Screening Assessment for the Challenge

Rosin, hydrogenated
Chemical Abstracts Service Registry Number
65997-06-0

Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol
Chemical Abstracts Service Registry Number
64365-17-9

Resin acids and Rosin acids, hydrogenated, esters with glycerol
Chemical Abstracts Service Registry Number
65997-13-9

Resin acids and Rosin acids, hydrogenated, esters with triethylene glycol
Chemical Abstracts Service Registry Number
68648-53-3

Environment Canada
Health Canada

January 2011

Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment on Rosin, hydrogenated (HR), Chemical Abstracts Service Registry Number 65997-06-0; Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol (HRPE), Chemical Abstracts Service Registry Number 64365-17-9; Resin acids and Rosin acids, hydrogenated, esters with glycerol (HRGE), Chemical Abstracts Service Registry Number 65997-13-9; and Resin acids and Rosin acids, hydrogenated, esters with triethylene glycol (HRTE), Chemical Abstracts Service Registry Number 68648-53-3, these substances will be referred to by their derived acronyms, HR, HRPE, HRGE and HRTE, respectively, in this assessment. These substances were identified as high priorities for screening assessment and were included in the Challenge initiative under the Chemicals Management Plan because they were found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and are believed to be in commerce in Canada. HR, HRPE, HRGE and HRTE were not considered to be a high priority for assessment of potential risks to human health, based upon application of the simple exposure and hazard tools developed for categorization of substances on the Domestic Substances List.

HR, HRPE, HRGE and HRTE are organic UVCBs (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products or **Bi**ological Materials) substances that are used in Canada for various purposes, which may include application in adhesives and sealers, cosmetics, electronics, paints and coatings, and inks and paper. Resin acid components of these substances are present naturally in some plants, however, hydrogenated resin acids and hydrogenated resin acid esters are not known to be naturally produced. These substances are not reported to be manufactured in Canada; however, import volumes in 2006 were 10 000–100 000 kg/year for HR and HRPE, 100 000–1 000 000 kg/year for HRGE, and 1000–10 000 kg/year for HRTE.

Based on certain assumptions and reported use patterns in Canada, it is expected that the majority of these substances end up at waste disposal sites. Generally, 5% or less is estimated to be released to water based on industrial and consumer/commercial uses, and no releases are predicted to air or soil. HR, HRPE, HRGE and HRTE are reported to have low experimental solubilities in water. However, HR solubility may depend on pH with higher solubility found at a higher pH. HR, HRPE, HRGE and HRTE are expected to partition to sediments when released in water. However a significant fraction of HR may still remain in the water column.

Based on their physical and chemical properties, experimental biodegradation data for HR, HRPE and HRGE, analogue biodegradation data for HRTE and predicted data for all four substances are expected to be persistent in the environment. New experimental data relating to bioconcentration of components of HR along with predicted bioaccumulation potential of additional components suggest that HR has a low potential to accumulate in the lipid tissues of organisms. The lower molecular weight components of HRPE, HRGE

and HRTE do not show a high predicted bioaccumulation potential based on multiple model results, suggesting that metabolism will mitigate bioaccumulation potential. It has been predicted that the larger, higher molecular weight components would have limited bioavailability, such that significant bioaccumulation would not be expected. Based on the available information, HR, HRPE, HRGE and HRTE do not have the potential to bioaccumulate in the environment.

Experimental toxicity data for a chemical analogue UVCB substance of HRPE and HRGE suggest that saturated solutions of the substance do not cause acute harm to aquatic organisms, including fish, daphnids and algae test species.

Experimental toxicity data for a chemical analogue UVCB substance of HR indicated that saturated solutions of the substance do not cause acute harm to test fish and algae species. However, effects were seen at the highest concentration tested for daphnids. Thus, component based toxicity was used to determine a conservative predicted no-effect concentration (PNEC) for HR. For HR, a conservative exposure scenario was applied in which two major industrial operations discharge HR into the aquatic environment. The predicted environmental concentration (PEC) in water was many orders of magnitude below the PNECs calculated for HR. As no suitable chemical analogue was found for HRTE, predicted component-based toxicity values were used to determine a conservative PNEC value. A conservative exposure scenario was selected in which an industrial operation discharges HRTE into the aquatic environment. The PEC in water was, similarly, many orders of magnitude below the conservative PNECs calculated for HRTE.

No empirical data were identified for concentrations of these compounds in environmental media. The potential for exposure of the general population to HR, HRPE, HRGE and HRTE from environmental media is expected to be low. In addition, there is potential for low levels of exposure from the use of a limited number of consumer products which may include lipstick, mascara, hair styling and hair removal products and consumer adhesives. Based on the physical-chemical properties of the substances, inhalation exposure is not expected from these products; however, there is potential for low levels of dermal or oral (lipstick) exposure. The health effects database for HR, HRPE, HRGE and HRTE is limited. Chronic studies for HR and selected analogues indicated no evidence of carcinogenicity in experimental animals and the available data does not indicate genotoxic potential. Positive skin sensitization reactions appear to be associated with consumer products containing concentrations of ≥ 20% HRGE or HRPE, and possibly HRTE. However, there is evidence to indicate that HR may be a possible skin sensitizer at lower concentrations. Consumer use of products containing these substances is expected to be low.

The margins between upper-bounding estimates of exposure via environmental media or consumer products for HR, HRPE, HRGE or HRTE with the oral critical effect levels observed in studies with one or more of these compounds or related analogues, are considered adequate to address uncertainties in the health effects and exposure databases.

Based on comparison of the upper-bounding estimates of exposure via environmental media or consumer products for HR, HRPE, HRGE or HRTE with the oral critical effect levels observed in studies with one or more of these compounds or related analogues, a concern for human health was not identified.

Based on the information available, it is concluded that HR, HRPE, HRGE and HRTE are not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity or that constitute or may constitute a danger to the environment on which life depends.

Based on the information available, it is concluded that HR, HRPE, HRGE and HRTE are not entering the environment in a quantity or concentration or under conditions that constitute a danger in Canada to human life or health.

HR, HRPE, HRGE and HRTE do not meet any of the criteria set out in section 64 of the *Canadian Environmental Protection Act, 1999*.

HR, HRPE, HRGE and HRTE do meet the persistence criteria but do not meet the bioaccumulation criterion as set out in the *Persistence and Bioaccumulation Regulations* of the *Canadian Environmental Protection Act, 1999*.

These substances will be considered for inclusion in the Domestic Substances List inventory update initiative. In addition and where relevant, research and monitoring will support verification of assumptions used during the screening assessment.

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that have met the categorization criteria set out in the Act to determine whether these substances present or may present a risk to the environment or to human health.

Based on the information obtained through the categorization process, the Ministers identified a number of substances as high priorities for action. These include substances that

- met all of the ecological categorization criteria, including persistence (P), bioaccumulation potential (B) and inherent toxicity to aquatic organisms (iT), and were believed to be in commerce in Canada; and/or
- met the categorization criteria for greatest potential for exposure (GPE) or presented an intermediate potential for exposure (IPE) and had been identified as posing a high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity.

The Ministers therefore published a notice of intent in the *Canada Gazette*, Part I, on December 9, 2006 (Canada 2006), that challenged industry and other interested stakeholders to submit, within specified timelines, specific information that may be used to inform risk assessment, and to develop and benchmark best practices for the risk management and product stewardship of those substances identified as high priorities.

The substances Rosin, hydrogenated (HR); Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol (HRPE); Resin acids and Rosin acids, hydrogenated, esters with glycerol (HRGE); and Resin acids and Rosin acids, hydrogenated, esters with triethylene glycol (HRTE), had been identified as high priorities for assessment of ecological risk, as they had been found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and are believed to be in commerce in Canada. The Challenge for these substances was published in the *Canada Gazette* on June 20, 2009 (Canada 2009). A substance profile for each of the four substances was released at the same time. The substance profiles presented the technical information available prior to December 2005 that formed the basis for categorization of these substances. As a result of the Challenge, submissions of information pertaining to the properties and uses of these substances were received.

Although HR, HRPE, HRGE, and HRTE were determined to be a high priority for assessment with respect to the environment, they did not meet the criteria for GPE or IPE and high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity. Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

Screening assessments focus on information critical to determining whether a substance meets the criteria as set out in section 64 of CEPA 1999. Screening assessments examine scientific information and develop conclusions by incorporating a weight-of-evidence approach and precaution.[1]

This final screening assessment includes consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under the Challenge. Data relevant to the screening assessment of these substances were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches, up to February–March 2010 for the ecological and human health sections of the document. Key studies were critically evaluated; modelling results may have been used to reach conclusions.

When available and relevant, information presented in hazard assessments from other jurisdictions was considered. The final screening assessment does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies and lines of evidence pertinent to the conclusion.

This final screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. The ecological portion of this assessment has undergone external written peer review/consultation.

Additionally, the draft of this screening assessment was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Health Canada and Environment Canada. Approaches used in the screening assessments under the Challenge have been reviewed by an independent Challenge Advisory Panel.

The critical information and considerations upon which the final assessment is based are summarized below.

[1] A determination of whether one or more of the criteria of section 64 are met is based upon an assessment of potential risks to the environment and/or to human health associated with exposures in the general environment. For humans, this includes, but is not limited to, exposures from ambient and indoor air, drinking water, foodstuffs, and the use of consumer products. A conclusion under CEPA 1999 on the substances in the Chemicals Management Plan (CMP) Challenge Batches 1-12 is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the *Controlled Products Regulations*, which is part of regulatory framework for the Workplace Hazardous Materials Information System [WHMIS] for products intended for workplace use. Similarly, conclusion based on the criteria contained in section 64 of CEPA 1999 does not preclude actions being taken under other sections of CEPA or other Acts.

Substance Identity

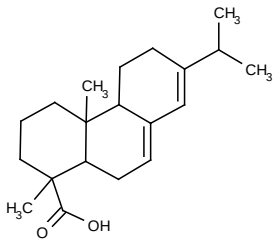
Substance Name

For the purposes of this document, these substances will be referred to as HR (Rosin, hydrogenated); HRPE (Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol); HRGE (Resin acids and Rosin acids, hydrogenated, esters with glycerol); and HRTE (Resin acids and Rosin acids, hydrogenated, esters with triethylene glycol), as derived from their Domestic Substances List (DSL) names. Note that the term "resin acids" is generic and includes those non-volatile terpenic acids found in plant resins in general while "rosin acids" is more colloquial and is highly specific to those resin acids that are present in Rosin (Zinkel and Russell 1989).

The evaluations of HR, HRPE, HRGE and HRTE have been grouped into a single assessment report due to the similarity of these substances in use profiles in Canadian commerce and structural features.

Hydrogenated rosins (i.e., HR) and their esterified derivatives (i.e., HRPE, HRGE and HRTE) are UVCB (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products or **B**iological Materials) substances that originate from biological materials that are processed to increase their commercial value. Table 1a summarizes the substance identity information for each of these substances. Rosins may be characterized by a variety of structures; however, to assist with this assessment, a limited number of structures and corresponding Simplified Molecular Input Line Entry System (SMILES) information were chosen to represent each substance. In choosing representative structures for HR, HRPE, HRGE and HRTE, representatives from the residual natural precursors (e.g., unmodified resin acids and neutrals present in rosin), residual reactants used in manufacturing (e.g., triethylene glycol) and significant products known to be present in each substance (e.g., hydrogenated and/or esterified resin acids) were considered. In the selection of representative structures, both compositional significance and potential ecological hazards were taken into account. A brief summary of these considerations are provided for each substance.

The production of HR involves the hydrogenation of the rosins, which consist primarily of the resin-acid-rich fraction from tall oil, wood and gum (see the following table for typical composition of resin acids in these three sources). Resin acids are mono-carboxylic diterpene acids, the most common of which have the molecular formula $C_{20}H_{30}O_2$. The most common resin acids are of the abietane skeletal class of which abietic acid (see [structure A] below) occurs most frequently.



[structure A]

Typical composition by percent of resin acids in various rosin sources (Zinkel and Russell 1989).

Components	**Tall oil**[3]	**Gum**[3]	**Wood**[3]
Abietic acid[1] [structure A]	38	24	51
Palustric acid[1]	8	21	8
Isopimaric acid[2]	11	17	16
Dehydroabietic acid[1]	18	5	8
Neoabietic acid[1]	3	19	5
Pimaric acid[2]	4	5	7

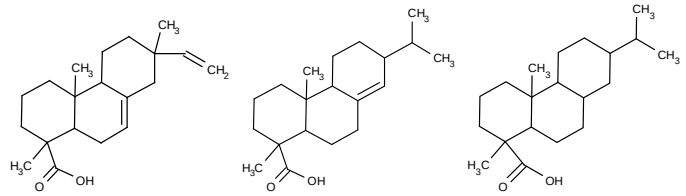
[1] Abietane class.
[2] Pimarane and isopimarane class.
[3] Percent of acid fraction.

