Substance Profile for The Challenge
1,2-Benzenediol
(Catechol)
CAS No. 120-80-9

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) required the Minister of Health and Minister of the Environment to categorize the approximately 23 000 substances on the Domestic Substances List (DSL). Categorization involved identifying those substances on the DSL that are a) considered to be persistent (P) and/or bioaccumulative (B), based on criteria set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada, 2000), and "inherently toxic" (iT) to humans or other organisms, or b) that present, to individuals in Canada, the greatest potential for exposure (GPE).

Further to this activity, the Act requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that meet the categorization criteria. A screening assessment involves a scientific evaluation of available information for a substance to determine whether the substance meets the criteria set out in section 64 of CEPA 1999. Based on the results of a screening assessment, the Ministers can propose taking no further action with respect to the substance, adding the substance to the Priority Substances List (PSL) for further assessment or recommending the addition of the substance to the List of Toxic Substances in Schedule 1 of CEPA 1999 and, where applicable, the implementation of virtual elimination of releases to the environment.

A number of substances have been identified by the Ministers as high priorities for action based on the information obtained through the categorization process. This includes substances:

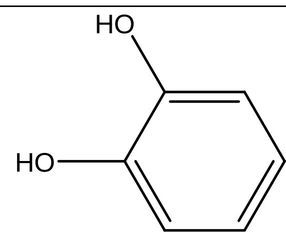
- that were found to meet all of the ecological categorization criteria, including persistence, bioaccumulation potential and inherent toxicity to aquatic organisms (PBiT), and that are known to be in commerce in Canada, and/or
- that were found either to meet the categorization criteria for GPE or to present an intermediate potential for exposure (IPE), and were identified as posing a high hazard to human health based on available evidence on carcinogenicity, mutagenicity, developmental toxicity or reproductive toxicity.

Based on a consideration of the ecological and/or human health concerns associated with these substances, and the requirement under section 76.1 of CEPA 1999 for the Ministers to apply a weight of evidence approach and the precautionary principle when conducting and interpreting the results of an assessment, sufficient data are currently available to consider these substances as meeting the criteria under Section 64 of CEPA 1999.

As such, the Ministers have issued a Challenge to industry and other interested stakeholders through publication in Canada Gazette Part I December 9, 2006 to submit, within the timelines stated in the Challenge section of this document, below, specific information that may be used to develop and benchmark best practices for risk management and product stewardship.

The substance catechol was identified as a high priority for action as it was determined to have a high potential for exposure to individuals in Canada (GPE or IPE), and is considered to present a high hazard to human health. The technical human health and ecological information that formed the basis for concern associated with this substance is contained in Appendices I and II, respectively.

Substance Identity

CAS Registry Number	120-80-9
Inventory names	1,2-Benzenediol; Catechol; Pyrocatechin; Pyrocatechol
Other names	1,2-Benzoldiol; 1,2-Dihydroxybenzene; 2-Hydroxyphenol; C.I. 76500; C.I. Oxidation Base 26; Durafur Developer C; Fouramine PCH; Fourrine 68; NSC 1573; o-Benzenediol; o-Dihydroxybenzene; o-Dioxybenzene; o-Hydroquinone; o-Hydroxyphenol; o-Phenylenediol; Oxyphenic acid; Pelagol Grey C; Phthalhydroquinone; Phthalic alcohol; Pyrocatechine; UN 2811
Chemical group	Discrete organics
Chemical sub-group	Phenols
Chemical formula	$C_6H_6O_2$
Chemical structure	
SMILES	Oc(c(O)ccc1)c1
Molecular mass	110.11 g/mol

Based on information submitted by the ten companies that notified this substance to the Domestic Substances List, approximately 120 tonnes of catechol were in commerce in 1986 for a variety of uses including, for example, the categories of: colourant (pigment/stain/dye/ink); analytical reagent; fragrance/deodourizer/flavouring agent; formulation component. Other potential uses of the substance in Canada include: photographic developer; chemical intermediate for antioxidants in rubber and lubricating oils, and a chemical intermediate for polymerization inhibitors. It can also be used in the synthesis of adhesives and insecticides, in electroplating, and in other sectors.

THE CHALLENGE

Respecting direction under section 76.1 of CEPA 1999, information obtained during conduct of categorization is sufficient to conclude that criteria under Section 64 of CEPA 1999 are met for this substance in that it "may enter the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health". As such, the Ministers are prepared to recommend to the Governor in Council that this substance be added to the List of Toxic Substances in Schedule 1 of CEPA 1999 with the intent of initiating the development of risk management measures taking into account socio-economic considerations. The measures will be subject to review in light of new scientific information, including monitoring and ongoing assessment activities.

