	ECHA CHEM 💋
(RS)-4-hydroxy-3-(3-oxo-1-phenylbutyl)coumarin (IUPAC Name) 81-81-2 (CAS Number) Member of Category: no View Dataset	Short-term toxicity to fish F Effect concentrations, Endpoint: LC50 Effect concentrations, Effect conc.: 34.3 µg/L	ECHA CHEM 🔂
(RS)-4-hydroxy-3-(3-oxo-1-phenylbutyl)coumarin (IUPAC Name) 81-81-2 (CAS Number) Member of Category: no View Dataset	Short-term toxicity to fish F Effect concentrations, Endpoint: LC50 Effect concentrations, Effect conc.: 37.7 µg/L	ECHA CHEM 🛂
(RS)-4-hydroxy-3-(3-oxo-1-phenylbutyl)coumarin (IUPAC Name) 81-81-2 (CAS Number) Member of Category: no View Dataset	Short-term toxicity to fish F Effect concentrations, Endpoint: LC50 Effect concentrations, Effect conc.: 46 µg/L	ECHA CHEM 🔂
-D-Galactopyranoside, 6-bromo-2-naphthalenyl (Unknown) 15572-30-2 (CAS Number) Member of Category: no View Dataset	Partition coefficient Partition coefficient: 1.57 (predicted by KowWin)	CCR 🗗



If you add a reliability of 1 then the results are now filtered to 121 results.



### **Property Search Result**

Back to Property Search CSV Excel Results 1 - 10 of 121(limited result)

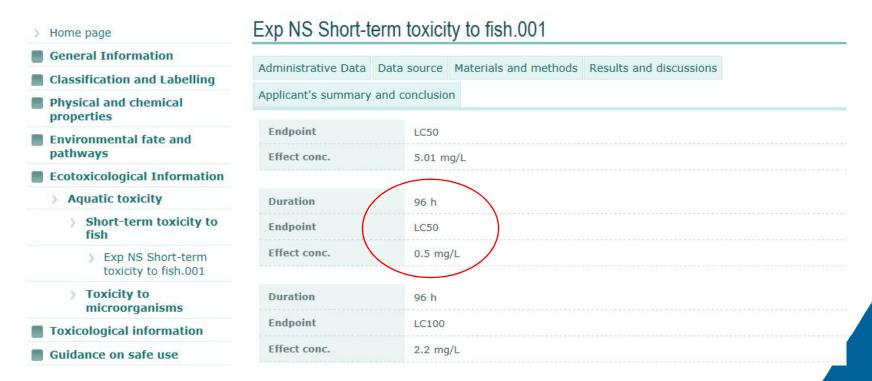
1 2 3 4 5 6 7 8 9 10 Next

Substance	Results	Source
2-Amino-5-chlorophenol (IUPAC Name) 28443-50-7 (CAS Number) Member of Category: no View Dataset	Partition coefficient  Partition coefficient: 1.24	ECHA CHEM
2-Amino-5-chlorophenol (IUPAC Name) 28443-50-7 (CAS Number) Member of Category: no View Dataset	Short-term toxicity to fish Reliability: 1 (reliable without restriction) Effect concentrations, Endpoint: LC50 Effect concentrations, Effect conc.: 0.5 mg/L	ECHA
2-benzyl-2-dimethylamino-4'- morpholinobutyrophenone (IUPAC Name) 119313-12-1 (CAS Number) Member of Category: no View Dataset	Partition coefficient  Partition coefficient, Partition coefficient: 2.91	ECHA CHEM 🚰
2-benzyl-2-dimethylamino-4'- morpholinobutyrophenone (IUPAC Name) 119313-12-1 (CAS Number) Member of Category: no View Dataset	Partition coefficient  Partition coefficient: 2.91	ECHA CHEM 🛂
2-benzyl-2-dimethylamino-4'- morpholinobutyrophenone (IUPAC Name) 119313-12-1 (CAS Number) Member of Category: no View Dataset	Short-term toxicity to fish  Reliability: 1 (reliable without restriction) Effect concentrations, Endpoint: LC50 Effect concentrations, Effect conc.: 0.46 mg/L	ЕСНА СНЕМ
2-benzyl-2-dimethylamino-4'-	Short-term toxicity to fish 🚜	ECHA