The hydrogenation process is generally conducted using a precious metal catalyst (e.g., palladium-type) under mild conditions (i.e., relatively low temperature and pressures) and has long been the most satisfactory method of stabilizing resin acids and rosin to oxidation (Zinkel and Russell 1989). Partial hydrogenation to saturate one of the conjugated double bonds and create dihydro products proceeds relatively easily. Full hydrogenation, to saturate the second double bond and create tetrahydro-products, is more difficult, because the residual double bond does not have the advantage of conjugation and is subject to increased steric hindrance (Zinkel and Russell 1989). As a result, commercially available hydrogenated rosin derivatives are not actually 100% hydrogenated; rather, they are generally in the range of 75% hydrogenated or greater depending upon the severity of reaction conditions (Panda 2005). The chemical characterization of the major products of hydrogenation has shown that the major component is dihydrogenated abietic acid (Table 1a – structure 2) (Burgstahler et al. 1969). Additionally, the presence of the tetrahydrogenated abietic acid derivative (Table 1a – structure 3) may also be significant in the composition of hydrogenated rosin despite the favourable formation of the dihydrogenated abietic acid (Duan et al. 2001; Kumooka 2008). Finally, due to the potential ecological hazard of residual unaltered resin acids, a representative of this class was also considered. Isopimaric acid (Table 1a – structure 1) was chosen based on the fact that it made up a significant amount (i.e., >10%) of tall oil

and provided a more conservative estimate of potential for harm compared with other unmodified resin acids based on higher potential toxicity (Geiger et al. 1985; Kutney et al. 1981a, 1981b) and potentially also persistence in the environment (Volkman et al. 1993) compared with other resin acids.

Certain components of the neutrals fraction of tall oil (4–15%), including unsaponafiables (i.e., non-hydrolyzable) such as beta-sitosterol, pinosylvin and dimerized abietic acid, may survive processing (i.e. fractionation, hydrogenation and/or esterification) and be present as residuals in the hydrogenated rosin. However, due to their expected low residual concentration and low relative potential for harm predicted for these various components, they are not considered to be of concern in processed rosin.

Table 1a. Substance identity for HR

Chemical Abstracts Service Registry Number (CAS RN)	**65997-06-0**
DSL name	**HR**
National Chemical Inventories (NCI) names[1]	*HR* (TSCA, EINECS, ENCS, AICS, PICCS, ASIA-PAC, NZIoC); *hydrogenated rosin* (ECL)
Other names	*Foral AX; Foral AX-E; Hypale; Hypale CH; KR 100; KR 100 (rosin); KR 610; KR 611; KR 612; Pinecrystal KR 610; Regalite M 335; Rosin, partially hydrogenated; SE 50; Selosol D 101; Staybelite; Staybelite Resin; Staybelite Resin E*
Chemical group (DSL Stream)	Biological UVCB
Major chemical class or use	Rosin
Major chemical sub-class	Carboxylic acid
Chemical formula	Variable
Representative chemical structures used to run the estimation model[2]	 Structure 1 (Isopimaric acid) Structure 2 Structure 3[3]
Representative SMILES used to run the estimation model[2]	CC1(CCC2C(C1)=CCC1C2(C)CCCC1(C)C(O)=O)C=C (structure 1) CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)=C1 (structure 2) CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)C1 (structure

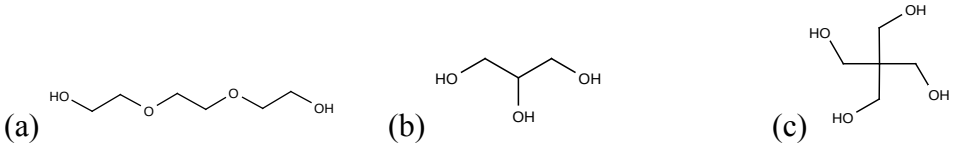
	3)
Molecular mass	302.5 g/mol (structure 1); 304.5 g/mol (structure 2); 306.5 g/mol (structure 3)

[1] National Chemical Inventories (NCI). 2007: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Commercial Chemical Substances); ENCS (Japanese Existing and New Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); PICCS (Philippine Inventory of Chemicals and Chemical Substances); and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

[2] This substance is a UVCB (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products, or **B**iological Materials); i.e., it is not a discrete chemical and thus may be characterized by a variety of structures. To assist with modelling, the structure and corresponding SMILES presented here were chosen to represent the substance.

[3] Structure used for Categorization

The esterification of rosin using polyhydroxyl alcohols such as (a) triethylene glycol,(b) glycerol and (c) pentaerythritol [structure 2 below] is generally carried out at elevated temperatures (e.g., 260–280ºC). It is generally desirable to decrease the acid number of the resultant product to reduce the number of free carboxylic acids and ensure a relatively high degree of esterification is achieved (Zinkel and Russell 1989).

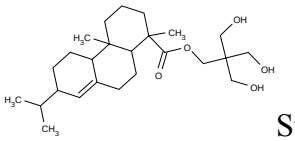
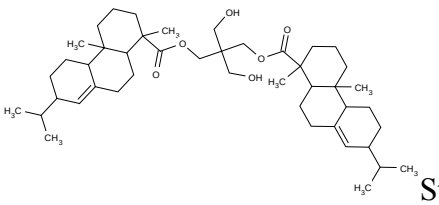


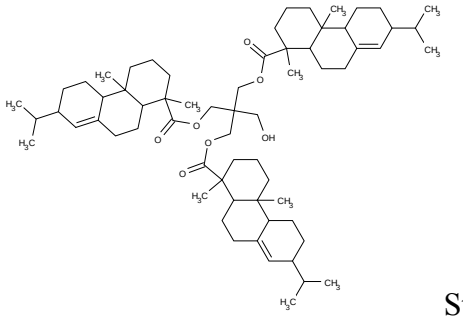
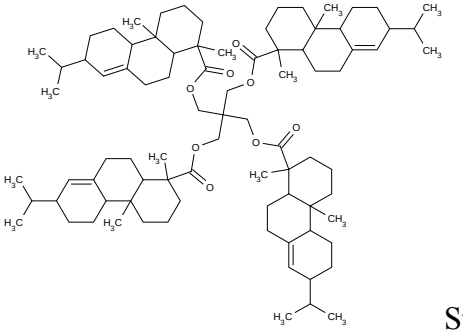
[Structure 2]

Generally, the highest level of esterification is preferred; however, in certain cases (e.g., tetraester with pentaerythritol), this may be minimized by increased steric hindrance. In the esterification process, by-products collectively known as "rosin oil" may form which results in undesirable impacts on product quality (e.g., softening point) (Hind et al. 1954). Thus, minimization of rosin oil formation is desirable through control of reaction conditions (e.g., temperatures < 300ºC) and physical removal of any excess rosin oil present in the reaction product. The main components of esterified rosin substances are mono-, di-, tri- and tetraesters, depending on the reactant alcohol (Structure 2) along with a small amount (<10%) of unreacted HR components. However, in general, an excess of alchohol is used to drive the reaction and minimize the amount of residual free resin acid that would have undesirable impacts on product quality (Panda 2005). As HR components will be assessed as part of this assessment, it was not necessary to reconsider the potential presence of these residual components in the esters, unless it was expected to impact the conclusions reached for the esters in this assessment. Representative structures were chosen based on expected compositions in final products, with a conservative approach taken by selecting the more bioavailable and thus likely hazardous components of lower molecular weight constituents. Several combinations of hydrogenated and unmodified resin acid esters with the alcohols (Structure 2a, Structure

2b and Structure 2c) are possible. However, the approach taken was to use the hydrogenated rosin acid esters that were most representative in composition (i.e., esters of dihydrogenated abietic acid), considering that the structural variations possible will lead to increased variation in the overall predicted properties. However, preliminary screening of several candidate structural variants (e.g., esters with isopimaric or tetrahydro-abietic acid) illustrated that the variation in resin acid components led to negligible differences in the predicted persistence, bioaccumulation and toxicity properties.

Table 1b. Substance identity for HRPE

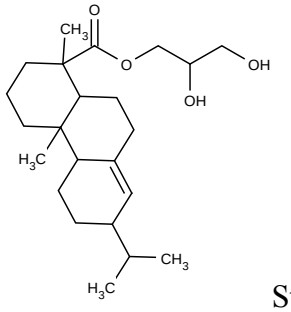
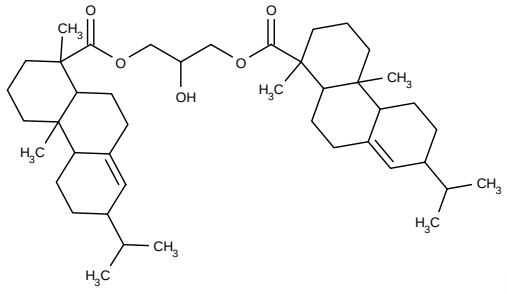
Chemical Abstracts Service Registry Number (CAS RN)	64365-17-9
DSL name	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol
National Chemical Inventories (NCI) names[1]	*Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol* (TSCA, EINECS, AICS, ECL, ASIA-PAC, NZIoC) *Hydrogenated rosin pentaerythritol ester* (ENCS)
Other names	*A 115; Ester Gum HP; Foral 105; Foral 105E; Foralyn 110; Hydrogenated resin acid pentaerythritol esters; Hydrogenated rosin, pentaerythritol ester; KE 359; Pentalyn C; Pentalyn H; Pentalyn H-E; Pentalyn K; Pinecrystal KE 359; Resin acids, hydrogenated, esters with pentaerythritol; Rikatac F 105; Rikatac PH; Super Ester 75; Super Ester A 115*
Chemical group (DSL Stream)	Biological UVCB
Major chemical class or use	Resin acids and Rosin acids
Major chemical sub-class	Ester
Chemical formula	Variable
Representative chemical structures used to run the estimation model[2]	 Structure 1  Structure 2

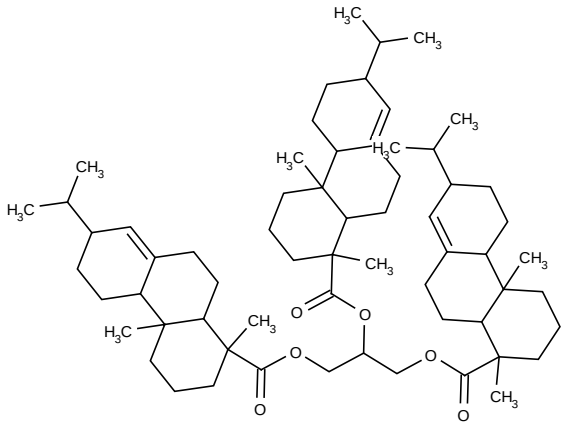
	 Structure 3  Structure 4
Representative SMILES used to run the estimation model[2]	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)CO)=C1 (structure 1) CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1 (structure 2) CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1 (structure 3) CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1 (structure 4)
Molecular mass	422.6 g/mol; 709.1 g/mol; 995.5 g/mol; 1282 g/mol

[1] National Chemical Inventories (NCI). 2007: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Commercial Chemical Substances); ENCS (Japanese Existing and New Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

[2] This substance is a UVCB (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products, or **B**iological Materials); i.e., it is not a discrete chemical and thus may be characterized by a variety of structures. To assist with modelling, the structure and corresponding SMILES presented here were chosen to represent the substance.