Section 71 Notice

Information needed for improved decision-making with regard to risk assessment and management of this substance is being gathered using section 71 of CEPA 1999. This notice applies to any person who, during the 2006 calendar year, manufactured or imported a total quantity greater than 100 kilograms of the substance, whether alone, in a mixture, in a product or in a manufactured item.

The 2006 information mandated through the notice relates to, among other things, quantity of the substance imported, manufactured or used, types of uses of the substance, and releases of the substance to the environment.

Copies of the section 71 notice and guidance on how to comply with it are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca), or from the contact provided below.

Responses to the section 71 notice must be received at the address provided below by June 5, 2007.

Opportunity to Submit Additional Information on Current Uses and Existing Control Measures to Inform the Risk Management Approach for this Substance

The Ministers of Health and Environment are inviting the submission of additional information that is deemed beneficial by interested stakeholders, relating to the extent and nature of the management/stewardship of substances listed under the Challenge.

Organizations that may be interested in submitting additional information in response to this invitation include those that manufacture, import, export or use this substance whether alone, in a mixture, in a product or in a manufactured item.

Additional information is being invited in the following areas:

- Import, manufacture and use quantities
- Substance and product use details
- Releases to the environment and spill management
- Current and potential risk management and product stewardship actions
- Existing legislative or regulatory programs controlling/managing the substance
- Information to support the development of a regulatory impact assessment.

A questionnaire is available which provides a detailed template as an example for the submission of this information. Guidance on how to respond to the challenge questionnaire is also available. Interested stakeholders are invited to provide available additional information, recognizing that not all questions in the questionnaire may be relevant to a particular substance, use, or industrial sector.

Copies of the questionnaire and associated guidance are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca)**,** or from the contact provided below.

Responses to the questionnaire should be received at the address provided below by June 5, 2007.

Request for Documents and Submission of Information

Documents and instructions may be requested from the following contact. Information in response to the above Challenge must be submitted to this address.

DSL Surveys Coordinator
Place Vincent Massey, 20th Floor
351 Saint Joseph Boulevard
Gatineau QC K1A 0H3
Tel: 1-888-228-0530 / 819-956-9313
Fax: 1-800-410-4314 / 819-953-4936
Email: DSL.surveyco@ec.gc.ca

Appendix I
Human Health Information
to Support The Challenge for
1,2-Benzenediol (catechol)
CAS No. 120-80-9

Introduction

Under the *Canadian Environmental Protection Act, 1999* (CEPA, 1999), Health Canada undertook to categorize all substances on the Domestic Substances List (DSL) to identify those representing the greatest potential for human exposure (GPE) and those among a subset of substances considered persistent (P) and/or bioaccumulative (B) that are also considered to be “inherently toxic” to humans.

In order to efficiently identify substances that represent the highest priorities for screening assessment from a human health perspective, Health Canada developed and applied a Simple Exposure Tool (SimET) to the DSL to identify those substances that meet the criteria for GPE, Intermediate Potential for Exposure (IPE) or Low Potential for Exposure (LPE), and a Simple Hazard Tool (SimHaz) to identify those substances that pose a high or a low hazard.

Catechol is considered to meet the criteria for IPE under SimET and for high hazard under SimHaz. This document summarizes the currently available information used to support the inclusion of this substance in the Challenge.

Exposure Information from Health Related Components of DSL Categorization

As mentioned above, SimET was developed and used to identify substances on the DSL considered to represent GPE. This approach was based on three lines of evidence: 1) the quantity in commerce in Canada, 2) the number of companies involved in commercial activities in Canada (i.e., number of notifiers), and 3) the consideration by experts of the potential for human exposure based on various use codes. The proposed approach was released for public comment in November 2003 and also enabled designation of substances as presenting an Intermediate (IPE) or Lowest Potential for Exposure (LPE), based on criteria for quantity and nature of use (Health Canada, 2003)

Results of the Application of SimET

Catechol has been determined to be IPE based on a consideration of the DSL nomination information listed below.

Nomination Information for DSL

Quantity in Commerce

The quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 123,000 kg.

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was 10.

Use Codes and Description

The following DSL use codes have been identified for the substance:

5	Analytical reagent
13	Colourant - pigment/stain/dye/ink
21	Formulation component
22	Fragrance/perfume/deodourizer/flavouring agent
51	Function other than that listed in codes 02-50
70	Leather/Tanning
77	Organic Chemicals, Specialty
84	Photographic/Photocopier
85	Pigment, Dye and Printing Ink
98	Used in industry other than those specified in codes 51-97

Potential Uses in Canada

The additional information below on potential uses of catechol was identified through searches of the available scientific and technical literature.

