

Toxics Information Clearinghouse Hazard Traits

Presentation to
Green Ribbon Science Panel Meeting
April 29-30

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What is the Clearinghouse?

- Established by SB 509:
 - “Decentralized Web-based system for the 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”
 - DTSC shall “operate the clearinghouse at the least possible cost to the state”

Clearinghouse content

- On or before January 1, 2011, OEHHA shall:
 - “...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.”
- Green Chemistry Initiative Final Report recommends starting with existing data from authoritative sources:
 - California and other states
 - Federal government
 - Other nations (e.g., Canada, European Union)
- Generating new data requires a prioritization process (AB 1879)

AB 1879 link to SB 509

- DTSC shall establish a process to identify and prioritize chemicals of concern in consumer products, which will include:
 - Volume in commerce
 - Exposure potential
 - Potential effects on sensitive subpopulations
- As part of the process, DTSC shall develop criteria for evaluating chemicals and alternatives, which will include:
 - “The traits, characteristics and endpoints that are included in the clearinghouse data”

Clearinghouse development to date

- Research on existing definitions, identification/evaluation methods, and data sources for hazard traits and endpoints
- Preliminary concepts
 - Identify chemical characteristics linked to hazard
 - Include “exposure traits”
 - Build in hierarchical structure linking early indicators to toxicological/environmental endpoints
 - Include evaluation - identify known and suspected hazards

Consultation process

- Ongoing meetings between OEHHA and DTSC
 - In contact with other states and countries regarding data sharing
- OEHHA public workshop on January 29, 2009
 - Brainstorming session
 - Input on broad questions from public and expert panel
- OEHHA, UCLA, UCB jointly applied for funding for workshop series
- Formal consultation with other state agencies planned

Jan 29 workshop on Clearinghouse

- Expert panel with members from:
 - Academia
 - Federal government
 - Industry
 - Nongovernmental organizations
- Included some members now on Green Ribbon Science Panel
- Wide range of stakeholders participated

Jan 29 workshop questions

- What characteristics should be considered a “hazard trait”?
- What hazard traits and toxicological/environmental endpoints should be included in Clearinghouse?
- What traits/endpoints/other data would be useful in identifying a chemical of concern without a full toxicological database?
- What traits/endpoints/other data would be useful in evaluating exposure potential?
- What traits/endpoints/other data would be useful in evaluating effects on sensitive subpopulations?

Jan 29 workshop highlights

- Cast broad net for “hazard traits” and chemicals
 - Prioritize hazard traits to consider first
 - Don’t just focus on data-rich chemicals, bad actors
- Incorporate emerging, “upstream endpoints”
 - E.g., endocrine disruption
 - Don’t extend too far into less well understood endpoints
- Don’t neglect traditional endpoints
 - Various lists of endpoints suggested
 - Include ecotoxicity - go beyond aquatic receptors
- Include physical chemical properties
- Use computational toxicology, structural alerts
- Include same set of hazard traits for all chemicals

Jan 29 workshop highlights, cont.

- Address exposure potential
 - Direct (e.g., biomonitoring) and indirect (e.g., production volume)
 - Persistence/bioaccumulation
 - Exposure timing, windows of vulnerability
- Address differential susceptibility
- Dose-response information critical
- Only address hazard, not dose/risk
- Leverage existing data sources
 - Clearly identify data source, potential conflict of interest
- Absence of adequate data a challenge
 - Illustrate data gaps
 - Missing information not necessarily a data gap

Examples of hazard traits

- Carcinogenicity
- Reproductive toxicity
- Developmental toxicity
- Genotoxicity
- Neurotoxicity
- Immunotoxicity
- Respiratory toxicity
- Cardiovascular effects
- Effects on other organs (e.g., liver)
- Endocrine disruption
- Perturbation of other hormone systems
- Ecotoxicity
- Sensory irritation
- Sensitization
- Persistence
- Bioaccumulation
- Flammability
- Reactivity
- Structural alerts
- Other physical chemical properties indicative of a hazard

Two examples of Internet data sources

- OECD eChemPortal
- US EPA Aggregated Computational Toxicology Resource (ACToR)



The Global Portal to Information on Chemical Substances

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by CAS Number:

or by Chemical name or synonym:

in

Search in:

All Databases



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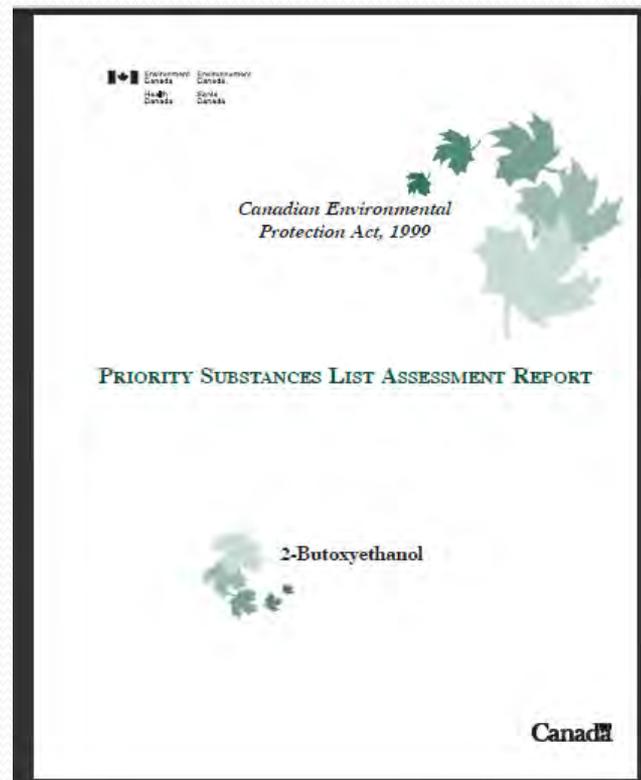
You searched "**Butoxyethanol, 2-**" which was identified as a synonym or trade name of the chemical substance "**Ethylene glycol monobutyl ether**"
CAS number related to the chemical substance: **111-76-2**

Found: 11

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

CESAR	Priority Substance List Assessment Report	Go to results
CESAR	Addendum to a Priority Substance List Assessment	Go to results
CHRIP		Go to results
EnviChem		Go to results
ESIS		Go to results
HSNO CCID		Go to results
INCHEM		Go to results
NICNAS PEC		Go to results
OECD HPV		Go to results
SIDS UNEP		Go to results

eChemPortal: Canada's Existing Substances Assessment Repository



eChemPortal: Japan's Chemical Risk Information Platform

National Institute of Technology and Evaluation

独立行政法人
製品評価技術基盤機構

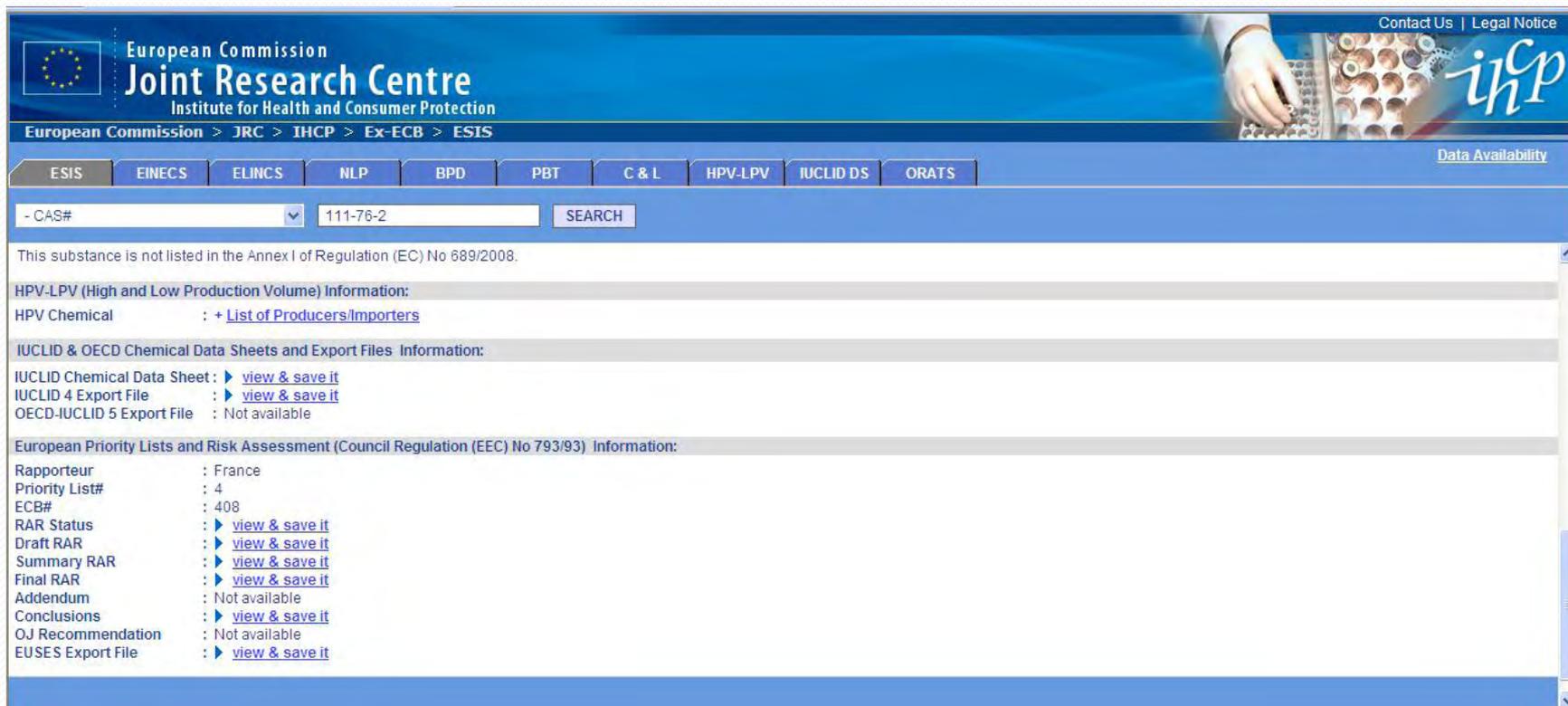
Biodegradation and Bioconcentration of Existing Chemical Substances under the Chemical Substances Control Law