Table 1c. Substance identity for HRGE

Chemical Abstracts Service Registry Number (CAS RN)	65997-13-9
DSL name	Resin acids and Rosin acids, hydrogenated, esters with glycerol
National Chemical Inventories (NCI) names[1]	*Resin acids and Rosin acids, hydrogenated, esters with glycerol* (TSCA, EINECS, AICS, ECL, PICCS, ASIA-PAC, NZIoC) *Hydrogenated rosin glycerin ester* (ENCS) *Resin acids and rosin acids ester of glycerol, hydrogenated* (PICCS) *HR, glycerol ester* (PICCS)
Other names	*A 100; Elkan A 120; Ester Gum H; Foral 69; Foral 85; Foral 85E; Foral 85-55WKX; Foralyn 90; Glycerides, rosin, hydrogenated; Glycerol ester of partially hydrogenated wood rosin; Hydrogenated rosin glycerides; hydrogenated rosin, disproportionated rosin, glycerol ester; KE 100; Pinecrystal KE 311; Pinecrystal KE 100; Resin acids, hydrogenated, esters with glycerol; Rikatac F 85; Rikatac SE 7; HR, ester with glycerol; Staybelite Ester 10; Staybelite Ester 10.55WK; Staybelite Ester 10E; Staybelite Ester 5; Staybelite Ester 5E; Staybelite Ester 5E-JQ; Staybelite Ester 610; Super Ester A 100; Wood HR, ester with 1,2,3-propanetriol*
Chemical group (DSL Stream)	Biological UVCB
Major chemical class or use	Resin acids and Rosin acids
Major chemical sub-class	Ester
Chemical formula	Variable
Representative chemical structures used to run the estimation mode[2]	 Structure 1  Structure 2

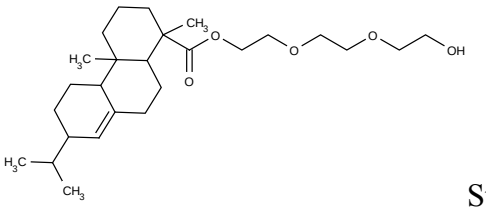
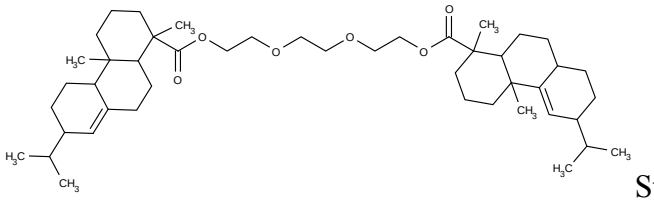
	 Structure 3
Representative SMILES used to run the estimation model[2]	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)CO)=C1 (structure 1) CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1 (structure 2) CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)OC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1 (structure 3)
Molecular mass	378.6 g/mol; 665.0 g/mol; 951.5 g/mol

[1] National Chemical Inventories (NCI). 2007: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Commercial Chemical Substances); ENCS (Japanese Existing and New Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); PICCS (Philippine Inventory of Chemicals and Chemical Substances); and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

[2] This substance is a UVCB (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products, or **B**iological Materials); i.e., it is not a discrete chemical and thus may be characterized by a variety of structures. To assist with modelling, the structure and corresponding SMILES presented here were chosen to represent the substance.

Table 1d. Substance identity for HRTE

Chemical Abstracts Service Registry Number (CAS RN)	68648-53-3
DSL name	Resin acids and Rosin acids, hydrogenated, esters with triethylene glycol
National Chemical Inventories (NCI) names[1]	*Resin acids and Rosin acids, hydrogenated, esters with triethylene glycol* (TSCA,,EINECS, AICS, ECL, PICCS, ASIA-PAC, NZIoC) *Hydrogenated rosin triethyleneglycol ester* (ENCS) *Staybelite Ester 3* (PICCS) *Resin Acids & Rosin Acids,hydrogenated, ester with triethylene*

	glycol (PICCS)
Other names	*Hydrogenated rosin, triethylene glycol ester* *Resin acids, hydrogenated, esters with triethylene glycol* *Staybelite Ester 3E*
Chemical group (DSL Stream)	Biological UVCB
Major chemical class or use	Resin acids and Rosin acids
Major chemical sub-class	Ester
Chemical formula	Variable
Representative chemical structures used to run the estimation model[2]	 Structure 1  Structure 2
Representative SMILES used to run the estimation model[2]	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCCOCCOCCO)=C1 (structure 1) CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCCOCCOCCOC(=O)C2(C)CCCC3(C)C2CCC2CCC(C=C32)C(C)C)=C1 (structure 2)
Molecular mass	436.6 g/mol; 723.1 g/mol

[1] National Chemical Inventories (NCI). 2007: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Commercial Chemical Substances); ENCS (Japanese Existing and New Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); PICCS (Philippine Inventory of Chemicals and Chemical Substances); and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

[2] This substance is a UVCB (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products, or **B**iological Materials); i.e., it is not a discrete chemical and thus may be characterized by a variety of structures. To assist with modelling, the structure and corresponding SMILES presented here were chosen to represent the substance.

Physical and Chemical Properties

Tables 2a, b, c and d contain experimental and modelled physical and chemical properties of HR, HRPE, HRGE and HRTE, respectively that are relevant to their environmental fate.

Quantitative structure-activity relationship (QSAR) models were used to generate data for some of the physical and chemical properties of HR, HRPE, HRGE and HRTE. These models (except WSKOWWIN 2000) are based on fragment addition methods, i.e. they rely on the structure of a chemical. Since these models generally only accept the neutral form of a chemical as input (in SMILES form), the modelled values shown in Table 2 are for the neutral form of these substances unless otherwise specified.

The modelled water solubility value for HR was determined using the experimental value adjustment (EVA) option in WATERNT (2002). This approach estimates water solubility for a queried chemical by comparing its structure to that of an analogue chemical that has an empirical water solubility value. The empirical water solubility value for the analogue is quantitatively adjusted based on the influence that structural differences are expected to have on water solubility when the two chemicals are compared.

Table 2a. Physical and chemical properties for HR

Property	Type	Value[1]	Temperature (°C)	Reference
Melting point (°C)				
Structure 1	Experimental	160		Suntio et al. 1988
Structure 2	Modelled	147		MPBPWIN 2008
Structure 3	Modelled	142		MPBPWIN 2008
Boiling point (°C)				
Structure 1	Modelled	391		MPBPWIN 2008

Structure 2	Modelled	391		MPBPWIN 2008
Structure 3	Modelled	387		MPBPWIN 2008
Density (kg/m3)				
		None available		
Vapour pressure (neutral form) (Pa)				
Structure 1	Modelled	7.54×10^{-5} (5.65×10^{-7} mmHg)	25	EPIWIN 2008
Structure 2	Modelled	1.05×10^{-4} (7.91×10^{-7} mmHg)	25	EPIWIN 2008
Structure 3	Modelled	1.5×10^{-4} (1.13×10^{-6} mmHg)	25	EPIWIN 2008
Henry's Law constant (neutral form) (Pa·m^3/mol)				
Structure 1	Modelled	6.04×10^{-1} (5.96×10^{-6} atm·m^3/mole)	25	HENRYWIN 2008
Structure 2	Modelled	8.10×10^{-1} (7.99×10^{-6} atm·m^3/mole)	25	HENRYWIN 2008
Structure 3	Modelled	7.80×10^{-1} (7.70×10^{-6} atm·m^3/mole)	25	HENRYWIN 2008
Log Dow[2] (Octanol-water distribution coefficient) (dimensionless)				
HR	Experimental	2.5–7.6[6]		USEPA 2008a
Structure 1	Modelled	5.5[3]		ACD/pKaDB

				2005
Structure 2	Modelled	6.0[3]		ACD/pKaDB 2005
Structure 3	Modelled	6.3[3]		ACD/pKaDB 2005
		Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)		
Structure 1	Modelled	3.2[4]		PCKOCWIN 2000
Structure 2	Modelled	3.5[4]		PCKOCWIN 2000
Structure 3	Modelled	3.6[4]		PCKOCWIN 2000
		Water solubility (mg/L)		
HR	Experimental	1.18	20	USEPA 2008a
Abietic acid [structure A]	Experimental	3.6[5]	20	Nyren and Back 1958
Structure 1	Modelled	2.42[7]		WATERNT 2008
Structure 2	Modelled	2.69[7]		WATERNT 2008
Structure 3	Modelled	2.00[7]		WATERNT 2008
		pK_a (Acid dissociation constant) (dimensionless)		
Abietic acid [structure A]	Experimental	6.4		Nyren and Back 1958
Structure 1	Modelled	4.90		ADME 2008
Structure 2	Modelled	4.90		ADME 2008
Structure 3	Modelled	4.90		ADME 2008
		Molecular diameter		

(Min-Max Dmax values; nm)				
Structure 1	Modelled	1.15–1.43		CPOPs 2008
Structure 2	Modelled	1.25–1.44		CPOPs 2008
Structure 3	Modelled	1.26–1.44		CPOPs 2008

[1] Values in parentheses represent the original ones as reported by the authors or as estimated by the models
[2] Log D_{ow} is the log of the distribution coefficient (D_{ow}) which represents the ratio of the sum of the concentration of all forms of the compound (ionized plus un-ionized) in octanol and water.
[3] Adjusted assuming a pH of 7 and pKa of 6.4 using $D = f_N K_{OW\text{-}N} + (1\text{-}f_N) K_{OW\text{-}I}$ where $K_{OW\text{-}Neutral}$ and $K_{OW\text{-}ionized}$ were obtained by determining log D_{ow} estimates for the substance using ACD/pKaDB (2005) at pH 14 and pH 1, respectively.
[4] Based on predicted log D_{ow} and thus takes into account influence of the more soluble ionic forms of the substance but does not account for acid-base pairing or electrostatic interactions with solid substrates.
[5] Solubility of the unionized / neutral form only (solubility will increase significantly upon increase in pH)
[6] Range of log D_{ow} values measured at pH 2 (un-ionized form) and may not be applicable to typical environmental conditions.
[7] WATERNT (2008) EVA method used with abietic acid and empirical water solubility of 3.6 mg/L (solubility will increase significantly upon increase in pH).

Table 2b. Physical and chemical properties for HRPE

Property	Type	Value[1]	Temperature (°C)	Reference
Melting point (°C)				
Structure 1	Modelled	223		MPBPWIN 2008
Structure 2	Modelled	309		MPBPWIN 2008
Structure 3	Modelled	350		MPBPWIN 2008
Structure 4	Modelled	350		MPBPWIN 2008
Boiling point (°C)				
Structure 1	Modelled	523		MPBPWIN 2008
Structure 2	Modelled	> 550 (707)		MPBPWIN 2008
Structure 3	Modelled	> 550 (908)		MPBPWIN 2008
Structure 4	Modelled	> 550 (1108)		MPBPWIN 2008

Property	Type	Value[1]	Temperature (°C)	Reference
Density (kg/m^3)				
		None available		
Vapour pressure (Pa)				
Structure 1	Modelled	<1.3x10^{-4} (3.32 x 10^{-12})	25	EPIWIN 2008
Structure 2	Modelled	<1.3x10^{-4} (1.33 x 10^{-15})	25	EPIWIN 2008
Structure 3	Modelled	<1.3x10^{-4} (3.35 x 10^{-25})	25	EPIWIN 2008
Structure 4	Modelled	<1.3x10^{-4} (1.85 x 10^{-26})	25	EPIWIN 2008
Henry's Law constant (Pa·m^3/mol)				
Structure 1	Modelled	3.94 x 10^{-5}*** (3.89 x 10^{-10} atm·m^3/mole)	25	HENRYWIN 2008
Structure 2	Modelled	3.74 x 10^{-5}*** (3.69 x 10^{-10} atm·m^3/mole)	25	HENRYWIN 2008
Structure 3	Modelled	3.56 x 10^{-5}*** (3.51 x 10^{-10} atm·m^3/mole)	25	HENRYWIN 2008
Structure 4	Modelled	3.38 x 10^{-2}*** (3.34 x 10^{-7} atm·m^3/mole)	25	HENRYWIN 2008
Log K_{ow} (Octanol-water partition coefficient)				

Property	Type	Value[1]	Temperature (°C)	Reference
(dimensionless)				
HRPE	Experimental	4.6–7.3[2]		USEPA, 2008b
Structure 1	Modelled	5.70		KOWWIN 2008
Structure 2	Modelled	> 9*		KOWWIN 2008
Structure 3	Modelled	> 9*		KOWWIN 2008
Structure 4	Modelled	> 9*		KOWWIN 2008
Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)				
Structure 1	Modelled	5.31		EPIWIN 2008 (Level III fugacity model v1.66)
Structure 2	Modelled	> 7**		PCKOCWIN 2000
Structure 3	Modelled	> 7**		PCKOCWIN 2000
Structure 4	Modelled	> 7**		PCKOCWIN 2000
Water solubility (mg/L)				
HRPE	Experimental	< 0.22	20	USEPA 2008b
Structure 1	Modelled	8.52		WATERNT 2008
Structure 2	Modelled	4.17×10^{-6}***		WATERNT 2008
Structure 3	Modelled	9.97×10^{-7}***		WATERNT 2008

Property	Type	Value[1]	Temperature (°C)	Reference
Structure 4	Modelled	1.28 x 10^{-6}***		WATERNT 2008
Molecular Diameter (Min-Max Dmax values; nm)				
Structure 1	Modelled	1.36–1.84		CPOPs 2008
Structure 2	Modelled	1.74–3.04		CPOPs 2008
Structure 3	Modelled	2.09–2.94		CPOPs 2008
Structure 4	Modelled	2.28–2.88		CPOPs 2008

[1] Values in parentheses represent the original ones as reported by the authors or as estimated by the models.
[2] Measured at pH 2.
* No values of log K_{ow} > 9 have been empirically measured for substances in the model training set. This prediction is considered uncertain, but will be at least 9 or theoretically greater.
** No values of log K_{oc} > 7 have been empirically measured for substances in the model training set. This prediction is considered uncertain, but will be at least 7 or theoretically greater.
***Outside parametric domain of model (molecular weight not represented by training set).

