

Substance Profile for The Challenge

Methyl oxirane

(propylene oxide)

CAS No. 75-56-9

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 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:

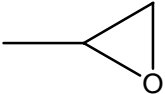
- that were found to meet all of the ecological categorization criteria, including persistence, bioaccumulation potential and inherent toxicity to aquatic organisms (PBiT), and that are known to be in commerce in Canada, and/or
- that were found either to meet the categorization criteria for GPE or to 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 propylene oxide 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	75-56-9
Inventory names	Oxirane, methyl-; Methyloxirane; Methyloxiranne; Propylene oxide
Other names	(±)-1,2-Epoxypropane; (±)-2-Methyloxirane; (±)-Epoxypropane; (±)-Methyloxirane; 1,2-Epoxypropane; 1,2-Propylene oxide; 2,3-Epoxypropane; AD 6; 1,2-Epoxypropane; Epihydrin; Epoxypropane; Methyl ethylene oxide; Methyloxacyclopropane; Oxypropylene; Propene oxide; Propozone; Propylene epoxide
Chemical group	Discrete organics
Chemical sub-group	Epoxides
Chemical formula	C ₃ H ₆ O
Chemical structure	
SMILES	O(C1C)C1
Molecular mass	58.08 g/mol

Based on information submitted by the 12 companies that notified this substance to the Domestic Substances List, approximately 10,000 tonnes of propylene oxide were in commerce in 1986 for a variety of uses, including (but not limited to) the categories of analytical reagent; formulation component; formulating and manufacture of pest control products; antioxidant/corrosion inhibitor; paint and coating. Other potential uses of the substance in Canada include three major areas: polymer production (e.g. production of propylene glycols), direct applications (e.g. stabilizer in fuels and heating oil), and a chemical intermediate. Health Canada has approved propylene oxide as food additive for use as starch modifying agent.

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
Methyl oxirane (propylene oxide)
CAS No. 75-56-9

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.

Propylene oxide is considered to meet the criteria for GPE 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

Propylene oxide has been determined to be GPE 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 10,200,000 kg.

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was 12.

Use Codes and Description

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

4	Adhesive/binder/sealant/filler
5	Analytical reagent
7	Antioxidant/corrosion inhibitor/tarnish inhibitor/scavenger/antiscaling agent
10	Chemical intermediate - organic
21	Formulation component
22	Fragrance/perfume/deodourizer/flavouring agent
28	Monomer
44	Solvent/carrier
51	Function other than that listed in codes 02-50
62	Explosive Materials
76	Organic Chemicals, Industrial
77	Organic Chemicals, Specialty
80	Paint and Coating
81	Pest Control Products, Formulating and Manufacture

Potential Uses in Canada

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

Usages of propylene oxide fall into three areas: polymer production, as a chemical intermediate and in direct applications.

Propylene oxide is used as monomer in polymer production of polyether polyols. Polyether polyols are used in the production of polyurethane foams for the furniture and automotive industries, and coatings, adhesives and sealants. It is also used in the manufacture of propylene glycol ether, for use as solvents in paints, inks, coatings, resins, cleaners, and waxes.

Propylene oxide is also used in the production of propylene glycols which can be used in the production of unsaturated polyester resin especially in the textile and construction industries, as a solvent in food, in pharmaceutical and cosmetics and in engine coolants and aircraft de-icers. It is also used for the manufacture of butanediol and related products for specialty resins and solvents (ECB, 2002).

Direct applications include its use as a stabilizer for dichloromethane and other chlorinated hydrocarbons. Propylene oxide also used as a stabilizer in fuels and heating oil, and as an anti-corrosion additive for liquid coolants. It is used as a package fumigant for certain fruit products & as a fumigant for bulk quantities of several food products, provided residues of propylene oxide & propylene glycol do not exceed specified limits (ECB, 2002).

Health Canada has approved propylene oxide as food additive for use as starch modifying agent (Health Canada, 2006).

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

Propylene oxide is considered to be a potentially high hazard substance based on its classification for carcinogenicity by the European Commission, United States National Toxicology Program (NTP), International Agency for Research on Cancer (IARC), United States Environmental Protection Agency (US EPA). Propylene oxide was also classified for mutagenicity by the European Commission.

In the 11th Report on Carcinogens, NTP concluded that propylene oxide is reasonably anticipated to be a human carcinogen based on sufficient evidence of carcinogenicity in experimental animals (NTP, 2005).

In 1994, IARC concluded that there is inadequate evidence in humans for the carcinogenicity of propylene oxide, but that there is sufficient evidence in experimental animals for the carcinogenicity of propylene oxide (IARC, 1994).