[Description](#) [Biodegradability](#)

Information on the chemical published in the Official Bulletin of Economy, Trade and Industry (Former title: The Official Bulletin of the Ministry of International Trade and Industry (published before Jan.6,2001))

Published Chemical Name	Published Date	Published result
2-n-butoxyethanol	1976/5/28	Chemical substance determined to be ready biodegradable

eChemPortal: European Chemical Substances Information System



The screenshot displays the eChemPortal interface. At the top, there is a blue header with the European Commission logo and the text "European Commission Joint Research Centre Institute for Health and Consumer Protection". Navigation links include "Contact Us" and "Legal Notice". Below the header is a breadcrumb trail: "European Commission > JRC > IHCP > Ex-ECB > ESIS". A menu bar contains tabs for "ESIS", "EINECS", "ELINCS", "NLP", "BPD", "PBT", "C & L", "HPV-LPV", "IUCLID DS", and "ORATS". A search bar shows "- CAS#" with a dropdown arrow, the input "111-76-2", and a "SEARCH" button. A "Data Availability" link is on the right. The main content area shows a message: "This substance is not listed in the Annex I of Regulation (EC) No 689/2008." Below this are sections for "HPV-LPV (High and Low Production Volume) Information:" and "IUCLID & OECD Chemical Data Sheets and Export Files Information:". The HPV-LPV section lists "HPV Chemical" with a link to "+ List of Producers/Importers". The IUCLID section lists "IUCLID Chemical Data Sheet", "IUCLID 4 Export File", and "OECD-IUCLID 5 Export File" with links to "view & save it" or "Not available". The "European Priority Lists and Risk Assessment (Council Regulation (EEC) No 793/93) Information:" section lists various fields: "Rapporteur" (France), "Priority List#" (4), "ECB#" (408), "RAR Status", "Draft RAR", "Summary RAR", "Final RAR", "Addendum", "Conclusions", "OJ Recommendation", and "EUSES Export File", each with a link to "view & save it" or "Not available".