Table 2c. Physical and chemical properties for HRGE

Property	Type	Value[1]	Temperature (°C)	Reference
Melting point (°C)				
Structure 1	Modelled	182		MPBPWIN 2008
Structure 2	Modelled	279		MPBPWIN 2008
Structure 3	Modelled	350		MPBPWIN 2008
Boiling point (°C)				

Property	Type	Value[1]	Temperature (°C)	Reference
Structure 1	Modelled	457		MPBPWIN 2008
Structure 2	Modelled	>550 (641)		MPBPWIN 2008
Structure 3	Modelled	>550 (846)		MPBPWIN 2008
Density (kg/m^3)				
		None available		
Vapour pressure (Pa)				
Structure 1	Modelled	$< 1.3 \times 10^{-4}$ (4.03×10^{-9})	25	EPIWIN 2008
Structure 2	Modelled	$< 1.3 \times 10^{-4}$ (1.54×10^{-15})	25	EPIWIN 2008
Structure 3	Modelled	$< 1.3 \times 10^{-4}$ (4.76×10^{-19})	25	EPIWIN 2008
Henry's Law constant ($Pa \cdot m^3/mol$)				
Structure 1	Modelled	6.11×10^{-4} (6.03×10^{-9} $atm \cdot m^3/mole$)	25	HENRYWIN 2008
Structure 2	Modelled	$5.81 \times 10^{-4***}$ (5.73×10^{-9} $atm \cdot m^3/mole$)	25	HENRYWIN 2008
Structure 3	Modelled	$5.52 \times 10^{-1***}$ (5.45×10^{-6} $atm \cdot m^3/mole$)	25	HENRYWIN 2008

Property	Type	Value[1]	Temperature (°C)	Reference
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)				
HRGE	Experimental	4.7–5.8[2]		USEPA 2008b
Structure 1	Modelled	5.23		KOWWIN 2008
Structure 2	Modelled	> 9*		KOWWIN 2008
Structure 3	Modelled	> 9*		KOWWIN 2008
Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)				
Structure 1	Modelled	4.84		EPIWIN 2008 (Level III fugacity model v.1.66)
Structure 2	Modelled	> 7**		PCKOCWIN 2000
Structure 3	Modelled	> 7**		PCKOCWIN 2000
Water solubility (mg/L)				
HRGE	Experimental	0.15	20	USEPA 2008b
Structure 1	Modelled	2.54		WATERNT 2008
Structure 2	Modelled	1.30×10^{-6}***		WATERNT 2008
Structure 3	Modelled	9.51×10^{-7}***		WATERNT 2008
Molecular diameter (Min-Max Dmax values; nm)				

Property	Type	Value[1]	Temperature (°C)	Reference
Structure 1	Modelled	1.27–1.90		CPOPs 2008
Structure 2	Modelled	1.59–3.05		CPOPs 2008
Structure 3	Modelled	1.98–2.72		CPOPs 2008

[1] Values in parentheses represent the original ones as reported by the authors or as estimated by the models.
[2] Measured at pH 2.
* No values of log K_{ow} > 9 have been empirically measured for substances in the model training set. This prediction is considered uncertain, but will be at least 9 or theoretically greater.
** No values of logK_{oc} > 7 have been empirically measured for substances in the model training set. This prediction is considered uncertain, but will be at least 7 or theoretically greater.
***Outside parametric domain of model (molecular weight not represented by training set).

Table 2d. Physical and chemical properties for HRTE

Property	Type	Value[1]	Temperature (°C)	Reference
Melting point (°C)				
Structure 1	Modelled	201		MPBPWIN 2008
Structure 2	Modelled	290.80		MPBPWIN 2008
Boiling point (°C)				
Structure 1	Modelled	483.58		MPBPWIN 2008
Structure 2	Modelled	> 550 (667)		MPBPWIN 2008
Density (kg/m^3)				
		None available		
Vapour pressure				

Property	Type	Value[1]	Temperature (°C)	Reference
(Pa)				
Structure 1	Modelled	< 1.3 x 10^{-4} (1.09 x 10^{-9})	25	EPIWIN 2008
Structure 2	Modelled	< 1.3 x 10^{-4} (1.84 x 10^{-13})	25	EPIWIN 2008
Henry's Law constant (Pa·m^3/mol)				
Structure 1	Modelled	3.04 x 10^{-6} (3.00 x 10^{-11} atm·m^3/mole)	25	HENRYWIN 2008
Structure 2	Modelled	2.89 x 10^{-3}*** (2.85 x 10^{-8} atm·m^3/mole)	25	HENRYWIN 2008
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)				
Structure 1	Modelled	5.31		KOWWIN 2008
Structure 2	Modelled	> 9*		KOWWIN 2008
Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)				
Structure 1	Modelled	4.92		EPIWIN 2008 (Level III fugacity model v.1.66))
Structure 2	Modelled	> 7**		PCKOCWIN 2000
Water solubility (mg/L)				

Property	Type	Value[1]	Temperature (°C)	Reference
Structure 1	Modelled	0.62		WATERNT 2008
Structure 2	Modelled	7.23×10^{-7}***		WATERNT 2008
Molecular diameter (Min-Max Dmax values; nm)				
Structure 1	Modelled	1.31–2.33		CPOPs 2008
Structure 2	Modelled	1.76–3.47		CPOPs 2008

[1] Values in parentheses represent the original ones as reported by the authors or as estimated by the models
* Outside of the prediction domain of the model.
* No values of log K_{ow} >9 have been empirically measured for substances in the model training set. This prediction is considered uncertain, but will be at least 9 or theoretically greater.
** No values of log K_{oc} >7 have been empirically measured for substances in the model training set. This prediction is considered uncertain, but will be at least 7 or theoretically greater.
***Outside parametric domain of model (molecular weight not represented by training set)

Sources

Unmodified resin acids (e.g., structure 1 of HR) occur in pine trees, among other plants and thus are present naturally in the environment. In addition, the processing of plant material (e.g. in the production of pulp for the production of paper) may lead to releases of unmodified resin acids into the environment. Most measurements of environmental levels are associated with pulp/paper production discharges (Leppänen et al. 2000; Lahdelma and Oikari 2005; Lee and Peart 1991; Owens et al. 1994; Quinn et al. 2003). The hydrogenated components of HR (i.e., structures 2 and 3), which make up the majority of the commercial substance, are not known to be naturally produced. Similarly, the ester components of HRPE, HRGE and HRTE are not known to be naturally produced.

Information gathered through CEPA 1999 section 71 notices for the 2005 and 2006 calendar years indicates that HR, HRPE, HRGE and HRTE were imported into Canada at a quantity above the prescribed reporting thresholds. Table 3 summarizes the numbers of notifiers and interested stakeholders, and associated notified volumes, of each substance for the years 2006, 2005 and DSL nomination year 1986 (Environment Canada 2009a, 2006, 1988).

Table 3. Information on the import of HR, HRPE, HRGE and HRTE into Canada

	Notifier (>100 kg/year)						**Stakeholder Interest**	
	2006		**2005**		**1986**		**2006**	**2005**
	N	V*	N	V*	N	V*	S	S
HR	13	10 000– 100 000	10 3 2	100–1000 1001– 100 000 > 100 000	12	1 000 000– 10 000 000	19	10
HRPE	6	10 000– 100 000	na	na	<4	> 10 000 000	15	na
HRGE	9	100 000– 1 000 000	na	na	<4	> 10 000 000	16	na
HRTE	<4	1000– 10 000	na	na	<4	1 000 000– 10 000 000	9	na

N = Number of notifications in that year.
V = Total volume, in kg, notified in that year.
S = Number of stakeholder interest forms received in that year.
na = Not available.
*Volume reported to be manufactured in, imported into or in commerce in Canada.

HR has been identified by the Organization for Economic Cooperation and Development (OECD) as a high production volume (HPV) chemical (OECD 2004), as a U.S. HPV (US EPA 2009) and, as an International Congress and Convention Association HPV (ICCA 2005). According to information from the U.S. Environmental Protection Agency (EPA), the import/production of HR was in the range of 45 000– 226 000tonnes (100 – 500

million pounds) in 1986. The import/production decreased to 4500 – 23 000 tonnes (10 – 50 million pounds) in 1990, 1994 followed up by a temporary increase in 1998 to 25 000-50 000 tonnes (50-100 million pounds), then decreased again to 4500 – 23 000 tonnes (10- 50 million pounds) in 2002 (US EPA 2009).

HRPE has been identified as a HPV chemical by the OECD (OECD 2004), the U.S. EPA (US EPA 2009), and the International Congress and Convention Association (ICCA 2005). According to information from the U.S. EPA, the import/production of HRPE was in the range of 23 000– 45 000 tonnes (50 – 100 million pounds) in 1986. The import/production decreased to 400 – 4500 tonnes (1 – 10 million pounds) in 1990, 1994, 1998 and 2002 (US EPA 2009).

HRGE has been identified as an HPV chemical by the OECD (OECD 2004), the U.S. EPA (US EPA 2009), and the International Congress and Convention Association (ICCA 2005). According to information from the U.S. EPA, the import/production of HRGE was in the range of 45 000-226 000 tonnes (>100 – 500 million pounds) in 1986. The import/production decreased to 5000 - 23 000 tonnes (10 - 50 million pounds) in 1990 and 1994, followed by a further decrease in 1998 to 5 - 23 tonnes (10-500 thousand pounds) to increase again in 2002 to 5000 - 23 000 tonnes (10 - 50 million pounds) (US EPA 2009).

HRTE import/production was in the range of > 450 – 4 500 tonnes (1 – 10 million pounds) in 1986 (US EPA 2009). The import/production decreased to 4.5 – 226 tonnes (10 – 500 thousand pounds) in 1990 and 1994, followed by a increase in 1998 and 2002 to 226 – 450 tonnes (500 000 - 1 000 000 pounds) (US EPA 2009).

Uses

HR, HRPE, HRGE and HRTE are used in adhesives, sealants, paints and coatings, dyes and pigments, printing inks, cosmetics and/or electronics based on information received from the Notice issued under section 71 of CEPA 1999 for the 2006 calendar year (Environment Canada. 2006).

HR, HRPE, HRGE and HRTE are used in soldering materials that are used in the manufacture of over seventy-five percent of electronics products, including sophisticated defence systems and telecommunications and transportation technologies. In the electronics industry, HR, HRPE, HRGE and HRTE are used in liquid soldering fluxes, both in the flux medium of solder paste and in the flux core of solder wire, in which they provide the chemical and electrical properties needed for the efficient and reliable assembly of most electronic products (IPC 2009).

HR, HRGE, HRPE and HRTE are used in the automotive industry for various purposes such as in patch sealer melt, coatings, brake noise dampeners, and other automotive parts (Environment Canada 2009a; HPD 2010).

HRPE is known to be used in medical devices including wound dressings marketed in Canada (Bristol Myers Squibb Company 1994; NPSS 2009).

HR, HRGE, HRPE and HRTE are also used in personal care products such as depilatory waxes and other cosmetic products (CNS 2010; Church & Dwight Co., Inc. 2008). The rosin esters HRGE and HRPE have been reported as ingredients in over one hundred cosmetic products in Canada that are listed in the Cosmetic Notification System database (CNS 2010). However, rosin esters do not appear on the Cosmetic Ingredient Hotlist, Health Canada's administrative list of ingredients that are intended to be prohibited or restricted for use in cosmetics in Canada (Health Canada 2009). The cosmetic products in Canada containing HRGE and HRPE are depilatory wax, lipstick and eye makeup (e.g., mascara) (CNS 2010). In addition, HR has been identified in a few hair styling products, primarily hair pomade and wax (CNS 2010).

As well, HR is used as an additive in pigments, dyes, and printing inks, and as a result may be found in colorants used for plastics, paints and coatings, and printing inks (Environment Canada 2009a; Ciba Canada Ltd. 2008; Ciba Canada Ltd. 2009; February 2010 email from Chemical Sector Directorate, Environment Canada, to Existing Substances Risk Assessment Bureau, Health Canada; unreferenced).

