Substance Profile for The Challenge
Phenol, 2,4,6-tris(1,1-dimethylethyl)-
(2,4,6-tri-tert-buthylphenol)
CAS No. 732-26-3

1. 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, or of commercial interest, 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 conclude whether these substances meet the criteria under Section 64 of CEPA 1999.

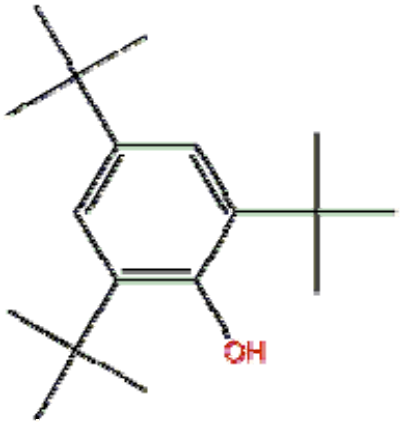
As such, the Ministers have issued a Challenge to industry and other interested stakeholders through publication in Canada Gazette Part I December 9, 2006 to submit, within the timelines stated in the Challenge section of this document, specific information that may be used to inform risk assessment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

The substance phenol, 2,4,6-tris(1,1-dimethylethyl)- was identified as a high priority for action as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The technical human health and ecological information, that formed the basis for the prioritization of this substance, is contained in Appendices I and II, respectively.

Substance Identity

For the purposes of this document, this substance will be referred to as 2,4,6-tri-tert-buthylphenol which has been derived from the PICCS inventory name.

CAS Registry Number	732-26-3
Inventory names	Phenol, 2,4,6-tris(1,1-dimethylethyl)- (TSCA, DSL, ENCS, AICS, SWISS, PICCS, ASIA-PAC) Phenol, 2,4,6-tris(1,1-dimethylethyl)- (English, French, German) (DSL, EINECS, PICCS) 2,4,6-tri-terc-butilfenol (Spanish) (EINECS) 2,4,6-Tris(1,1-dimethylethyl)phenol (ECL) 2,4,6-TRI-TERT.-BUTYLPHENOL (German) (SWISS) 2,4,6-TRI-TERT-BUTYL PHENOL (PICCS)
Other names	2,4,6-Tri-t-butylphenol 2,4,6-Tri-tert-butyl-1-hydroxybenzene 2,4,6-Tris(tert-butyl)phenol Alkofen B NSC 14459 P 23 P 23 (phenol) Phenol, 2,4,6-tri(1,1-dimethylethyl)- Phenol, 2,4,6-tri-tert-butyl- TM 02 Tri-tert-butylphenol Voidox
Chemical group	Discrete organics
Chemical sub-group	Phenols
Chemical formula	$C_{18}H_{30}O$

Chemical structure	
SMILES	Oc(c(cc(c1)C(C)(C)C)C(C)(C)C)c1C(C)(C)C
Molecular mass	262.44 g/mol

Based on information submitted in response to a legal Notice published in 2000 under section 71 of CEPA 1999, 2,4,6-tri-tert-buthylphenol was not manufactured in Canada in 2000 in a quantity meeting the 100 kg reporting thresholds. Five companies reported importing up to 100,000 kg into Canada in 2000 for activities described as a chemical intermediate in the production of antioxidants used in rubber and plastic; as a lubricating agent in the transport sector; as a by-product in the production of 4-tert-butylphenol; as an additive for gasoline and fuel oil distillate and use in the offshore sector.

THE CHALLENGE

Respecting direction under section 76.1 of CEPA 1999, and in the absence of additional relevant information as a result of this Challenge, the Ministers are predisposed to conclude, based on a screening assessment, that this substance satisfies the definition of toxic under section 64 of CEPA 1999. As such, the Ministers are prepared to then 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.