In 1994, the US EPA conducted a weight of evidence assessment of the carcinogenicity of propylene oxide and classified it as a Group B2 carcinogen (Probable human carcinogen). This conclusion was based on inadequate human data and an increased incidence of benign and malignant tumors at the site of exposure in two species of animals, when exposed by subcutaneous injection, by inhalation, and by gavage. There was also evidence of mutagenicity in a variety of test systems. Propylene oxide is structurally similar to other chemicals that demonstrate carcinogenic activity in animals (US EPA, 1994).

The European Commission classified propylene oxide as a Carcinogen Category 2 (Substance which should be regarded as if carcinogenic to man) and also as a Mutagen Category 2 (Substances which should be regarded as if they are mutagenic to man) (European Commission, 1999; European Commission, 2001; ECB, 2002; ESIS, 2006).

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.

References

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Appendix II
Ecological Information to Support The Challenge for
Methyl oxirane (propylene oxide)
CAS No. 75-56-9

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 propylene oxide which are relevant to its environmental fate.

Table 1a: Experimental physico-chemical properties for propylene oxide

Property	Value/Units	Reference
Boiling point (BP)	34.23 °C; 35.00 °C	Plunkett, 1987; SRC PHYSPROP Database, 2003
Melting point (MP)	-112.13 °C; -111.90 °C	Howard, 1989; SRC PHYSPROP Database, 2003
log K _{ow}	0.03	Howard, 1989; Hansch <i>et al.</i> , 1995
Vapour pressure (VP)	532.1 mm Hg; 538 mm Hg	Howard, 1989; Boublik <i>et al.</i> , 1984
Water solubility (WS)	590000 mg/L	Bogyo <i>et al.</i> , 1980

Table 1b: Modelled physico-chemical properties for propylene oxide

Property	Value/Units	Reference
Boiling point (BP)	31.32 °C	MPBPWIN v1.41
Melting point (MP)	-100.23 °C	MPBPWIN v1.41
Henry's Law constant (HLC)	1.226×10 ⁻⁴ atm·m ³ /mole	HenryWin v3.10
log K _{oc}	0.37	PCKOCWIN v1.66
log K _{ow}	0.37	KOWWIN v1.67
Vapour pressure (VP)	70930 Pa; 532 mm Hg	MPBPWIN v1.41
Water solubility (WS)	129300 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

Based on an estimated log K_{oc} value of 0.37 (Table 1b), propylene oxide is not expected to adsorb to suspended solids and sediments. Volatilization from water surfaces, based upon an estimated Henry's Law constant of $(1.2-1.6) \times 10^{-4}$ atm-m³/mole, is expected to be moderate. Thus, if water is a receiving medium, propylene oxide is expected to mainly remain in water and, to some extent, partition to air 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 propylene oxide

Receiving media	% in Air	% in Water	% in Soil	% in Sediment
Air (100%)	88.0	10.3	1.6	0.02
Water (100%)	4.5	95.3	0.1	0.18
Soil (100%)	7.6	18.0	74.4	0.03
Air, water, soil (33.3% each)	15.4	44.0	40.6	0.08

Terrestrial fate

Based on an estimated log K_{oc} value of 0.37 (Table 1b), propylene oxide is not expected to adsorb to soil and, therefore, will have very high mobility in this environmental compartment. Volatilization of propylene oxide from moist soil surfaces is expected to be a relatively important fate process given an estimated Henry's Law constant of $(1.2-1.6) \times 10^{-4}$ atm-m³/mole. The potential for volatilization of propylene oxide from dry soil surfaces may exist based upon a vapour pressure of 532-538 mm Hg (Tables 1a and 1b).

Atmospheric fate

According to a model of gas/particle partitioning of semi-volatile organic compounds in the atmosphere (Bidleman, 1988), this chemical, having a vapour pressure of 532-538 mm Hg (Tables 1a and 1b), is expected to exist solely as a vapour in the ambient atmosphere. Propylene oxide may also be removed from the atmosphere by wet

deposition processes, considering the very high water solubility of this chemical (Tables 1a and 1b).

Presence in the Environment

No data concerning 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

Vapour-phase propylene oxide is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 20.6 days (Table 3a), calculated from its experimental rate constant of $5.2 \times 10^{-13} \text{ cm}^3/\text{molecule} \cdot \text{sec}$ (Atkinson, 1989). The anticipated products of the atmospheric reaction with hydroxyl radicals have been cited as oxomethyl acetate, propanedial, formaldehyde, and diformyl ether (Cupitt, 1980). This compound is not expected to 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.

The empirical biodegradation data (Chemicals Inspection and Testing Institute, 1992) show 93-98% biodegradation over 28 days in a ready-biodegradation test for propylene oxide (Table 3a). This indicates that its half-life in water is less than 182 days (6 months).