HR, HRPE, HRGE and HRTE are not listed as approved food additives under Division 16 of the *Food and Drug Regulations* (Canada 1978). HR is used as a tackifier in select inks for food packaging materials used primarily in non-food contact applications. For example, HR has been identified in two colour concentrates that may be used in the manufacture of bottle caps and in one component of an adhesive coating that is used in contact with milk (December 2009 email from Food Directorate, Health Canada, to Risk Management Bureau, Health Canada; unreferenced). HRGE may be present in inks used in food packaging materials for non-food contact applications (December 2009 email from Food Directorate, Health Canada, to Risk Management Bureau, Health Canada; unreferenced). Neither HRTE nor HRPE were identified as being used in food packaging applications (December 2009 email from Food Directorate, Health Canada, to Risk Management Bureau, Health Canada; unreferenced). HR, HRTE, HRPE and HRGE were not identified as being used in incidental additives (December 2009 email from Food Directorate, Health Canada, to Risk Management Bureau, Health Canada; unreferenced).

HR, HRTE, HRPE and HRGE are not listed in the Drug Product Database (DPD 2010), the Therapeutic Products Directorate's Non-Medicinal Ingredient Database, the Natural Health Products Ingredients Database (NHPID 2010) nor the Licensed Natural Health Products Database (LNHPD 2010) as medicinal nor non-medicinal ingredients present in final pharmaceutical products, natural health products or veterinary drugs (November 2009 to January 2010 emails from Therapeutic Products Directorate, Natural Health Products Directorate and Veterinary Drugs Directorate, Health Canada, to Risk Management Bureau, Health Canada; unreferenced; Health Canada DPD, NHPID and LNHPD websites).

HR and HRPE are List 2 formulants in the Pest Management Regulatory Agency List of Formulants (PMRA 2007). HR is a formulant in dyes used in four seed treatment fungicides at a concentration of 0.036–0.23 % by weight of pest control product (February 2010 email from Pest Management Regulatory Agency, Health Canada to Existing Substances Risk Assessment Bureau, Health Canada; unreferenced). HRPE is a formulant in one antifouling paint product for non-food use at a concentration of 1.72% by weight (February 2010 email from Pest Management Regulatory Agency, Health Canada, to Existing Substances Risk Assessment Bureau, Health Canada; unreferenced).

In addition, there is older use profile information from the DSL nomination (1984–1986).

The following DSL use codes have been identified for HR:

4 - Adhesive/binder/sealant/filler
13 - Colorant–pigment/stain/dye/ink
21 - Formulation component
30 - Paint/coating additives
44 - Solvent/carrier
45 - Stripper/etcher/discharge printing agent/de-inker
51 - Function other than that listed in codes 02-50
52 - Adhesive and Sealant Production
61 - Electrical or Electronic Products
80 - Paint and Coating
84 - Photographic/Photocopier
85 - Pigment, Dye and Printing Ink
86 - Plastics
89 - Printing and Publishing

The following DSL use codes have been identified for HRPE and HRGE:

4 - Adhesive/binder/sealant/filler
21 - Formulation component
30 - Paint/Coating additive
52 - Adhesive and Sealant Production

The following DSL use codes have been identified for HRTE:

4 - Adhesive/binder/sealant/filler
52 - Adhesive and Sealant Production

Releases to the Environment

The releases of HR, HRPE, HRGE and HRTE to the environment depend upon various losses of these substances from their manufacture, industrial use, and/or consumer/commercial use. These losses can be grouped into seven types: (1) discharge to wastewater; (2) emission to air; (3) loss to land; (4) chemical transformation; (5) disposal to landfill; (6) disposal by recycling; and (7) disposal by incineration. They are estimated using regulatory survey data, industry data and data published by different organizations. To assist in estimating these losses, a spreadsheet (Mass Flow Tool) was used that incorporates all data and assumptions required for the estimation (Environment Canada 2008). Unless specific information on the rate of release or potential for release of the substance from landfills and incinerators is available, the Mass Flow Tool does not quantitatively account for releases to the environment from waste disposal sites.

In the context of the estimation assisted by the Mass Flow Tool, the discharge to wastewater refers to raw wastewater prior to any treatment, either on-site industrial wastewater treatment or off-site municipal wastewater treatment. In a similar manner, the loss via chemical transformation refers to changes in substance identity that occur within the manufacture, industrial use, or consumer/commercial use stages, but excludes those during waste management operations such as incineration and wastewater treatment.

The losses estimated for HR, HRPE, HRGE and HRTE over their lifecycles are presented in Table 4 (Environment Canada 2010a, 2010b, 2010c, 2010d). These substances are expected to be released to wastewater at up to 5% of the total quantity used in Canadian commerce. The 2006 volumes reported in Canadian commerce (Table 3) were 10,000-100,000 kg/year for HR and HRPE, 100,000-1,000,000 kg/year for HRGE, and 1,000-10,000 kg/year for HRTE. The total volume released to wastewater is estimated to be highest for HRGE, followed by HR, and then HRPE; HRTE was expected to be released to wastewater in the least amount. In general, loss to wastewater results in some effluent releases to surface water and potentially also to soil through application of biosolids from wastewater treatment facilities.

Table 4. Estimated losses of HR, HRPE, HRGE and HRTE during their life cycles*

	Proportion (%)			
Type of Loss	**HR**	**HRPE**	**HRGE**	**HRTE**
Wastewater	3.9	0.9	2.4	5.4
Air emission	-	-	-	-
Land	-	-	-	-
Chemical transformation	-	-	-	-
Landfill	79.2	92.8	94.5	91.8
Recycling	14.5	2.6	-	-
Incineration	2.4	2.9	2.9	2.8

*Pertinent lifecycle stages are industrial and consumer/commercial use

HR, HRPE, HRGE and HRTE may also be released to the environment via routes other than wastewater. For example, the substance entering recycling facilities can find its way in minor amounts to water and/or soil, depending upon the operational characteristics of these facilities. The substances disposed of in landfills also have the potential to leach in small quantities into groundwater.

These substances are expected to be used in some consumer products and manufactured items. Although some information is available on the quantity of consumer products and manufactured items containing HR, HRPE, HRGE and/or HRTE that are imported into Canada, it is anticipated that additional material may be imported for which no information exists. However, the total amounts lost to wastewater are not expected to be significantly different from those estimated in this assessment, although, the quantities sent to waste management operations may be higher, if importation of these items were taken into consideration.

Environmental Fate

HR

Based on its physical and chemical properties, this substance is expected to predominantly reside in water and sediment or water and soil, depending on the compartment of release.

The relatively high model-derived acid dissociation constant (pK_a) of 4.9 for the carboxylic acid functional group in HR indicates that half of the substance will be dissociated at pH 4.9. However, the larger empirical pK_a of 6.4 (Table 2a) for the analogous chemical abietic acid [structure A] suggests that even more of the HR substance could be in the neutral form than predicted for HR at environmentally relevant pHs. There is additional empirical evidence that the pKa of most resin acids, including hydrogenated derivatives should be ~6-7 (Sundberg et al. 2009; Holmbom 2010). This along with the close structural similarities between abietic acid [structure A] and representative structures of HR (particularly structures 2 and 3), suggests that the empirically derived pK_a of 6.4 should be considered and is more appropriate than the predicted value of 4.9. The presence (i.e., abietic acid [structure A]) or absence of double bonds in the cyclic groups far from the carboxylic functional group is thought to have a negligible impact on the pK_a of this acid.

Based on the pK_a of 6.4, in water bodies at environmentally relevant pHs (6-9), some of the HR substance will be dissociated, which indicates that the biotic exposure to HR may be from the neutral and the ionized form of the substance. At pH 6, 30% would be in the ionized form, with 70% in the neutral form; at pH 7, 80% would be in the ionized form, with 20% in the neutral form; at pH 9, almost all of the substance would be in the ionized form. Note that a higher proportion would be in ionized form, assuming a pK_a of 4.9.

In view of the high proportion of dissociated chemical at environmentally relevant pHs partitioning behaviour may be described using the log D_{ow} and corrected log K_{oc}. Although electrostatic interactions between the ionized form of the substance and positively charged particles (i.e., soil or sediment) may influence partitioning in the aquatic environment, the extent of this influence is not known.

Based on a relatively low modelled vapour pressure ($3.24 \times 10^{-4} – 7.54 \times 10^{-5}$ Pa) and Henry's law constant ($6.04 \times 10^{-1} – 8.10 \times 10^{-1}$ Pa m^3/mole), HR in the neutral form is considered to be only slightly volatile, whereas the ionized form of the substance would not be volatile at all. Based on these modelled parameter values together with expected aquatic releases, and ionization at environmentally relevant pHs, it would be expected that if released to water, negligible amounts of HR would partition into the atmosphere.

The hydrophobic nature of resin acids causes them to partition to suspended solids during biological wastewater treatment and receiving aquatic environments (Leppanen et al. 2000). Isopimaric acid (structure 1, Table 1a) was found to be present at concentrations of 0.02 mg/L in water and 11.7 mg/kg (dry weight) in sediments adjacent to a pulp and paper mill effluent outfall (Volkman et al. 1993). The magnitude of these environmental concentrations is not directly relevant because the resin acids in this study come primarily from natural pine wood processed at the pulp and paper mill and not the commercial HR substance under evaluation in this assessment. However, the relative partitioning between water and sediment gives an indication of the proportion of HR that may be expected to partition to sediment from water. The hydrogenated derivatives of resin acids, which make up the bulk of HR, may even have a greater tendency to partition to sediments based on their slightly larger predicted organic carbon - water partitioning coefficients (log K_{oc} of 3.5-3.6 for representative structures 2 and 3 in Table 2a) compared with the unmodified resin acid (log K_{oc} of 3.2 for representative structure 1 in Table 2a). The low measured water solubility (1.18 mg/L) for HR would also suggest that if released to water these components would tend to partition to sediments. In addition, the ionized form of a substance (i.e. carboxylate in this case) may undergo chelation with counter-charged substrates, and therefore exhibit an affinity for sediment solids. Chelation and adsorption of ionized substances is important when considering media partitioning of the substance in the environment and the resulting exposure pathway(s). A moderate modelled Log K_{oc} (3.2-3.6) for HR suggests that if released to water, HR is expected to partition to sediments, with a lesser amount remaining in the water column. Similarly, if released to soil, HR is expected to partition to a limited extent into water (e.g., soil pore water, or groundwater) with a greater amount remaining in the soil.

Rosin Esters (HRPE, HRGE and HRTE)

Since these substances do not ionize appreciably at environmentally relevant conditions as they are esters, the use of standard Level III fugacity modelling is appropriate. Based on their physical and chemical properties (Table 2b, c and d), the results of Level III fugacity modelling (Table 5) suggest that HRPE, HRGE and HRTE (as predicted using

all representative structures) are expected to predominantly reside in soil or sediment, depending on the compartment of release, with less than 10% of any substance component predicted to reside in water when released to water.

Table 5. Results of the Level III fugacity modelling (EQC 2003) at 20ºC

	Percentage of HRPE[1] partitioning into each compartment			
Substance released to:	**Air**	**Water**	**Soil**	**Sediment**
Air (100%)	0	0	99.6–99.7	0.3–0.4
Water (100%)	0	0.9–3.4	0.1	96.6–99.1
Soil (100%)	0	0	99.6–99.7	0.3–0.4
	Percentage of HRGE[2] partitioning into each compartment			
Substance released to:	**Air**	**Water**	**Soil**	**Sediment**
Air (100%)	0	0	99.6–99.7	0.3–0.4
Water (100%)	0	0.4–8	0	92–99.6
Soil (100%)	0	0	99.6–99.7	0.3–0.4
	Percentage of HRTG[3] partitioning into each compartment			
Substance released to:	**Air**	**Water**	**Soil**	**Sediment**
Air (100%)	0	0	99.6–99.7	0.3–0.4
Water (100%)	0	0.9–6.9	0	93.1–99.1
Soil (100%)	0	0.3–0.4	99.6–99.7	0

[1]Based on all representative structures shown in Table 1b.
[2]Based on all representative structures shown in Table 1c.
[3]Based on all representative structures shown in Table 1d.

If released into water, HRPE, HRGE and HRTE are expected to strongly adsorb to suspended solids and sediment based upon high estimated log K_{oc} values of ≥4.8. Volatilization from water surfaces is expected to be an unimportant fate process based upon the vapour pressure and Henry's Law constants of HRPE, HRGE and HRTE. Thus, if water is a receiving medium, HRPE, HRGE and HRTE are expected to mainly partition to sediment (see Table 5).

If released to soil, HRPE, HRGE and HRTE are expected to have high adsorptivity to soil (i.e., expected to be relatively immobile) based upon their estimated log K_{oc} values. Volatilization from moist soil surfaces seems to be an unimportant fate process based upon their estimated Henry's Law constants. Therefore, if released to soil, HRPE, HRGE and HRTE will mainly reside in this environmental compartment, which is illustrated by the results of the Level III-fugacity modelling (see Table 5).