If it is determined that the substance meets the virtual elimination criteria in subsection 77(4) of CEPA 1999, then subsequent risk management activities will be based on the objective of eliminating the release of any measurable quantity of the substance to the environment. In the absence of further information on existing management practices for a substance, actions would be proposed based on the assumption of worst-case practices. The management actions being considered for such substances at this time include prohibition through regulations, of the manufacture, use, sale, offer for sale and import of this substance, except for those activities controlled under the *Pest Control Products Act* and/or the *Food and Drugs Act.*

Exceptionally, should no information be identified to indicate that this substance is in commerce in Canada, the Ministers will conclude, based on a screening assessment, that this substance does not satisfy the definition of toxic under section 64 of CEPA 1999. However, given the properties of this substance, there is concern that new activities for the substance that have not been identified or assessed under CEPA 1999 could lead to the substance meeting the criteria set out in section 64 of the Act. Therefore it would be recommended that this substance be subject to the Significant New Activity provisions specified under subsection 81(3) of the Act, to ensure that any new manufacture, import or use of this substance in quantities greater than 100 kg/year is notified, and that ecological and human health risk assessments are conducted as specified in section 83 of the Act prior to the substance being introduced into Canada.

Section 71 Notice

Under the Challenge, information deemed necessary for improved decision making may be gathered by the Minister of Environment using section 71 of CEPA 1999. This information may be used for the purpose of assessing whether a substance is toxic or is capable of becoming toxic as defined under section 64 of CEPA 1999, or for the purpose of assessing whether to control, or the manner in which to control a substance.

The information mandated through the notices may relate to, among other things; quantity of the substance imported, manufactured, used, or released, concentrations, suppliers, customers, as well as types of uses of the substance.

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.

Opportunity to Submit Additional Information to Inform Screening Assessment

The Ministers of Health and Environment are inviting the submission of additional information for consideration during screening assessment of this substance. Data of the types described in the following paragraphs are considered most relevant, although other submitted information will be considered.

Data on the persistence, bioaccumulation, and potential for toxicity of the substance to organisms in different environmental media – Through the categorization exercise, available experimental data were collected up to December 2005. Where acceptable experimental data were not available, Quantitative Structure Activity Relationships (QSARs) or read across data were used to fill the data gaps. Since experimental data are preferred, interested parties have an opportunity to provide new or additional relevant experimental study information on the persistence, bioaccumulation, and potential for toxicity of this substance to organisms in different environmental media (air, water, sediment, soil). Efforts should focus on providing data for the endpoints for which quality experimental data does not already exist, as demonstrated by the information summarized in Appendix II of this document. As submitted data will be evaluated for completeness and robustness, it is recommended that stakeholders follow the guidance for test protocols and alternative approaches for test data, as described in Section 8 of the "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers".[1]

Data on the toxicity of the substance to human health - Through the categorization exercise, the high health priorities for action were those substances identified by various agencies as representing a high health hazard on the basis of potential to induce cancer, and/or adversely affect reproduction and development, two critical determinants of the health of Canadians of all ages. The hazard classifications used were those developed by national or international agencies in which large numbers of substances have been classified for endpoint-specific hazard based on original review and critical evaluation of data, assessments of weight of evidence and extensive peer review. Interested parties have an opportunity to provide new or additional relevant experimental study information on the toxicity of the substance to human health which could inform the screening assessment.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

[1] "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers (version 2005)", Government of Canada, Available from http://www.ec.gc.ca/substances/nsb/eng/cp_guidance_e.shtml

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 this part of the challenge for this substance should be received at the address provided below by September 11th, 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
Phenol, 2,4,6-tris(1,1-dimethylethyl)-
(2,4,6-tri-tert-buthylphenol)
CAS No. 732-26-3

Introduction

Under the *Canadian Environmental Protection Act, 1999* (CEPA, 1999), Health Canada undertook to categorize 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 persistant (P) and/or bioaccumulative (B) by Environment Canada 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 low hazard.

2,4,6-tri-tert-buthylphenol is considered to meet the criteria for LPE under SimET and does not meet the criteria for high hazard under SimHaz. This document summarizes the currently available information on which the SimET and SimHaz results are based.

Exposure Information from Health Related Components of DSL Categorization

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 IPE or LPE, based on criteria for quantity and nature of use (Health Canada, 2003)

Results of the Application of SimET

2,4,6-tri-tert-buthylphenol has been determined to be LPE 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 10,000,000 kg

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was less than 4.

Use Codes and Description

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

07 Antioxidant/corrosion inhibitor/tarnish inhibitor/scavenger/antiscaling agent
27 lubricating agent/lubricant additive/mould release agent

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, 2005)

Results of the Application of SimHaz

2,4,6-tri-tert-buthylphenol has not been classified for hazard by any of the agencies considered under the SimHaz tool and therefore does not meet the criteria for high hazard under SimHaz

Uncertainties

SimET and SimHaz have been developed as robust tools for effectively identifying substances from the DSL considered to be human health 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.