Table 3a: Experimental persistence values for propylene oxide

Medium	Fate Process	Degradation Value	Degradation Endpoint/Units	Reference
Air	Photodegradation	5.2×10^{-13}	Rate constant, $\text{cm}^3/\text{molecule} \cdot \text{sec}$	Atkinson, 1989
Air	Photodegradation	20.57	Half-life, days	Atkinson, 1989
Water	Biodegradation	93-98	Biodegradation, % (28 days, ready)	Chemicals Inspection and Testing Institute, 1992

Table 3b: Predicted persistence data for propylene oxide

Medium	Fate Process	Degradation Value	Degradation Endpoint	Reference
Air	Atm. oxidation	17.87	Half-life (days)	AOPWIN v1.91
Air	Ozone reaction	Non-reactive	Half-life (days)	AOPWIN v1.91
Water	Hydrolysis	1042	Half-life (days)	HYDROWIN v1.67
Water/Soil	Biodegradation	15	Half-life (days)	BIOWIN v4.01, Ultimate Survey
Water/Soil	Biodegradation	2.33	Half-life (days)	BIOWIN v4.01, Primary Survey
Water/Soil	Biodegradation	0.5734	Probability	BIOWIN v4.02 (MITI Linear)
Water/Soil	Biodegradation	0.7044	Probability	BIOWIN v4.02 (MITI Non-linear)
Water/Soil	Biodegradation	0.968	Probability	Topkat v.6.1

For estimating biodegradation in water, QSAR modeling was used (Table 3b). Based on these results, the estimated timeframe for biodegradation indicates that, propylene oxide 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 ($t_{1/2 \text{ water}} : t_{1/2 \text{ soil}} : t_{1/2 \text{ sediment}} = 1 : 1 : 4$, BIOWIN v4.01). Using these factors, it may be concluded that propylene oxide is not expected to be persistent in soil and sediments

Considering abiotic degradation, this substance is not expected to hydrolyse in water and in moist soils.

Therefore, the empirical and modelled data demonstrate that propylene oxide does not meet the persistence criteria in soil and water (half-lives ≥ 182 days) and in sediments (half-life ≥ 365 days); however, it does meet the persistence criterion in air (half-life ≥ 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 0.03 and 0.37, respectively (Tables 1a and 1b) indicate that the potential for bioaccumulation of propylene oxide in aquatic organisms is likely to be low.

Experimental BAF and 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 substance propylene oxide does not have the potential to bioaccumulate in the fish. The three BCF models provide a weight-of-evidence to support a low bioconcentration potential of this substance (BCF=1-13 L/kg, Table 4).

Table 4: Predicted bioaccumulation values for propylene oxide

Test Organism	Endpoint/Units	Value	Reference
Fish	BAF (wet weight, L/kg)	1	Modified GOBAS BAF T2MTL (Arnot & Gobas, 2003)
Fish	BCF (wet weight, L/kg)	1 – 13	OASIS; Modified GOBAS BCF 5% T2LTL (Arnot & Gobas, 2003); BCFWIN v2.15

Therefore, modelled data indicate that the substance propylene oxide 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 at low concentrations, propylene oxide is not expected to cause significant harm to aquatic organisms (Table 5a). For fish, acute LC50 values vary within a narrow range of 89-219 mg/L. Predicted acute toxicity values (Table 5b) are, in general, in a reasonably good agreement with the empirical results.

Table 5a: Experimental aquatic toxicity values for propylene oxide

Test Organism	Endpoint	Test Type	Value (mg/L)	Reference
Fish (<i>Carassius auratus</i> , <i>Gambusia affinis</i> , <i>Lepomis macrochirus</i> , <i>Mugil cephalus</i>)	LC50	Acute	89 - 219	Bridie <i>et al.</i> , 1979; Crews, 1974

Table 5b: Modelled aquatic toxicity values for propylene oxide

Organism	Endpoint	Duration	Toxicity value (mg/L)	Reference
Daphnia	EC50	Acute	416	TOPKAT v6.1
Daphnia	EC50	Acute	38.9	ECOSAR v.0.99g
Fish	LC50	Acute	4400	TOPKAT v6.1
Fish	LC50	Acute	278	AI Expert
Fish	LC50	Acute	12509	OASIS Forecast
Fish	LC50	Acute	13.83	ECOSAR v.0.99g
Fish	LC50	Acute	2050	ECOSAR v.0.99g
Fish	LC50	Acute	21.51	ECOSAR v.0.99g
Fish	LC50	Acute	14.66	ECOSAR Neutral Org. SAR

Therefore, according to the most of the experimental and modelled data, acute LC50/EC50 values are in the order of tens to hundreds mg/L, which may indicate that propylene oxide is expected to pose a moderate or low (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, propylene oxide persists in the environment (in air) and is not bioaccumulative, based on criteria defined in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000). Information on concentrations of this chemical in the environment has not been identified at this time.

Experimental ecotoxicological data indicate that propylene oxide is expected to pose a moderate or even low 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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