### Result in local data source







# Search and property search: CAS Number <142-96-1>

Check	Number	Name	Remark	Level	Result	Source
	142-96-1 (CAS Number)	n-Butylether (Unknown)		<b>b</b>	ゼ	EnviChem
	142-96-1 (CAS Number)	Butane, 1,1'-oxybis - (Unknown)		\$	샵	HSNO CCID
V	142-96-1 (CAS Number)	Butyl ether (Unknown)		<b>b</b>	松	J-CHECK
	142-96-1 (CAS Number)	Butyl ether, n- (Unknown)		•	굡	INCHEM
V	142-96-1 (CAS Number)	1,1'-oxydibutane (IUPAC Name)	dibutyl ether	<u>d</u>	怪	ECHA CHEM
	142-96-1 (CAS Number)	Butyl ether (Unknown)		9	怪	ACTOR
	142-96-1 (CAS Number)	Butane, 1,1'-oxybis - (Unknown)		<u></u>	<b>&amp;</b>	US EPA SRS
7	142-96-1 (CAS Number)	1,1'-oxydibutane (IUPAC Name)	dibutyl ether (IUC4 DSN 142)	4	<b>៤</b>	OECD SIDS IUCLID
	142-96-1 (CAS Number)	Butane, 1,1 -oxybis - (Unknown)		<b>d</b>	嵒	CCR
	142-96-1 (CAS Number)	dibutyl ether (EC Name)	ESIS : CLP/GHS (Classification.	•	嵒	ESIS

Select All Deselect All

Continue with Property Search

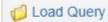


### Search and property search

### **Property Search**

### Select Query Block Type

Select a section for which to define query criteria.



- + Physical and chemical properties
- Environmental fate and pathways
- Ecotoxicological Information
- Toxicological information
- Toxicokinetics, metabolism and distribution

Basic toxicokinetics

Dermal absorption

Acute Toxicity

Acute toxicity: oral

Acute toxicity: inhalation

Acute toxicity: dermal

Acute toxicity: other routes

THE PERSON ASSESSED TO BE SHOULD BE



# Search and property search criteria: Acute toxicity: oral

You can search on a data point without entering additional criteria.





### Search and property search criteria:

Biodegradation in water: screening test

### **Property Search**





# Search and property search result

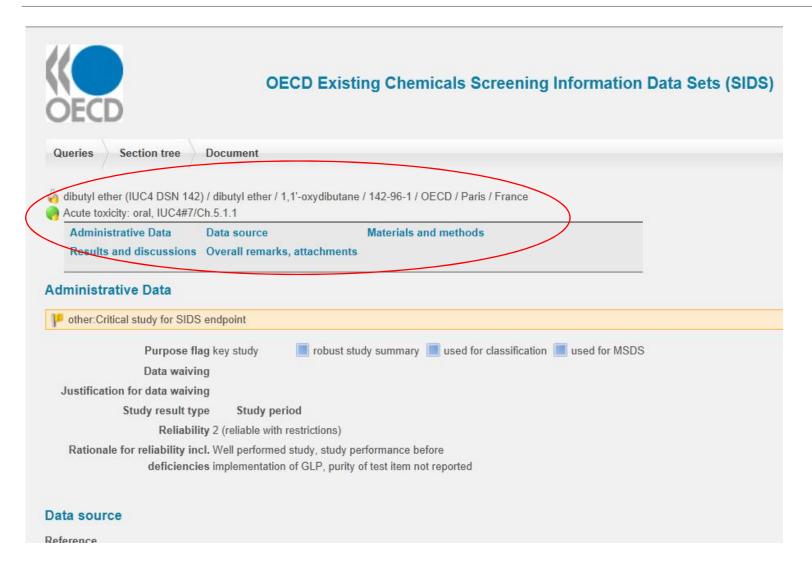
### **Property Search Result**

Back to Property Search	CSV Excel	Results 1 - 4 of 4

Substance	Results	Source
1,1'-oxydibutane (IUPAC Name) 142-96-1 (CAS Number) Member of Category: no View Dataset	Acute toxicity: oral	OECD SIDS IUCLID
1,1'-oxydibutane (IUPAC Name) 142-96-1 (CAS Number) Member of Category: no View Dataset	Acute toxicity: oral	OECD SIDS IUCLID
1,1'-oxydibutane (IUPAC Name) 142-96-1 (CAS Number) Member of Category: no View Dataset	Acute toxicity: oral	ECHA CHEM
1 1 Lovudihutana	Acute toxicity: oral 🛃	ECHA CHEM 🛂



### Result in local data source

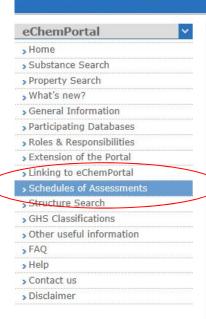




# Assessment scheduling information on existing industrial chemicals

#### The Global Portal to Information on Chemical Substances





### A Roadmap to National and Regional Programmes' work on Chemicals Assessment

Efforts continue to be made in OECD to create, maintain and improve the various parts of a process which looks at sharing in a mutually beneficial manner work from National and Regional Chemicals Programmes while saving resources and avoiding inefficiencies caused by duplicative work.