References

Health Canada. 2003. Proposal for Priority Setting for Existing Substances on the Domestic Substances List under the Canadian Environmental Protection Act, 1999: Greatest Potential for Human Exposure. http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/existsub/exposure/greatest_potential_human_exposure-risque_exposition_humaine_e.pdf

Health Canada. 2005. Proposed Integrated Framework for the Health-Related Components of Categorization of the Domestic Substances List under CEPA 1999 http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/contaminants/existsub/framework-int-cadre_e.pdf

Appendix II
Ecological Information
to Support The Challenge for
Phenol, 2,4,6-tris(1,1-dimethylethyl)-
(2,4,6-tri-tert-buthylphenol)
CAS No. 732-26-3

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. In addition, an industry survey was conducted for the year 2000 through a Canada Gazette Notice issued pursuant to section 71 of CEPA 1999 (Environment Canada, 2001). This Notice requested data on the Canadian manufacture, import, uses and releases for the 2000 survey.

Physical and Chemical Properties

Table 1 contains experimental and modelled physical-chemical properties of 2,4,6-tri-tert-buthylphenol which are relevant to its environmental fate

Table 1. Physical and chemical properties for 2,4,6-tri-tert-buthylphenol.

Property	Type	Value	Temperature (°C)	Reference
Melting point (°C)	Experimental	131 ^{o}C	--	SRC 2003
Boiling point (°C)	Experimental	278 ^{o}C	--	SRC 2003
Vapour Pressure (Pa)	Modelled	0.03 (*2E-4 mm Hg*)	25	MPBPWIN 2000
	Modelled	0.027 (*2E-4 mm Hg*)	--	HENRYWIN 2000
Henry's Law Constant ($Pa \cdot m^3/mol$)	Modelled	0.70-0.98 (*(6.9-9.7) ×10^{-6} atm-m3/mole*)	25	EPIWIN 2000
log Kow (octanol-water partition coefficient) (dimensionless)	Modelled	6.39	25	KOWWIN 2000
	Experimental	6.06		MITI (1992)

Water solubility (mg/L)	Experimental	35	15 – 25	MITI (1992)
log Koc (organic carbon-water partition coefficient) (dimensionless)	Modelled	5.01 - 5.12		PCKOCWIN 2000
Log Koa (Octanol-air partition coefficient) (dimensionless)	Modelled	9.79		OctanAir 2004

Manufacture, Importation, and Uses

Manufacture and Importation

In Canada, no manufacture of 2,4,6-tri-tert-buthylphenol was reported in response to a CEPA section 71 survey notice for the 2000 calendar year. However, five companies reported importing a total of between 10,000 and 100,000 kg of 2,4,6-tri-tert-buthylphenol into Canada in 2000 (Environment Canada, 2001).

Elsewhere, 2,4,6-tri-tert-buthylphenol has been identified as a OECD HPV chemical (1997), as a United State HPV Challenge programme (USEPA 1994) and a European Union Low Production Volume Chemical. Production within the EU has been estimated to be of the order of 10 tonnes; however, the Oslo-Paris (OSPAR) commission received information indicating possible uses at 33 tonnes in Denmark and 1 tonne in Norway (OSPAR commission 2004).

Uses

In Canada, greater than 98% of 2,4,6-tri-tert-buthylphenol has been reported for use as a fuel and oil additive. Based on these uses, the substance may be destroyed or released to the environment in a dispersive manner (Environment Canada 2001).

Although, there is still some uncertainty about the actual use pattern of 2,4,6-tri-tert-buthylphenol in Canada, but five categories of potential production and use have been identified or suggested worldwide: as a chemical intermediate in the production of antioxidants used in rubber and plastic; as a lubricating agent in the transport sector; as a by-product in the production of 4-tert-butylphenol; as an additive for gasoline and fuel oil distillate and use in the offshore sector.

Releases, Fate and Presence in the Environment

Releases

The substance 2,4,6-tri-tert-buthylphenol is not naturally produced in the environment. Only one of the 5 companies importing 2,4,6-tri-tert-buthylphenol reported a release of the substance, corresponding to 20 kg in 2000 (Environment Canada 2001). Because the s.71 survey did not gather release information from users of the substance, and because of the dispersive use of the chemical, it is expected that environmental releases to the environment were underestimated in the 2000 survey.