Catechol is prepared by treating salicyladehyde with hydrogen peroxide, or from its monomethyl ether (guaiacol) by treatment with hydrobromic acid (O'Neil, 2001).

Catechol is found in nature in the tannin layer of mycorrhiza of the Douglas pine, and in the leaves/branches of oak and willow. In addition, it has been found in onions, crude beet sugar coal and apples (NLM, 2005).

Catechol is used as a photographic developer, a developer in fur dyes (NLM, 2005), as an intermediate for antioxidants in rubber and lubricating oils, in polymerization inhibitors and in pharmaceuticals (US EPA, 2000). It may be used as an oxidizing agent in hair colourants (Winter, 2005), however it is currently listed on Health Canada's Cosmetic Hotlist prohibiting its use in cosmetic products (Health Canada, 2005a). Catechol may also be used as a reagent; used in the synthesis of adhesives, insecticides and electroplating; in fax papers, specialty inks, as an antioxidant for perfumes and essential oils and as a fur/leather dyeing reagent (Ash and Ash, 2002). This substance has also been detected in cigarette smoke (US EPA, 2000).

Hazard Information from Health Related Components of DSL Categorization

Simple Hazard Tool (SimHaz)

SimHaz is a tool that has been used to identify, among all of the approximately 23 000 substances on the DSL, those considered to present either high or low hazard to human health based on formalized weight of evidence criteria and/or peer review/consensus of experts. This tool has been developed through extensive compilation of hazard classifications of Health Canada and other agencies and consideration of their robustness based on availability of transparent documentation of both process and criteria (Health Canada, 2005b).

Results of the Application of SimHaz

Catechol is considered to be a potentially high hazard substance based on its classification for carcinogenicity by the International Agency for Research on Cancer (IARC).

IARC has classified catechol as Group 2B for carcinogenicity (Possibly carcinogenic to Humans). IARC noted that no epidemiologic data relevant to the carcinogenicity of catechol were available, but there is sufficient evidence in experimental animals for the carcinogenicity of this compound (IARC, 1999).

Uncertainties

SimET and SimHaz have been developed as robust tools for effectively identifying substances from the DSL considered to be human health related priorities for further consideration. It is recognized that they do not include a number of elements normally considered in a human health risk assessment such as a comprehensive characterization of exposure and hazard, a comparison of exposure metrics to hazard metrics and a detailed analysis of uncertainties. However, as a result of the combination of the severe hazard properties of these substances and their high potential for exposure to humans, evaluation of whether there is a need for preventative and protective actions is required.

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Appendix II
Ecological Information
to Support The Challenge for
1,2-Benzenediol (catechol)
CAS No. 120-80-9

Introduction

The information in this document will form the basis of a screening assessment under section 74 of CEPA, 1999. Data relevant to an ecological screening assessment were identified in original literature, review documents, commercial and government databases prior to December 2005. Properties and characteristics may also have been estimated using Quantitative Structure Activity Relationship (QSAR) models.

Physical and Chemical Properties

Tables 1a and 1b contain experimental and modelled physical-chemical properties of catechol which are relevant to its environmental fate.

Table 1a: Experimental physico-chemical properties for catechol

Property	Value/Units	Reference
Boiling point	245 ºC	SRC PHYSPROP Database 2003
Melting point	105 ºC	SRC PHYSPROP Database 2003
Henry's Law constant	3.14×10^{-9} atm-m^3/mole	SRC PHYSPROP Database 2003
Dissociation constant	9.45	Serjeant, E.P. & Dempsey, B. (1979)
Log K_{ow}	0.88	Hansch *et al*., 1995
Vapour pressure	0.01 mmHg	Boublik *et al*. 1984
Water solubility	461000 mg/L	Granger & Nelson, 1921

Table 1b: Modelled physico-chemical properties for catechol

Property	Value/Units	Reference
Boiling Point	229.69 ºC	MPBPWIN v1.41
Melting Point	45.73 ºC	MPBPWIN v1.41
Henry's Law Constant	8.099×10^{-11}atm · m3/mol; 5.833×10^{-11}atm · m3/mol	HenryWin v3.10
log Koc	2.65	PCKOCWIN v1.66
log Kow	1.03	KOWWIN v1.67
Vapour Pressure	0.152 Pa; 1.14×10^{-3} mm Hg	MPBPWIN v1.41
Water Solubility	73230 mg/L	WSKOWWIN v1.41

Manufacture, Importation, and Uses

Refer to Appendix I.

Releases, Fate and Presence in the Environment

Releases

Refer to Appendix I.