The links below lead to existing scheduling information of national/regional and international assessments notified to the OECD by OECD member countries and stakeholders. They are provided here with the aim to assist in avoiding duplication across national/regional programmes in the area of chemical assessment.

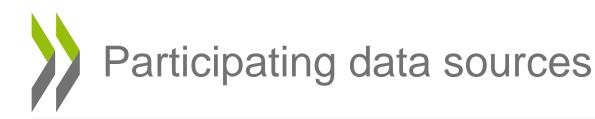
A project is underway to provide a more integrated access to this information in the future.

#### Links

- \*Australia
  - National Industrial Chemicals Notification and Assessment Scheme (NICNAS) PEC Declarations: Priority Existing Chemicals under assessment and the expected date of completion 母
- · Canada's Chemicals Management Plan
  - Overview of the Substances Grouping Initiative English , French
  - Forward Agenda: English ♥, French ♥, EXCEL (EN & FR) ♥
  - Summary of Previous Assessments English . French .
- FU RFACH
  - List of registered substances
  - Candidate List of Substances of Very High Concern
  - Registry of Intentions (SVHC , Harmonised C&L , Restrictions )
- · The United States
  - National Center for Risk Assessment IRIS Substance Assessment Tracking System:



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- 28 data sources participate in substance search
  - Australia, Canada, Finland, France, Japan, New Zealand, UK, USA, EU, IOs
- 4 data sources in property data search
  - Canada (CCR); EU (ECHA CHEM); Japan (J-CHECK); OECD (OECD SIDS IUCLID)
- The number of data sources participating in eChemPortal is continuously increasing



### Participating data sources

- U.S. EPA Aggregated Computational Toxicology Resource (ACToR)
- AGRITOX Base de données sur les substances actives phytopharmaceutiques
- The Australian Pesticides and Veterinary Medicines Authority (APVMA) database
- Canadian Categorization Results (Env. & Human Health)
- Canada's Existing Substances Assessment Repository
- Collection of Case Studies on Risk Assessments of Combined Exposures to Multiple Chemicals
- ECHA's Dissemination portal with information on chemical substances registered under REACH.
- Data Bank of Environmental Properties of Chemicals (EnviChem)
- US EPA Human Health Benchmarks for Pesticides
- US EPA Office of Pesticide Programs' Aquatic Life Benchmarks
- European Chemical Substances Information System (ESIS)
- Gefahrstoffdatenbank der Länder
- The Result of the GHS Classification by the Japanese Government
- US High Production Volume Information System (HPVIS)
- Hazardous Substance Data Bank (HSDB)
- New Zealand Hazardous Substances and New Organisms Chemical Classification Information Database (HSNO CCID)

- Chemical Safety Information from Intergovernmental Organizations INCHEM
- Japan CHEmicals Collaborative Knowledge database (J-CHECK)
- Japan Existing Chemical Data Base (JECDB)
- Australian National Industrial Chemicals Notification and Assessment Scheme (NICNAS) assessments of existing chemicals other than Priority Existing Chemical assessments
- NICNAS Priority Existing Chemical Assessment Reports (NICNAS PEC)
- OECD Existing Chemicals Database
- OECD Existing Chemicals Screening Information Data Sets (SIDS) Database
- OECD Initial Assessment Reports for HPV Chemicals including Screening Information Data Sets (SIDS) as maintained by United Nations Environment Programme (UNEP) Chemicals
- Substances in Preparations In the Nordic countries (SPIN)
- UK Coordinated Chemicals Risk Management Programme Publications
- US EPA Integrated Risk Information System (IRIS)
- US EPA Substance Registry Services (US EPA SRS)

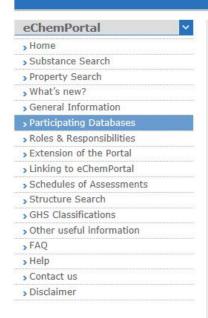


### Description of data source

### The Global Portal to Information on Chemical Substances

Participating Databases





### **Participating Databases**

nite

National Institute of Technology and Evaluation

独立行政法人 製品評価技術基盤機構

The Result of the GHS Classification by the Japanese Government

GHS-J

#### Type of information that can be found via eChemPortal:

National GHS classifications.