Persistence and Bioaccumulation Potential

Environmental Persistence

Resin acids are commonly found in the oleoresin of coniferous trees such as pines, spruce and firs, where they may account for up to 0.2– 0.8% of the total weight of wood (Fengel and Wegner 1985; Liss et al. 1997). As has been mentioned previously, these substances such as the HR structure 1 (isopimaric acid), are therefore commonly found in pulp mill effluents (Liss et al. 1997). Aerobic biological wastewater treatment systems have been shown to reduce resin acids concentrations from pulp and paper mill effluent (MacLeay and Associates Ltd. 1986; Liss et al. 1997, Stuthridge et al. 1991). The performance of the aerobic biological treatment systems in degrading resin acids however, is greatly influenced by the variation in composition of the effluent components, nutrient availability, and the status of the microbial community (Liss et al. 1997). Due to the inhibiting properties of some resin acid components, biodegradation of resin acid mixtures can experience a lag period of variable duration (Hemingway and Greaves 1973). In nature, some bacteria and fungi have been observed to biodegrade resin acids (Kutney et al. 1981a, 1981b, Kutney et al. 1985, Liss et al. 1997, Nilsson et al. 1992, Singh et al 1994, Wilson et al. 1996). Pimarane/isopimarane type resin acids such as isopimaric acid (structure 1 of HR – Table 1a) were observed to be less readily removed than abietane type resin acids such as abietic acid [structure A], due to the presence of the vinyl group (Liss et al. 1997). While biodegradation occurs in the natural environment, these rates are often slow and only a few bacteria are able to use resin acids as a sole carbon source (Liss et al. 1997). However, it has been well-supported that one relatively persistent resin acid metabolite, retene (7-isopropyl-1-methylphenantrene), dominates in anaerobic conditions by microbial activity (Tavendale et al. 1997, Leppänen et al. 2000).

Table 6a presents empirical biodegradation data that indicates 0.95%, 3.0% and 47.3% biodegradation over 28 days in a ready-biodegradation test for HR, HRPE and HRGE respectively (US EPA 2008a; US EPA 2008b). These ready-biodegradation tests were conducted according to the 1992 OECD protocol 301B *Modified Sturm Test*, which specifically applies to substances with low solubility (e.g., <10 mg/l), negligible volatility and high adsorption potential. The test results indicate that the half-life in water for HR and HRPE is likely to be longer than 182 days, and that these two substances will be persistent in the aquatic environment. Although HRGE cannot be considered "ready biodegradable" according to the criteria specified in the OECD 301B protocol, this substance could have a degradation half-life value in water of less than 182 days,

considering that almost 50% biodegradation was observed after 28 days. However, as HRGE is a multi-component substance (see three representative structures in Table 2c), the components remaining after the 28 day study may be relatively recalcitrant and it is possible that further biodegradation would be slow and limited. As such, the persistence status of HRGE is to some extent unclear, based solely on this empirical information.

Based on these experimental results, the U.S. EPA classified HR and HRPE as highly persistent (US EPA 2008a; US EPA 2008b) while HRGE was classified as being moderately persistent (US EPA 2008b).

Table 6a. Empirical data for biodegradation of HR, HRPE and HRGE

Substance	Medium	Fate process	Degradation value	Degradation endpoint / units	Reference
Hydrogenated rosins (CAS RN 65977-06-0)	Water	Biodegradation	0.95	28-day biodegradation / %	US EPA 2008a
HRPE (CAS RN 64365-17-9)	Water	Biodegradation	3.0	28-day biodegradation / %	US EPA 2008b
HRGE (CAS RN 65997-13-9)	Water	Biodegradation	47.3	28-day biodegradation / %	US EPA 2008b

Since experimental biodegradation data are not available for HRTE, empirical biodegradation data from the analogue substance Rosin, diethylene glycol ester (RDE); (CAS RN 68153-38-8), was used to fill data gaps. The biodegradation data also generated according to OECD protocol (1992) 301B *Modified Sturm Test* indicate that HRTE will be persistent in the aquatic environment (US EPA 2008b). It is noted that while this substance contains a diethylene glycol component that is expected to have similar properties to triethylene glycol, the resin acid component of this analogue is not hydrogenated like the resin acid components of HRTE which may affect the measured persistence of HRTE versus that of the analogue (see Appendix IIc for structural comparison between RDE and HRTE). Based on these uncertainties, these analogue empirical data may not be sufficient on their own, to confidently conclude on the persistence status of HRTE.

Table 6b. Analogue empirical data for degradation of HRTE

Substance	Analogue for	Medium	Fate process	Degradation value	Degradation endpoint / units	Reference

Substance	Analogue for	Medium	Fate process	Degradation value	Degradation endpoint / units	Reference
RDE (CAS RN 68153-38-8)	HRTE	Water	Biodegradation	19.7	28-day biodegradation / %	US EPA 2008b

Since few experimental and analogue data are available on the degradation of HR, HRPE, HRGE and HRTE or their components, a QSAR-based weight-of-evidence approach (Environment Canada 2007) was also applied using the degradation models shown in tables 6c, 6d and 6e.

As illustrated by the Level III fugacity model (EQC 2003), HRGE, HRPE and HRTE are essentially non-volatile and will not partition into the atmospheric compartment upon their release to the environment. Atmospheric degradation predictions were solely generated for the three representative structures of HR (see Table 6c), as some of the constituents of this substance were considered slightly volatile. In air, a predicted atmospheric oxidation half-life value of 0.082 days, 0.098 days and 0.365 days for HR representative structures 1, 2 and 3 respectively (see Table 6c) demonstrates that these substances are likely to be rapidly oxidized. Representative structures 1 and 2 for HR are also expected to react at higher rates with other photo-oxidative species in the atmosphere, such as ozone (O_3). With half-lives for all three sub-structures ranging from 0.027 to 0.365 days, HR is considered not persistent in air.

Table 6c. Modelled data for degradation of HR in the atmosphere

HR substructure	Fate process	Model and model basis	Model result and prediction	Extrapolated half-life (days)
Structure 1	Atmospheric oxidation	AOPWIN 2008[1]	$t_{1/2}$ = 0.082 days (~ 1 hrs)	< 2
	Ozone reaction	AOPWIN 2008[1]	$t_{1/2}$ = 0.027 days (~ 0.63 hrs)	< 2
Structure 2	Atmospheric oxidation	AOPWIN 2008[1]	$t_{1/2}$ = 0.098 days (~ 1.2 hrs)	< 2
	Ozone reaction	AOPWIN 2008[1]	$t_{1/2}$ = 0.027 days (~ 0.63 hrs)	< 2
Structure 3	Atmospheric oxidation	AOPWIN 2008[1]	$t_{1/2}$ = 0.365 days (~ 4.4 hrs)	< 2

HR substructure	Fate process	Model and model basis	Model result and prediction	Extrapolated half-life (days)
	Ozone reaction	AOPWIN 2008[1]	n/a[2]	n/a[2]

[1] EPIsuite (2008)
[2] Model does not provide an estimate for this type of structure.

Given the ecological importance of the water compartment, the fact that most of the available models apply to water, and the fact that these substances are expected to be released to this compartment, degradation in water was examined, primarily. Table 6d summarizes the results of available QSAR models for hydrolysis potential of HRPE, HRGE and HRTE. Since clear and reliable empirical biodegradation data are already available for HR and HRPE, and because of uncertainties surrounding the persistence status of HRGE and the absence of empirical degradation data for HRTE, modelled persistence results are only presented for these latter two substances. Table 6e summarizes the results of available QSAR models for degradation in water for HRGE and HRTE.

In water, predicted hydrolysis half-life values ranging from 3.7 to 58 years (pH 7) and from 137 days to 5.8 years (pH 8) for the HRPE, HRGE and HRTE representative structures (see Table 6d) demonstrates that while these chemicals possess hydrolyzable functional groups, the reaction rates will be slow, likely due to the steric hindrance of the ester bonds and possibly also the lack of appreciable solubility of these substances in water. These hydrolysis values must be interpreted with caution, however,as substitute fragments were used by HYDROWIN (2008) to complete structural features for which no data were available in the substance fragments library.

Table 6d. Modelled data for hydrolysis of HRPE, HRGE and HRTE

Fate process	**Hydrolysis**	
Model and model basis	**HYDROWIN 2008**	
	Model result and prediction	
Substances	**pH 7**	**pH 8**
HRPE		
Structure 1	$t_{1/2}$ = 58 yrs	$t_{1/2}$ = 5.8 yrs
Structure 2	$t_{1/2}$ = 29 yrs	$t_{1/2}$ = 2.9 yrs
Structure 3	$t_{1/2}$ = 19 yrs	$t_{1/2}$ = 1.9 yrs
Structure 4	$t_{1/2}$ = 14 yrs	$t_{1/2}$ = 1.4 yrs
HRGE		
Structure 1	$t_{1/2}$ = 19 years	$t_{1/2}$ ~ 2 yrs
Structure 2	$t_{1/2}$ = 9.6 yrs	$t_{1/2}$ = 350 days
Structure 3	$t_{1/2}$ = 3.7 yrs	$t_{1/2}$ = 137 days
HRTE		

Structure 1	$t_{1/2}$ = 8.8 yrs	$t_{1/2}$ = 322 days
Structure 2	$t_{1/2}$ = 4.4 yrs	$t_{1/2}$ = 161 days

Results from Table 6e for HRGE and HRTE show variable degrees of primary and ultimate biodegradation, depending on the chemical structures investigated and their complexity. In general, modelled biodegradation results indicate that larger and more complex rosin esters (i.e., oligo-esters) will be more persistent than smaller molecules (i.e., mono-esters). Since HRGE and HRTE typically contain lesser amounts of mono-esters due to an industry desire to reach high esterification levels (Zinkel and Russell 1989), the persistence status of these substances will be weighted more heavily on the persistence of the oligo-esters (i.e., di-, tri- and tetra-esters). The following evaluation of the biodegradation of HRGE and HRTE therefore focuses on results for the oligo-esters.

Table 6e. Modelled data for biodegradation HRGE and HRTE in the aquatic environment

Fate process		**Primary bio-degradation**	**Ultimate biodegradation**				
Model and model basis		BIOWIN 2008	BIOWIN 2008			TOPKAT 2004 Probability[4]	CATABOL 2008 % BOD[5]
		Sub-model 4: Expert Survey (qualitative results)[3]	Sub-model 3: Expert Survey (qualitative results)[3]	Sub-model 5: MITI linear probability[4]	Sub-model 6: MITI non-linear Probability[4]		
HRGE							
Structure 1 (mono-ester)	Model result and prediction	3.5 "biodegrades fast"	2.4 "biodegrades fast"	0.6 "biodegrades fast"	0.25 "biodegrades slowly"	0.0 "biodegrades slowly"	30.9 "may biodegrade fast"
	Extrapolated half-life	≤ 182	≤ 182	≤ 182	> 182	> 182	≤ 182
Structure 2 (di-ester)	Model result and prediction	2.9 "biodegrades slowly"	1.3 "biodegrades slowly"	0.2 "biodegrades slowly"	0.0 "biodegrades very slowly"	0.0 "biodegrades slowly"	27.3 "may biodegrade fast"
	Extrapolated half-life	> 182	> 182	> 182	> 182	> 182	≤ 182
Structure 3 (tri-ester)	Model result and prediction	2.2 "biodegrades slowly"	0.2 "biodegrades very slowly"	-0.2 "biodegrades very slowly"	0 "biodegrades very slowly"	0.0 "biodegrades slowly"	25.3 "may biodegrade fast"
	Extrapolated half-life	> 182	> 182	> 182	> 182	> 182	≤ 182
HRTE							

Structure 1 (mono-ester)	Model result and prediction	3.2 “biodegrades fast”	2.1 “biodegrades slowly”	0.5 “biodegrades fast”	0.0 “biodegrades very slowly”	0.0 "biodegrades slowly"	34.8 “biodegrades fast”
	Extrapolated half-life	≤ 182	> 182	≤ 182	> 182	> 182	≤ 182
Structure 2 (di-ester)	Model result and prediction	2.6 “biodegrades slowly”	1.0 “biodegrades slowly”	0.1 “biodegrades slowly”	0.0 “biodegrades very slowly”	0.0 "biodegrades slowly"	27.5 “may biodegrade fast”
	Extrapolated half-life	> 182	> 182	> 182	> 182	> 182	≤ 182

[1] EPIsuite (2008)
[2] Model does not provide an estimate for this type of structure.
[3] Output is a numerical score from 0 to 5.
[4] Output is a probability score.
[5] BOD = Biochemical Oxygen Demand

Contrary to empirical results (see table 6a), most model biodegradation results indicate that HRGE may be persistent. Primary biodegradation model results from BIOWIN sub-model 4 estimate that the primary biodegradation half-lives of structures 2 and 3 will proceed relatively slowly, i.e, ≥ 182 days. Additionally, the ultimate biodegradation models BIOWIN 3, 5 and 6 as well as TOPKAT indicate that HRGE structures 2 and 3 will have a half-life in water ≥ 182 days. CATABOL results indicate that the persistence of structures 2 and 3 (27.3% and 25.3 % degradation respectively, over 28 days) is uncertain, signifying that their ultimate degradation half-lives could be slightly below or above 182 days. While more weight is normally attributed to empirical data, due to the variable composition of this substance the ready biodegradation value of 48% over 28 days presented in Table 6a is not sufficiently elevated to confidently conclude that no major components of HRGE will be persistent in the environment (i.e., the remaining 52% could contain a high proportion of larger molecular weight recalcitrant components). Therefore, based on model and empirical results with consideration of the compositional variability of this substance along with the presence of structural features associated with chemicals that are not easily biodegraded (i.e., two or more rings and hydrogenation), the biodegradation half-life in water for HRGE is ≥ 182 days.