Fate

The high log K_{ow} and K_{oc} values indicate that this substance will likely partition to soil and sediments. Indeed, the results of the Level III Fugacity modelling indicates that if the chemical is released equally to the three major environmental compartments (air, water, and soil), it will mainly partition in soil and sediments (Table 2), where the chemical has been indicated to persist (see Table 3).

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

	Fraction of substance partitioning to each medium (%)			
Substance release to:	**Air**	**Water**	**Soil**	**Sediment**
Air (100%)	15.60	2.64	25.2	56.6
Water (100%)	0.00	4.46	0.0	95.5
Soil (100%)	0.00	0.00	99.9	0.1
Air, water, soil (33.3% each)	0.16	2.84	36.3	60.7

A vapour pressure of 0.03 Pa and Henry's Law constant of 0.7-0.98 $Pa \cdot m^3/mol$ indicates that 2,4,6-tri-tert-buthylphenol is semi/slightly volatile. Therefore, if released solely to air, it will tend to some extent to remain in this compartment; but even so, the major two media where this substance will partition will be soil and sediment (~82%, Table 2). In air, the chemical seems to be rapidly oxidized, indicated by an atmospheric oxidation half-life value of 0.67 day (Table 3a**).**

If released to soil, 2,4,6-tri-tert-buthylphenol is expected to have extremely high adsorptivity to soil (i.e. expected to be immobile) based upon an estimated Log K_{oc} of ~5. Volatilization from moist soil surfaces is likely a relatively unimportant fate process based upon an estimated Henry's Law constant of 0.7-0.98 $Pa \cdot m^3/mol$. This chemical may slightly volatilize from dry soil surfaces based upon its vapor pressure. 2,4,6-tri-tert-buthylphenol is practically non-biodegradable according to the Japanese MITI test (MITI 1992). Therefore, if released to soil, 2,4,6-tri-tert-buthylphenol will mainly remain in this environmental compartment, as illustrated by the results of the Level III fugacity modelling (Table 2).

If released into water, 2,4,6-tri-tert-buthylphenol is expected to strongly adsorb to suspended solids and sediment based upon extremely high values of estimated Log K_{oc}. Volatilization from water surfaces is expected to be a relatively unimportant fate process based upon this compound's estimated Henry's Law constant. Thus, if water is a receiving medium, 2,4,6-tri-tert-buthylphenol is expected to mainly partition into sediments and, to some extent, remain in water (Table 2).

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

Once released into the environment, 2,4,6-tri-tert-buthylphenol appears to be relatively persistent, mainly in water, soil and sediments.

No experimental persistence data in air are available for 2,4,6-tri-tert-buthylphenol. A predicted atmospheric oxidation half-life value of 0.67 days (Table 3a) demonstrates that in air, this chemical seems to be rapidly oxidized. This compound is not expected to react, or react appreciably, with other photo oxidative species in the atmosphere, such as O_3 and NO_3, nor is it likely to degrade via direct photolysis. Therefore, it is expected that reactions with hydroxyl radicals will be the most important fate process in the atmosphere for 2,4,6-tri-tert-buthylphenol. With a half life of 0.67 days via reactions with hydroxyl radicals, 2,4,6-tri-tert-buthylphenol is not persistent in air.

Table 3a. Modeled data for persistence of 2,4,6-tri-tert-buthylphenol.

Medium	Fate Process	Degradation Value	Endpoint/Units	Model/Reference exp.
Air	Atm. oxidation	0.6685	Half-life, days	AOPWIN 2000
Air	Ozone reaction	Not reactive	Half-life, days	AOPWIN 2000
Water/Soil	Biodegradation	60	Half-life, days	BIOWIN 2000
Water/Soil	Biodegradation	0.0497	Probability	BIOWIN 2000
Water/Soil	Biodegradation	0.002	Probability	TOPKAT 2004

Table 3b. Empirical data for persistence of 2**,4,6-tri-tert-buthylphenol.**

Medium	Fate Process	Degradation Value	Endpoint/Units	Model/Reference exp.
Water	Biodegradation	0	Biodegradation, %	MITI 1992

For estimating degradation in water, soil and sediment, a QSAR weight-of-evidence approach (ESD, 2006a) was applied using the models shown in Table 3a. Based on these results shown in table 3a, the estimated timeframe for biodegradation indicates that, 2,4,6-tri-tert-butylphenol can be considered as persistent in water and soil. This substance is not expected to hydrolyse.