European Commission
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European Commission > JRC > IHCP > Ex-ECB > ESIS

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

- CAS# 111-76-2 SEARCH

Data Availability

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

HPV-LPV (High and Low Production Volume) Information:
HPV Chemical : + [List of Producers/Importers](#)

IUCLID & OECD Chemical Data Sheets and Export Files Information:
IUCLID Chemical Data Sheet : [view & save it](#)
IUCLID 4 Export File : [view & save it](#)
OECD-IUCLID 5 Export File : Not available

European Priority Lists and Risk Assessment (Council Regulation (EEC) No 793/93) Information:
Rapporteur : France
Priority List# : 4
ECB# : 408
RAR Status : [view & save it](#)
Draft RAR : [view & save it](#)
Summary RAR : [view & save it](#)
Final RAR : [view & save it](#)
Addendum : Not available
Conclusions : [view & save it](#)
OJ Recommendation : Not available
EUSES Export File : [view & save it](#)

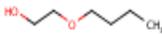
ACToR: Initial search results

Chemical Name Parameters Match by

Search on Chemical Names Exact
 Search on CAS Numbers Any

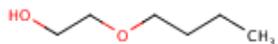
Enter Chemical Name:

Previous [Next 10](#)

Structure	CASRN	Name	Generic	Hazard	Carcinogenicity	Genotoxicity	Developmental	Reproductive	Chronic	Food Safety
	111-76-2	Ethylene glycol monobutyl ether	Details	Ha	Ca	G	D	R	Cr	FS

ACToR: Chemical summary

Chemical Summary : Ethylene Glycol Monobutyl Ether



GCID	205
CASRN	111-76-2
Formula	C ₆ H ₁₄ O ₂
MW	118.1742
SMILES	CCCCOCCO
INCHI	InChI=1/C6H14O2/c1-2-3-5-8-6-4-7/h7H,2-6H2,1H3

- ▶ [Show Substances](#)
- ▶ [Show Synonyms](#)

Data By Toxicology Phenotype

- ▶ [Show Hazard](#)
- ▶ [Show Carcinogenicity](#)
- ▶ [Show Genetic Toxicity](#)
- ▶ [Show Reproductive Toxicity](#)
- ▶ [Show Developmental Toxicity](#)
- ▶ [Show Chronic Toxicity](#)
- ▶ [Show Food Safety](#)

Data by Toxicology Data Category

- ▶ [Show In vivo toxicology \(tabular, primary data\)](#)
- ▶ [Show In vivo toxicology \(tabular, secondary data\)](#)
- ▶ [Show In vivo toxicology \(listing of studies performed\)](#)
- ▶ [Show In vivo toxicology \(summary calls of toxicity\)](#)
- ▶ [Show In vivo toxicology \(links to summary reports on the web\)](#)

Non-Toxicology Data

- ▶ [Show Physico-Chemical Data](#)
- ▶ [Show Biochemical Assays](#)
- ▶ [Show Links to chemical summary reports on the web](#)
- ▶ [Show Chemical Categories](#)
- ▶ [Show Chemical Manufacturing and Use Levels](#)
- ▶ [Show Descriptive Data](#)
- ▶ [Show Pesticidal Mode of Action](#)
- ▶ [Show Material Safety Data Sheet](#)
- ▶ [Show Regulations to which chemical is subject](#)
- ▶ [Show PubMed via MESH](#)
- ▶ [Show Notes](#)
- ▶ [Show External Searches by Name or CAS](#)

ACToR: Hazard results (portion)

NIOSH ChemHazard
 Result Group:

Component Name	Value
NIOSH ChemHazard URL	Link Out EXIT Disclaimer

OSHA/EPA Occupational Chemical Database - Full report
 Result Group:

Component Name	Value
OSHA EPA URL	Link Out EXIT Disclaimer

Risk Assessment Information System Toxicity Metadata
 Result Group:
 Previous **1-10 of 18** [Next 8](#)

Component Name	Value
EPA Cancer Class	C
RfC Basis	BMC
RfC Confidence Level	medium to high
RfC Critical Effect	changes in RBC count
RfC Modifying Factor	1
RfC Study Reference	NTP
RfC Study Date	1998
RfC Study Species	rat
RfC Target Organ	blood
RfC Uncertainty Factor	30.0

Screening Information Data Sets (SIDS) for High Volume Chemicals
 Result Group:

Component Name	Value
OECD SIDS URL	Link Out EXIT Disclaimer

Result Group:

Component Name	Value
DISP - DISPOSAL METHODS	The following wastewater treatment technologies have been investigated for Ethylene glycol monobutyl ether: Concentration process: Activated carbon. [USEPA; Management of Hazardous Waste Leachate, EPA Contract No.68-03-2766 p.E-152 (1982)]**PEER REVIEWED*

Result Group:

Component Name	Value
TOXS - TOXICITY SUMMARY	2-Butoxyethanol is a high production volume glycol ether. It is a colorless liquid that is miscible in water and soluble in most organic solvents. 2-Butoxyethanol is used widely as a solvent in surface coatings, such as spray lacquers, quick dry lacquers.