Fate

Aquatic fate

The relatively high acid dissociation constant of 9.45 (Table 1a) indicates that half of the chemical will be dissociated at pH 9.45. At environmentally relevant pH of surface waters (6-8), catechol will be primarily in the undissociated form, The estimated log K_{oc} value of 2.65 (Table 1b) indicates that if released to water, adsorption of catechol to sediment and suspended organic matter will not be important. Volatilization from water surfaces to the atmosphere, based upon an experimental (3.1×10^{-9} atm · m^3/mole) and estimated (8.1×10^{-11} and 5.8×10^{-11} atm · m^3/mol) Henry's Law constant, will be too low to be environmentally important. Thus, if released to water, catechol is expected to mainly partition to water, which can be illustrated by the results of Level III Fugacity modelling (Table 2).

Table 2: Results of the Level III fugacity modelling (EPIWIN V3.12) for catechol

Receiving media	% in Air	% in Water	% in Soil	% in Sediment
Air (100%)	0.18	22.5	77.3	0.04
Water (100%)	0.00	99.8	0.00	0.20
Soil (100%)	0.00	18.6	81.4	0.04
Air, water, soil (33.3% each)	0.06	37.1	62.8	0.07

Terrestrial fate

Since the acid dissociation constant of this chemical is 9.45 (Table 1a), at environmentally relevant pH of soils (4-8), catechol will be mostly in the undissociated form. Based on an estimated log K_{oc} value of 2.65 (Table 1b), catechol should have moderate sorption to soil and, therefore, moderate mobility in this environmental compartment. Volatilization of this chemical from moist soil surfaces is not expected to occur to any significant extent, given the experimental (3.1×10^{-9} atm · m^3/mole) and estimated (8.1×10^{-11} and 5.8×10^{-11} atm · m^3/mol) Henry's Law constant. The potential for volatilization of catechol from dry soil surfaces is low, based upon experimental (0.01 mmHg) and estimated (1.1×10^{-3} mm Hg) values of vapour pressure (Tables 1a and 1b).

Thus, if released to soil, catechol is expected to remain in soil and, in a lesser degree, partition to water, which can be illustrated by the results of Level III Fugacity modelling (Table 2).

Atmospheric fate

If catechol is released to the atmosphere, it is expected to be rapidly oxidized. Catechol may also be removed from the atmosphere by wet deposition processes, considering very high water solubility of this substance (Tables 1a and 1b).

Presence in the Environment

No monitoring data relating to the presence of this substance in environmental media (air, water, soil, sediment) have yet been identified.

Evaluation of P, B and iT Properties

Environmental Persistence

The empirical rate constant for the vapour-phase reaction of catechol with photochemically-produced hydroxyl radicals has been reported to be 1.04×10^{-10} cm^3/molecule · sec at 25 ºC (Table 3a), which corresponds to an atmospheric half-life of 0.10 days. The EPIWIN-estimated atmospheric-oxidation half-life for catechol is ~0.5 days, assuming an average atmospheric hydroxyl radical concentration of 1.5×10^{6} molecule/cm^3 (Table 3b). Therefore, in air, catechol seems to be rapidly oxidized. This compound is not expected to react appreciably, with other photo-oxidative species in the atmosphere such as O_3. However, during the night-time, vapour-phase reaction with nitrate radicals may be a degradation process (Hazardous Substances Data Bank).

Therefore, it is expected that reactions with hydroxyl radicals will be the most important fate processes in the atmosphere for catechol, while reaction with nitrate radicals may be another removal process in night-time air.

Table 3a: Experimental persistence values for catechol

Medium	Fate Process	Degradation Value	Degradation Endpoint/Units	Reference
Air	Photodegradation	1.04×10^{-10}	Rate constant, cm^3/molecule · sec	Atkinson, 1989
Air	Photodegradation	0.103	Half-life, days	Atkinson, 1989
Water	Biodegradation	83	Biodegradation, %	Chemicals Inspection and Testing Institute, 1992

Table 3b: Modelled persistence values for catechol

Medium	Fate Process	Degradation Value	Endpoint/Units	Reference
Air	Atm. oxidation	0.4606	Half-life, days	AOPWIN v1.91
Air	Ozone reaction	Non-reactive	Half-life, days	AOPWIN v1.91
Water/Soil	Biodegradation	15	Half-life, days	BIOWIN v4.02, Ultimate survey
Water/Soil	Biodegradation	0.691	Probability	BIOWIN v4.02, MITI Non-linear Probability
Water/Soil	Biodegradation	0.546	Probability	BIOWIN v4.02, MITI Linear Probability
Water/Soil	Biodegradation	0.998	Probability	Topkat v.6.1

Experimental biodegradation data (Chemicals Inspection and Testing Institute, 1992) show 83% biodegradation of catechol in water over 28 days in a ready-biodegradation test (Table 3a). This indicates that its half-life in water is less than 182 days (6 months).