HRTE model biodegradation results indicate that this substance will biodegrade slowly in the aquatic environment. Primary biodegradation model results from BIOWIN sub-model 4 show that the diester will undergo primary biodegradation at a relatively slow rate, with a half-life value > 182 days if full mineralization is considered. Furthermore, ultimate biodegradation model results from BIOWIN 3, 5, and 6 and TOPKAT for representative structure 2 (a di-ester) indicate that the half-life of this substance in water will be ≥ 182 days. However, the CATABOL model result (27.5 %) is only slightly above the threshold value of 20 %, indicating that the half-life value in water for this substance could be slightly below or above 182 days. The interpretation of the model results for the mono-ester component (structure 1) of HRTE is not clear. However, this component would be present in smaller quantities in HRTE compared with the di-ester (structure 2), due to the high level of esterification required to meet quality requirements in manufacturing of this substance. Therefore, based on modelled data for the more representative structure (i.e.

structure 2 – di-ester) of HRTE, experimental analogue biodegradation data (i.e. Table 6b) and the presence of structural features associated with chemicals that are not easily biodegraded (e.g., two or more rings and hydrogenation), the degradation half-life in water for HRTE is ≥ 182 days.

Considering empirical biodegradation data, analogue empirical data, model results as well as structural features, there is sufficient consistent evidence that the ultimate biodegradation half-lives of HR, HRPE, HRGE and HRTE are ≥ 182 days in water.

Using an extrapolation ratio of 1:1:4 for a water:soil:sediment biodegradation half-life (Boethling et al. 1995), the half-life in soil is also > 182 days and the half-life in sediments is > 365 days. Thus HR, HRGE, HRPE and HRTE are expected to be persistent in soil and sediment.

As HRGE, HRPE, and HRTE do not partition to air, it can be concluded that HR, HRGE, HRPE and HRTE are persistent in water, soil and sediment and HR is not persistent in air based on criteria set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

The evaluation of bioaccumulation was based on the available experimental and model data. Experimental data on the bioconcentration of resin acids in aquatic organisms were obtained. Rainbow trout (*Oncorhynchus mykiss*) were exposed to representative structure 1 of HR, isopimaric acid, in combination with other resin acids in a flow-through system for 20 days, followed by 10 days of depuration. The mean waterborne concentration of isopimaric acid was 2.7 ± 0.8 µg/L, and pH was approximately 8. The mean bioconcentration factor (BCF) for isopimaric acid was calculated to be 34 ± 14 L/kg based on the 14- and 20-day BCF values which were determined during the period when the fish had reached steady-state concentrations. Depuration half-lives for the resin acids could not be calculated as no free or conjugated acids were detected in fish sampled 4 to 10 days into the depuration period. However, the authors estimate that half-lives for all free and conjugated resin acids are less than 4 days in rainbow trout (Niimi and Lee 1992). It has been observed that in the bile of fish exposed to point-source emissions of resin acids (i.e., pulp and paper mill effluents) 90–98% of the resin acids are found in the form of metabolic conjugates (Oikari et al. 1984). Thus, excretion of resin acids from fish is primarily active and involves conjugation in the hepatocytes and secretion to the bile in the form of glucuronides, within the time frame of several days.

Another bioconcentration study (Burggraaf et al. 1996) measured the accumulation of isopimaric acid, and other resin acids and resin acid derivatives in freshwater mussels (*Hyridella menziesi*). Mussels were exposed to kraft pulp and paper mill effluent for 8 weeks, followed by a 21-day depuration period. The mean exposure levels of isopimaric acid, ranged from 4.5 to 5 µg/L, and the pH of the experiment ranged from 7.3 to 7.6. Resin acids were rapidly accumulated by the mussels and reached steady state in 7 days or less. The mean BCF for isopimaric acid, was calculated to be 180±30 L/kg dry weight

based on the 7-, 14-, and 28-day BCF values. Isopimaric acid had a depuration rate constant (i.e., k_2) of 0.24/day, and a half-life of 3 days.

The empirical bioconcentration data for fish and mussels are summarized in Table 7.

Table 7. Empirical data for bioaccumulation of HR

	Test organism	Depuration rate constant (1/days)	Endpoint	Value (L/kg)	Reference
Structure 1 (isopimaric)	*Oncorhynchus mykiss*	n/a	BCF	34[1]	Niimi and Lee 1992
Structure 1 (isopimaric)	*Hyridella menziesi*	0.24	BCF	180[2]	Burggraaf et al. 1996

[1]Wet weight; [2]Dry weight

Since few experimental BCF data for HR were available, and none were available for HRPE, HRGE and HRTE, a predictive approach was also applied using available bioaccumulation factor (BAF) and BCF models as shown in Tables 8a, b, c, and d. According to the *Persistence and Bioaccumulation Regulations* (Canada 2000) a substance is bioaccumulative if its BCF or BAF is $\geq$ 5000. However, measures of BAF are the preferred metric for assessing the bioaccumulation potential of substances. This is because BCF may not adequately account for the bioaccumulation potential of substances via the diet, which predominates for substances with log $K_{ow} > \sim 4.0$ (Arnot and Gobas 2003). Kinetic mass-balance modelling is in principle considered to provide the most reliable prediction method for determining the bioaccumulation potential because it is based on first principles of bioaccumulation kinetics. This assumes that the log K_{ow} used as input is within the log K_{ow} domain of the model and uptake and elimination follow a passive diffusion mode.

BCF and BAF estimates, corrected for potential biotransformation, were generated using the BCFBAF model (EPIsuite 2008). For HRPE, HRGE and HRTE, metabolic rate constants were derived using structure activity relationships described further in Arnot et al. (2008a, 2008b and 2009). Since metabolic potential can be related to body weight and temperature (Hu and Layton 2001; Nichols et al. 2007), the BCFBAF model further normalizes the k_M for a 10g fish at 15^{o}C to the body weight of the middle trophic level fish in the Arnot-Gobas model (184 g) (Arnot et al. 2008b). The middle trophic level fish was used to represent overall model output as suggested by the model developer and is most representative of fish weight likely to be consumed by an avian or terrestrial piscivore. However, for HR, metabolic rate constants were derived using an *in vivo* BCF normalization routine based on the maximum estimated depuration half-life for resin acids including structure 1 (isopimaric) of 4 days in rainbow trout (Niimi and Lee 1992). This value represents a conservative estimate of the metabolic rate for several free and conjugated resin acids in rainbow trout (*Oncorhynchus mykiss*) exposed to waterborne concentrations.

Table 8a: Modelled data for bioaccumulation for HR

	Test organism	$LogD_{ow}$[1]	Metabolic rate (k_M) 10 g fish at 15°C (1/days)	Endpoint	Value wet weight (L/kg)	Reference
Structure 1	Fish	5.5	n/a	BCF	10	BCFBAF 2008 (linear model)
	Fish	5.5	0.34	BCF	1096	BCFBAF 2008 (mass balance BCF model)
	Fish	5.5	0.34	BAF	1738	BCFBAF 2008 (mass balance BAF model)
	Fish	5.5	0.046	BCF	92	BBM with mitigating factors (Dimitrov et al. 2005)
Structure 2	Fish	6.0	n/a	BCF	10	BCFBAF 2008 (linear model)
	Fish	6.0	0.34	BCF	1000	BCFBAF 2008 (mass balance BCF model)
	Fish	6.0	0.34	BAF	2884	BCFBAF 2008 (mass balance BAF model)
	Fish	6.0	0.056	BCF	112	BBM with mitigating factors (Dimitrov et al. 2005)
Structure 3	Fish	6.3	n/a	BCF	56	BCFBAF 2008 (linear model)
	Fish	6.3	0.34	BCF	871	BCFBAF 2008 (mass balance BCF model)
	Fish	6.3	0.34	BAF	3981	BCFBAF

						2008 (mass balance BAF model)
	Fish	6.3	0.058	BCF	140	BBM with mitigating factors (Dimitrov et al. 2005)

[1] Adjusted log D_{ow} values for pH 7 were taken from table 2a..

Table 8b: Modelled data for bioaccumulation for HRPE

	Test organism	**Log K_{ow}**	**Metabolic rate (k_M) 10 g fish at 15°C (1/days)**	**Endpoint**	**Value wet weight (L/kg)**	**Reference**
Structure 1	Fish	5.7	n/a	BCF	2670	BCFBAF 2008 (linear model)
	Fish	5.7	1.6	BCF	227	BCFBAF 2008 (mass balance BCF model)
	Fish	5.7	1.6	BAF	259	BCFBAF 2008 (mass balance BAF model)
	Fish	5.7	6.1×10^{-6}	BCF	2745	BBM with mitigating factors (Dimitrov et al. 2005)
Structure 2	All model results were outside of the estimation domain of the model					

Structure 3	All model results were outside of the estimation domain of the model
Structure 4	All model results were outside of the estimation domain of the model

Table 8c: Modelled data for bioaccumulation for HRGE

	Test organism	**Log K_{ow}**	**Metabolic rate (k_M) 10 g fish at 15°C (1/days)**	**Endpoint**	**Value wet weight (L/kg)**	**Reference**
Structure 1	Fish	5.22	n/a	BCF	1290	BCFBAF 2008 (linear model)
	Fish	5.22	1.3	BCF	289	BCFBAF 2008 (mass balance BCF model)
	Fish	5.22	1.3	BAF	306	BCFBAF 2008 (mass balance BAF model)
	Fish	5.22	2.04×10^{-6}	BCF	2094	BBM with mitigating factors (Dimitrov et al. 2005)
Structure 2	All model results were outside of the estimation domain of the model					

Structure 3	All model results were outside of the estimation domain of the model

Table 8d: Modelled data for bioaccumulation for HRTE

	Test organism	**Log K_{ow}**	**Metabolic rate (k_M) 10 g fish at 15°C (1/days)**	**Endpoint**	**Value wet weight (L/kg)**	**Reference**
Structure 1	Fish	5.31	n/a	BCF	1480	BCFBAF 2008 (linear model)
	Fish	5.31	0.87	BCF	432	BCFBAF 2008 (mass balance BCF model)
	Fish	5.31	0.87	BAF	479	BCFBAF 2008 (mass balance BAF model)
	Fish	5.31	$2.0x10^{-6}$	BCF	1127	BBM with mitigating factors (Dimitrov et al. 2005)
Structure 2	All model results were outside of the estimation domain of the model					

The BCF values predicted by BBM and the linear BCFBAF model for HR (Table 8a) are expected to be reliable as their molecular weights and log D_{ow} values are well within the estimation domains of the models. The representative structures of HR are also within the structural domain of BBM. In addition, the BCF values for several resin acids with structures resembling those of HR structures 1, 2 and 3 (Table 1a) were included in the BCFBAF ionic compound training set. The BCFBAF (2008) steady-state mass balance models are not intended to be applied to substances that ionize appreciably, however,

based on the estimated pK_a for HR components (4.9-6.4) at pH 6, up to 70% could be in the neutral form, and thus the results for this model are presented in Table 8a as well.