To extrapolate to a half-life in sediments, an approach as been developed using Boethling's extrapolation factors (Boethling et al. 1995), which involves extrapolating the half life in sediment from that estimated for water ($t_{1/2\ water} : t_{1/2\ soil} : t_{1/2\ sediment} = 1:1:4$). Therefore, in sediments, the half-life is expected to exceed 365 days.

In addition, the empirical biodegradation data (MITI 1992), show 0% biodegradation over 28 days in a ready-biodegradation test for 2,4,6-tri-tert-buthylphenol (Table 3b). This indicates that the half-life in water and soil is longer than 182 days (6 months).

The long-range transport potential (LRTP) of 2,4,6-tri-tert-buthylphenol from its point of release to air is estimated to be low according to the model prediction presented in Table 3c. The TaPL3 model was used to estimate Characteristic Travel Distance (CTD), defined as the maximum distance traveled by 63% of the substance; or in other words, the distance that 37% of the substance may travel beyond. Beyer et al (2000) have proposed CTD's of >2000 km as representing high LRTP, 700-2000 km as moderate, and <700 km as low. Based on the result shown in Table 3c, this substance is expected to remain primarily in areas close to its emission sources.

Table 3c – Model Predicted Characteristic Travel Distance (CTD) for 2,4,6-tri-tert-buthylphenol.

Characteristic Travel Distance	Model (Reference)
166 km	TaPL3 (CEMC, 2003)

The empirical and modelled data (Tables 3a and 3b) demonstrate that the substance *meets the persistence criteria (half-lives in soil and water ≥ 182 days; half-life in sediments ≥ 365 days)* as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Potential for Bioaccumulation

Experimental and modelled log K_{ow} values for 2,4,6-tri-tert-buthylphenol indicate that this chemical has the potential to bioaccumulate in the environment (Table 4a&b).

The experimental bioconcentration factor (BCF) value in fish is reported to be 10317 to 13903 L/kg (MITI 1992).

QSAR modelled bioaccumulation and bioconcentration values also agree quite well with the experimental value (Table 4b). The Modified GOBAS BAF middle trophic level model produced a bioaccumulation factor (BAF) of 16982 L/kg, indicating that 2,4,6-tri-tert-buthylphenol has the potential to bioconcentrate and biomagnify in the environment. The three other BCF models also provide a weight-of-evidence to support the bioconcentration potential of this substance.

Table 4a. Empirical data for bioaccumulation

Test Organism	Endpoint	Value wet wt	Reference
Fish	BCF	10317-13903 L/kg	MITI 1992

Table 4b. Modelled data for bioaccumulation

Test Organism	Endpoint	Value wet wt	Reference
Fish	BAF	16982 L/kg	Arnot and Gobas 2003
Fish	BCF	3388 L/Kg	Arnot and Gobas 2003
Fish	BCF	67608 L/kg	OASIS Forecast 2005
Fish	BCF	3311 L/kg	BCFWIN 2000

The modelled bioaccumulation values do not take into account the potential of the substance to be metabolized. However, the experimental BCF value is high enough to indicate that metabolic degradation is not likely significant. Also, due to its type of structure (hindered phenol), this substance is not likely to have a high rate of metabolism.

The weight of evidence indicates that the substance meets the bioaccumulation criterion (BCF, BAF > 5000) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada 2000).

Ecological Effects

In the Aquatic Compartment

There is modelled and experimental evidence that the substance causes harm to aquatic organisms at relatively low concentrations (e.g., LC50 < 1 mg/L) [Table 5a and b].