#### General information:

The GHS-J is a database of GHS classification results by the Japanese government since 2006. This database includes GHS classification guidance by the Japanese government and classification results (classification, symbol, signal word and hazard statement) in accordance with the guidance, etc. These classification are an advisory classification and intended to be used as reference for preparing GHS labelling and SDS by enterprises.



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## National GHS classifications

- Currently 7 databases disseminate GHS information via eChemPortal
  - AGRITOX (European CLP Regulation) (France)
  - INCHEM by WHO/IPCS via its International Chemical Safety Cards
  - ECHA CHEM (Registration dossiers' section 2.1 on C&L) (Europe)
  - HSNO CCID (based on GHS) (New Zealand)
  - GDL (European CLP Regulation) (Germany)
  - GHS-J (Japan)
  - ESIS (Europe)
- ECHA public C&L inventory (in 2014)
- Video tutorial on how to find classification information (in 2014)



# Future developments – 2014 (1)

- Filter results by type
  - Property information
  - Exposure & use information
  - National GHS classifications

Type:	Databases:	
Property information	Source 1	Source 7
Exposure and use information	Source 2	Source 8
National GHS classifications	Source 3	Source 9
Select All Deselect All	Source 4	Source 10
Select one or more of the types of information for your search	Source 5	Source 11
	▼ Source 6	Source 12
	Select All Deselect Al	I
	Select one or more of t	he participating databases for your search.



## Future developments – 2014 (2)

- GHS classification search
  - By chemical substance
  - By classification hazard category
  - A combination of both
- Only Harmonised / "Reviewed"\*



\*"Reviewed C&L" means that the C&L has undergone a review by a regulatory body or similar international organisation e.g. substances listed in table 3.1 of the Annex VI to the CLP Regulation in Europe



## Future developments – 2014 (2b)

View
"in a glance"
all GHS
classifications
available for
same substance

The second table includes results from data sources which indicate they contain C&L data but cannot submit in the correct format or contain self-classifications.

### Query Result - Reviewed / harmonised classification and labelling Ways to proceed

· You can click a link in the "Result" column to see the substance in the participants database

Regulatory number	Substance name	Substance number	Form	Classification	Labelling	Qualifier	Result	Source
XXX-XXX-X	Chemical 1 (IUPAC name)	XXX-XXX-X (EC number)	Liquid	Acute Tox - oral 3 Acute Tox - dermal 3 Acute Tox - inhalation 3 Skin Corr. 18 Skin Sens. 1 Carc 2	Danger		&	Source 1
ID69	Chemical 1 (IUPAC name)	XXX-XX-X (CAS rumber)	Gas	Acute Tex. ral 4 Acute	Not submitted by participant		S.	Source 2

### Other classification and labelling information

Number	Name	Remark	Level	Result	Source
(XX-XX-X CAS Number)	Chemical 1 (IUPAC Name)		9	<b>E</b>	Source 3



## Future developments – 2014 (2c)

View all substances with specific classification hazard category/ies

### Classification and labelling search

#### Search history

You searched for

Classification: Carc. 1A

Number of hits: 2

· Download results in CVS or EXCEL format

#### Query Result - Reviewed / harmonised of ssift ation and labelling

Ways to proceed

. You can click a link in the "Result" column . hee the substance in the participants database

Regulatory number	Substance name	Substance number	Form	Classification	Labelling	Qualifier	Result	Source
XXX-XXX-XX-X	Chemical 1	XXX-XXX-X (CAS Number)		Acute Tox. 3 Skin Corr. 1B Skin Sens. 1 Acute Tox. 2 Muta. 2 Carc. 1A	Danger	YES	&	Source 1
ID261	Chemical 2	XXX-XXX-X (CAS Number)		Ox. Sol. 2 Skin Corr. 1A Skin Corr. 1B Skin Corr. 1C Muta. 1A Carc. 1A Asp. Tox. 1	Not submitted by participant		&	Source 2
2 Hit(s)								



- OECD
- What eChemPortal is
- How to use eChemPortal
- Data sources
- Information classifications according to the GHS
- Conclusion



### Achieving the Vision:

- make relevant data freely available on the Internet (authorities & IOs).
- identify relevant data to be linked to eChemPortal (OECD Stakeholders).
- implement IT systems with the OECD Harmonised Templates (Data sources).
- develop processes to submit data to eChemPortal (authorities & IOs).



# Thank you