Result Group:

Component Name	Value
ANTR - ANTIDOTE AND EMERGENCY TREATMENT	Maintain an open airway and assist ventilation if necessary. Administer supplemental oxygen. Treat coma, convulsions, cardiac arrhythmia and metabolic acidosis if they occur. Observe the patient for several hours to monitor for development of metabolic ac

Result Group:

Component Name	Value
MEDS - MEDICAL SURVEILLANCE	The urinary excretion of /ethoxyacetic and butoxyacetic acids/ appears to correlate closely with the degree of occupational exposure, making them useful markers for medical surveillance. This usage is appropriate because there is evidence that the alkoxya

Result Group:

Component Name	Value
HTOX - HUMAN TOXICITY EXCERPTS	/HUMAN EXPOSURE STUDIES/ As a vapor at 100 ppm and higher, ethylene glycol mono-n-butyl ether (EGBE) was a sensory irritant... [Bingham, E.; Cohrssen, B.; Powell, C.H.; Pattys Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001).,

Result Group:

Component Name	Value
HTOX - HUMAN TOXICITY EXCERPTS	/HUMAN EXPOSURE STUDIES/ In several, single, 8 hour exposures of humans at concentrations of 100 or 200 ppm, no objective effects were seen except for urinary excretion of butoxyacetic acid. No increased osmotic fragility was observed in these short term

Result Group:

Component Name	Value
HTOX - HUMAN TOXICITY EXCERPTS	/HUMAN EXPOSURE STUDIES/ No clinical signs of adverse effects nor subjective complaints occurred among seven male volunteers exposed at 20 ppm for 2 hours during light physical exercise. [American Conference of Governmental Industrial Hygienists. Docume

ACToR: Physico-chemical properties (portion)

AOP - Hydroxyl Radical Rate Constants	
Result Group:	
Component Name Value	
OH est	2.351344E-11 sec-1
OH exp	1.86E-11 sec-1
BCF - Bioconcentration Factors	
Result Group:	
Component Name Value	
BCF	3.162
log BCF	0.5
log Kow	0.83
BIOHC - Biodegradation Half Life	
Result Group:	
Component Name	Value
log-iodegradation half-life	-99.0
DERMWIN - Dermal Permiability Estimators	
Result Group:	
Component Name Value	
Kp	0.00141
DA(Frick)	0.023
DA(Eq.5)	0.085
MW	118.18 daltons
log Kow	0.83
Henrys Law Constants	
Result Group:	
Component Name Value	
HLC(bond)	9.79E-8 L-atm/mol

KOA - Octonal Air partition coefficient (KOAWIN)	
Result Group:	
Component Name Value	
log Koa(1)	5.014
log Koa(2)	5.968
HLC	1.6E-6 L-atm/mol
log Kow	0.83
MPBPWIN - melting and boiling points	
Result Group:	
Component Name Value	
BP(est)	181.14 K
MP(est)	-20.31 K
VP(est)	0.475 atm
BP(exp)	168.4 K
MP(exp)	-74.8 K
VP(exp)	0.88 atm
VP temp	25.0 K
PCKOC - The Soil Adsorption Coefficient	
Result Group:	
Component Name Value	
Koc	1.0 (ug absorbed/g organ)
mci	3.9142
log Koc	0.0

Possible ways that Clearinghouse could add scientific value?

- Include California-specific information
 - New legislation implementing electronic system for California data on hazardous chemicals at regulated sites
- Show relationships between early indicators and toxic effects
- Compare chemicals
 - Data gaps
 - Safer alternatives
- Consider cumulative/synergistic effects

Questions for Panel

- Which are the highest priority hazard traits for inclusion in the Clearinghouse?
- Should the hazard traits be organized and/or evaluated in some way?
- How would you deal with data gaps?
- Which data sources should be included first?

Next steps

- Continue work to evaluate and specify hazard traits
- Hold additional public workshops
- Coordinate with DTSC to:
 - Consult with other state agencies
 - Pursue data sharing with other jurisdictions
 - Seek ongoing input from Panel

➤ Input welcome: shoover@oehha.ca.gov