Table 5a Empirical data for aquatic toxicity

Test Organism	Type of Test	Endpoint	Value (mg/L)	Reference
Fish	Acute	LC_{50}	0.06	Geiger et al. 1990

Table 5b Modelled data for aquatic toxicity

Test Organism	Type of Test	Endpoint	Value (mg/L)	Model / Reference
Fish	Acute	LC_{50}[1]	NP[3] 0.076 NP 0.1016 0.078	Topkat 2004 ECOSAR 2004; USEPA 1999 OASIS 2005; AI Expert 2005
Daphnia	Acute	EC_{50}[2]	NP NP	ECOSAR 2004; TOPKAT 2004
Algae	Acute	EC_{50}[2]	0.017	ECOSAR 2004

[1] Lethal concentration affecting 50% of the test population
[2] Concentration affecting 50% of the test population
[3] NP = Not predictable or not a reliable prediction

A range of aquatic toxicity predictions were obtained from the various QSAR models considered. Table 5b list those predictions that were considered reliable and were used in the QSAR weight-of-evidence approach for aquatic toxicity (ESD 2006a). These results

indicate a high potential for toxicity to aquatic organisms (i.e. acute LC/EC50<1.0 mg/L and chronic NOEC<0.1 mg/L).

In Other Media
Effects studies to non-aquatic non-human organisms have not yet been identified for this compound.

Potential to Cause Ecological Harm

Evidence that a substance is highly persistent and bioaccumulative as defined in the Persistence and Bioaccumulation Regulations of CEPA 1999 (Government of Canada, 2000) together with evidence of commercial activity provides a significant indication of its potential to be entering the environment under conditions that may have harmful long term ecological effects (ESD, 2006b). Substances that are persistent remain in the environment for a long time after being released, increasing the potential magnitude and duration of exposure. Substances that have long half-lives in mobile media (air and water) and partition into these media in significant proportions, have the potential to cause widespread contamination. Releases of small amounts of bioaccumulative substances may lead to high internal concentrations in exposed organisms. Highly bioaccumulative and persistent substances are of special concern, since they may biomagnify in food webs, resulting in very high internal exposures, especially for top predators. Evidence that a substance is both highly persistent and bioaccumulative, when taken together with other information (such as evidence of toxicity at relatively low concentrations, and evidence of uses and releases) may therefore be sufficient to indicate that the substance has the potential to cause ecological harm.

The relatively large importation volumes of 2,4,6-tri-tert-buthylphenol into Canada along with its dispersive uses indicate potential for releases into the Canadian environment. Once released in the environment, because of its resistance to degradation, it will remain in water, sediment and soil for long times. As it persists in the environment, and because of its lipophyllic character, it will likely bioaccumulate and may be biomagnified in trophic food chains. It has also been demonstrated to have relatively high toxicity. This information suggests that 2,4,6-tri-tert-buthylphenol has the potential to cause ecological harm in Canada.

Uncertainties

Based on information collected, there is some uncertainty about the precise use patterns of 2,4,6-tri-tert-buthylphenol. In addition, information and data on concentrations in the Canadian environment are currently lacking. Yet, the relatively high volume imported into Canada in 2000 and its dispersive uses is evidence of its potential for widespread release into the Canadian environment.

The evidence for high persistence and bioaccumulation potential is considered strong, since both modelled estimates and empirical data indicate that 2,4,6-tri-tert-buthylphenol meets the criteria set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000). Similarly convincing evidence that 2,4,6-tri-tert-

buthylphenol can harm organisms at relatively low exposure concentrations, is provided by results from QSAR modelling and toxicity testing for a fish species. However, it must be acknowledged that there were a limited number of empirical studies available relating to the persistence, bioaccumulation and toxicity of 2,4,6-tri-tert-buthylphenol.

Regarding toxicity, based on the predicted partitioning behaviour of this chemical, the significance of soil and sediments as important media of exposure is not well addressed by the effects data available. Indeed, the only effects data identified apply primarily to pelagic aquatic exposures, although the water column may not be the medium of primary concern based on partitioning estimates.

There is also uncertainty associated with basing the overall conclusion that 2,4,6-tri-tert-buthylphenol may be causing ecological harm, solely on information relating to its persistence, bioaccumulation, relative toxicity and use pattern. Typically quantitative risk estimates (i.e., risk quotients or probabilistic analyses) are important lines of evidence when evaluating a substances potential to cause environmental harm. However when risks for persistent and bioaccumulative substances such as 2,4,6-tri-tert-buthylphenol are estimated using such quantitative methods, they are highly uncertain and are likely to be underestimated (ESD, 2006b). Given that long term risks associated with persistent and bioaccumulative substances cannot at present be reliably predicted, quantitative risk estimates have limited relevance. Furthermore since accumulations of such substances may be widespread and are difficult to reverse, a conservative response to uncertainty (that avoids underestimation of risks) is justified.

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