For estimating degradation in water, QSAR modeling was used (Table 3b). Based on these results, the estimated timeframe for biodegradation indicates that catechol can be considered as not persistent in water.

To extrapolate half-life in water to half-lives in soils and sediments, Boethling's extrapolation factors can be used ($t_{1/2\ water} : t_{1/2\ soil} : t_{1/2\ sediment}$ = 1: 1: 4, BIOWIN v4.01). Using these factors, it may be concluded that propylene oxide is not expected to be persistent in soil and sediments

Therefore, the empirical and modelled data demonstrate that catechol does not meet the persistence criteria (half-lives in soil and water ≥182 days, in sediments ≥365 days, in air ≥2 days) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Potential for Bioaccumulation

Experimental and modelled log K_{ow} values of 0.88 and 1.03 (Tables 1a and 1b, respectively) indicate that catechol does not have the potential to bioaccumulate in aquatic organisms.

Experimental BCF values for this substance are not available. The middle-trophic-level modified GOBAS BAF model produced a BAF of 1 L/kg, indicating that catechol does not have the potential to bioaccumulate in the fish. Furthermore, the three BCF models provide a weight-of-evidence (BCF=1-19 L/kg, Table 4) that catechol has a low potential for bioconcentration in aquatic organisms.

Table 4: Predicted bioaccumulation values for catechol

Test Organism	Endpoint/Units	Value	Reference
Fish	BAF (wet weight, L/kg)	1	Gobas BAF T2MTL (Arnot & Gobas, 2003)
Fish	BCF (wet weight, L/kg)	1 - 19	OASIS; Modified GOBAS BCF 5% T2LTL (Arnot & Gobas, 2003); BCFWIN v2.15

Therefore, modelled data indicate that the substance catechol does not meet the bioaccumulation criteria (BCF/BAF≥5000) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Ecological Effects

In the Aquatic Compartment

Experimental ecotoxicological data provide evidence that catechol does not cause significant harm to aquatic organisms at low concentrations (Table 5a). For two species of fish, acute LC50 values vary within a narrow range of 3.5-10 mg/L. Toxicity values for aquatic plants are slightly higher (13-27.5 mg/L), while for invertebrates (shrimp), the LC50 exceeds 40 mg/L. Predicted toxicity values (Table 5b) are, in general, in a reasonable agreement with the empirical results.

Table 5a: Experimental aquatic toxicity values for catechol

Test Organism	Endpoint	Test Type	Value (mg/L)	Reference No. (ECOTOX database)
Fish (*Pimephales promelas, Oncorhynchus mykiss*)	LC50	Acute (2-4 days)	3.5 - 10.0	569; 3217; 6573; 15031; 59196
Bay shrimp (*Crangon septemspinosa*)	LC50	Acute (4 days)	> 44	5810
Aquatic plants (*Elodea Canadensis, Lemna minor*)	EC50 (population growth rate)	Acute (≤ 9-12 d.)	13.2 - 27.5	14483

Table 5b: Modelled aquatic toxicity values for catechol

Organism	Endpoint	Duration	Toxicity value (mg/L)	Reference
Green algae	EC50	Acute	395	ECOSAR v.0.99h
Daphnia	EC50	Acute	22	TOPKAT v6.2
Fish	LC50	Acute	103	TOPKAT v6.2
Fish	LC50	Acute	6.77	AI Expert
Fish	LC50	Acute	152	ASTER
Fish	LC50	Acute	1773	OASIS Forecast
Fish	LC50	Acute	64	ECOSAR v.0.99h
Fish	LC50	Acute	6.7	ECOSAR v.0.99h (Neutral Org. SAR)

Therefore, according to the most of the experimental data, acute LC50/EC50 values are in the order of tens mg/L (or, sometimes, slightly below 10 mg/L), which may indicate that catechol is expected to pose a moderate (acute or immediate) hazard to aquatic organisms.

In Other Media

No effects studies for non-aquatic non-mammalian organisms were found for this compound.

Potential to Cause Ecological Harm

Based on the available information, catechol does not persist in the environment and is not bioaccumulative, based on criteria defined in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000). Information on concentrations of catechol in the environment has not been identified at this time. Experimental and modelled ecotoxicological data indicate that catechol is expected to pose a moderate hazard for aquatic organisms exposed to the chemical in water. Information on potential impacts in other environmental compartments has not been identified.

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