Some of the modelled values for representative structures in Tables 8b, c and d are not presented; they were considered to be reliable as no chemicals of structural comparability were contained in the model training sets. HRPE structure 4 has a molecular weight of 1282 g/mol, which is outside the estimation domain of BBM and the BCFBAF models. In addition, log K_{ow} values for HRPE structures 2, 3 and 4, and HRGE structure 2 and 3 are all outside the estimation domains for BBM and the BCFBAF models. HRPE structure 2 and HRTE structure 2 have predicted log K_{ow} values of >9 which is outside the estimation domains for the BCFBAF and BBM models. All valid model results for mono-ester (structure 1) components of HRPE, HRGE and HRTE suggest that these components will not bioaccumulate mainly due to significant metabolism rates (k_m). Some large discrepancies in predicted metabolism rate constants are apparent between BCFBAF and BBM models in Tables 8b, c and d. However, even at the lower predicted metabolism rates for the various components (i.e. BBM k_m prediction for HRPE structures 1, HRGE structures 1 and HRTE structure 1), the predicted BCF values were not high enough to consider these components bioaccumulative. For components with significantly larger log K_{ow} such that they were out of the domain of the models, it should be noted that growth dilution combined with slow rates of uptake may be an important factor that would limit the potential for bioaccumulation (Arnot and Gobas 2003). Additional mitigating factors that would limit potential bioaccumulation for these substances (including HRPE structures 2, 3 and 4; HRGE structures 2 and 3; and HRTE structure 2) are discussed more fully below.

It has been stated by ETAD (1995) that the molecular characteristics indicating the absence of bioaccumulation are a molecular weight of > 450 g/mol and a cross-sectional diameter of > 1.05 nm. More recent investigations relating fish BCF data and molecular size parameters (Dimitrov et al. 2002; Dimitrov et al. 2005; BBM 2008) suggest that the probability of a molecule crossing cell membranes as a result of passive diffusion declines significantly with increasing maximum diameter (D_{max}). The probability of passive diffusion falls appreciably when a maximum diameter is greater than ~1.5 nm and falls more significantly when molecules have a maximum diameter of > 1.7 nm. Sakuratani et al. (2008) have also investigated the effect of cross-sectional diameter on passive diffusion in a test set of about 1200 new and existing chemicals. They observed that substances that do not have a very high bioconcentration potential (BCF < 5000) often have a D_{max} of > 2.0 nm and an effective cross-sectional diameter (D_{eff}) of > 1.1 nm.

As Arnot et al. (2010) have noted, there are uncertainties associated with the thresholds proposed by Dimitrov et al. (2002, 2005) and Sakuratani et al. (2008) since the BCF studies used to derive them were not critically evaluated. Arnot et al. (2010) pointed out that molecular size influences solubility and diffusivity in water and organic phases (membranes), and larger molecules may have slower uptake rates. However, these same kinetic constraints apply to diffusive routes of chemical elimination (i.e., slow in = slow out). Thus, significant bioaccumulation potential may remain for substances that are

subject to slow absorption processes, if they are slowly biotransformed or slowly eliminated by other processes. Consequently, when evaluating bioaccumulation potential molecular size information should be considered with care, and used together with other relevant lines of evidence in a weight of evidence approach.

The D_{max}s for representative components of HRPE are estimated to range from 1.84 nm (structure 1) to > 2 nm for structures 2, 3 and 4, and their molecular weights range from 422.61 g/mol (structure 1) to 1281.99 g/mol (structure 4), which exceed some of the threshold values cited above for di-, tri- and tetra-esters (i.e., structures 2, 3 and 4) and suggest that the uptake rate of these components may be slower compared to that of smaller, more compact substances, thus mitigating the overall bioconcentration potential, given the biotransformation potential of these substances.

The same is true for HRGE and HRTE. The maximum diameters for HRGE are estimated to range from 1.90 nm (structure 1) to > 2 nm for structures 2 and 3, and their molecular weights range from 378.56 g/mol (structure 1) to 951.48 g/mol (structure 3), which exceed some of the threshold values cited above for di- and tri-esters (i.e. structures 2 and 3) and suggest that the uptake rate of these components may be slower compared to that of smaller, more compact substances, thus mitigating the overall bioconcentration potential. Finally, the maximum diameter for HRTE is estimated to be > 2 nm for both structure 1 and 2, and its molecular weight ranges from 436.64 g/mol (structure 1) to 723.10 g/mol (structure 2) which exceeds some of the threshold values cited above for mono- and di-esters (i.e., structures 1 and 2) and suggest that the uptake rate of these components may be slower compared to that of smaller, more compact substances, thus mitigating the overall bioconcentration potential given the biotransformation potential of these substances.

It is acknowledged that strict cut-offs for molecular weight and size should be applied with caution in predicting bioaccumulation potential, as, in some cases, large molecules with slow uptake rates may show even slower elimination rates, which could lead to bioaccumulation. However, realistically considering that the log K_{ow} values for these larger substances, which were out of the domains for BCFBAF and BBM models, were > 9, they will likely have such low uptake rates that growth dilution would mitigate the bioaccumulation potential of these substances, given the biotransformation potential of these substances (Arnot and Gobas 2003).

The available evidence indicates that HR is expected to have low bioaccumulation potential due to its physical and chemical properties (i.e., ionizing capabilities) and low experimental BCFs (34-180) for component structures (i.e., isopimaric acid). Metabolism-corrected QSAR-estimated BCF values range from 10-1096 L/kg depending on the model used and which component was modelled. Furthermore, the metabolism-corrected QSAR-estimated BAF values were 1738-3981 L/Kg based on which component was modelled. Based on the available empirical and kinetic-based modelled values corrected for metabolism, and considering empirical evidence for metabolic potential, HR does not meet the bioaccumulation criterion (BAF $\geq$ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

HRPE, HRGE and HRTE are also expected to have low bioaccumulation potentials due to their physical and chemical properties (i.e., high molecular weights, large cross-sectional diameters of some components), slow uptake potential estimated for larger components and low predicted BCF and BAF for smaller components. Predicted metabolism corrected BCF and BAF values for the monoester components range from 259 to 2745 L/kg for HRPE, 289 to 2094 L/kg for HRGE, and 432 to 1480 L/kg for HRTE, depending on the model used. The available predicted BAF results for HRPE, HRGE, and HRTE are up to 259, 306-140 and 479 L/kg, respectively. The larger structures for HRPE, HRGE and HRTE were generally outside of the domain of the BCFBAF and BBM models. However, based on their high predicted molecular size (D_{max} > 2nm), weights (> 450 g/mol) and log K_{ow} (> 9), these components would have such slow uptake rates that metabolism and growth dilution would effectively mitigate bioaccumulation. Thus, HRPE, HRGE and HRTE do not meet the bioaccumulation criterion (BAF $\geq$ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

A - In the Aquatic Compartment

There is experimental evidence that HRPE and HRGE do not cause harm to aquatic organisms following short-term (acute) exposure at relatively low concentrations. However, some experimental evidence suggests that components of HRTE and HR may cause harm to aquatic organisms following short-term (acute) exposure at relatively low concentrations.

The aquatic toxicity of analogues of HRPE, HRGE and HR has been determined with the Water Accommodated Fraction (WAF) method (OECD 2000). This method has been developed for the aquatic toxicity testing of hydrophobic mixtures. Only a fraction of the total mass of multi-component substances responsible for the composition of a WAF may be present in the WAF solution. The "loading rate" has therefore been advocated for expressing exposures of mixtures that neither wholly dissolve nor completely form a stable dispersion or emulsion over the required test range (Girling et al., 1992). The loading rate is the mass-to-volume ratio of the mixture to medium used in the preparation of a WAF. WAFs may thus be considered analogous to the term "nominal concentration" used for typical test substances, with all the limitations inherent in that term (OECD 2000).

Effects concentrations in tests based upon WAFs can thus be calculated from (1) the loading rates, which are identified as either lethal loading 50 (i.e., a loading rate that is lethal to 50% of the test population) (LL_{50}) or effective loading 50 (i.e., a loading rate that has a non-lethal effect on 50% of the test population) (EL_{50}) values and/or (2) the

measured mass of test substance in the test water which is identified as either LC_{50} or EC_{50} values. LL_{50} or EL_{50} values are analogous to nominal LC_{50} or EC_{50} values determined for pure substances tested within their solubility range. Similarly, the NOEC (no-observable-effect-concentration) is analogous to the NOELR (no-observable-effect-loading-rate). The statistical methods used to determine LL_{50}, EL_{50} and NOELR values are the same as those used to determine LC_{50}, EC_{50} and NOEC values (OECD 2000).

For the WAF tests reported in this assessment, the test material was dissolved in water by stirring for 48 hours in sealed containers (i.e.,to avoid loss of volatile components) prior to toxicity testing, to ensure adequate time for all the components to reach equilibrium under the test conditions.

HR

The aquatic toxicity data pertinent to HR presented in Table 9a for Rosin (CAS RN 8050-09-7) were generated using the WAF method.

This material serves as an analogue for HR, as many of the same structural components would be present however, the major components would be structures 2 and 3 (Table 1a) with two double bonds still present (e.g. abietic acid [structure A]) (see Appendix IIa for structure-based comparison). It is acknowledged that these structural variations may lead to slight differences in aquatic toxicity. However, comparison of log K_{ow}, water solubility and representative chemical structures, molecular weights, and cross-sectional diameters all suggest that this analogue may be closely related to HR in terms of overall *in situ* and *in vivo* bioavailability. Loading rates for HR analogue Rosin (CAS RN 8050-09-7) were 0, 1, 10, 100 or 1000 mg/L for algae, fish and *Daphnia*. In addition, the effects of filtering and a lower pH on the observed toxicity were examined and no mortality or other effects were observed for fathead minnow (*Pimephales promelas*) or green algae (*Pseudokirchneriella subcapitatum*) at the highest concentrations tested (1000 mg/L). For *Daphnia sp*. however, there was a 60% mortality in the 1000 mg/L-filtered treatment group and 90% mortality in the pH adjusted (i.e. pH 6.7 versus pH >8 in non-pH adjusted tests) 1000 mg/L treatment. In the definitive test conducted without filtering or use of pH adjustments and concentrations gradients of 0, 125, 250, 500 and 1000 mg/L, 85% mortality was found at 1000 mg/L after 48 hours (this was the basis of the EL_{50} of 911 mg/L shown in Table 9a).

Table 9a. Empirical data for aquatic toxicity for HR analogues and representative structure 1 (isopimaric acid)

Test organism	Type of test	Endpoint	Value (mg/L)	Reference
Rosin (CAS RN 8050-09-7)				
Green algae (*Selenastrum*	Acute (72 hours)	EC_{50}[1]	NES[4]	US EPA 2008a

capriconutum)				
Daphnia sp.	Acute (48 hours)	EL_{50}[3]	911	US EPA 2008a
Fathead minnow (*Pimephales promelas*)	Acute (96 hours)	LC_{50}[2]	NES[4]	US EPA 2008a
HR structure 1 (isopimaric acid; Table 1a)				
Daphnia sp.	Acute (24 hours) (48 hours) (96 hours)	 LC_{50}[2] LC_{50}[2] LC_{50}[2]	 0.26 0.07 0.02	Peng and Roberts 2000
Coho salmon *(Oncorhynchus kisutch)*	Acute (96 hour)	LC_{50}	0.22	Leach and Thakore 1977
Fathead minnow *(Pimephales promelas*)	Acute (96 hours)	LC_{50}[2]	0.87	Geiger et al. 1985
Sockeye salmon *(Oncorhynchus nerka)*	Acute (96 hours)	LC_{50}[2]	0.7	Kutney et al.1981b
Daphnia sp.	Acute (96 hours)	EC_{50}[1]	1.3	Kutney et al.1981b

[1] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.
[2] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[3] EL_{50} – Effective loading rate that is estimated to be lethal to 50% (not equivalent to LC_{50} or EC_{50} of the substance).
[4] NES – No effects observed at saturation at loadings of up to 1000 mg/L.

The evaluation of available WAF toxicity data for fish and an alga (Table 9a) show that no effects were observed at the water solubility limit (saturation) of the HR analogue Rosin (CAS RN 8050-09-7). The evaluation of available WAF toxicity data for the HR analogue exposed to Daphnia sp. (Table 9a) shows that some effects were seen at high loading rates where an EL_{50} of 911 mg/L was reported. The observed toxicity of the analogue Rosin, which is a mixture of resin acids, may in part be due to other similar components such as HR structure 1 (isopimaric acid). Due to combined toxicity and other matrix factors, the toxicity potential of Rosin versus the individual pure compound, represented by isopimaric acid (structure 1), can be expected to differ substantially (Spurgeon et al. forthcoming). Ultimately, the weight of evidence based on the LC_{50} measurements with isopimaric acid (structure 1) suggest that components of HR would be acutely hazardous to aquatic organisms at relatively low concentrations (i.e., <1 mg/L). The most sensitive toxicity estimate was reported by Peng and Roberts (2000) based on toxicity tests with *Daphnia magna*, where the 24-, 48- and 96-hour LC_{50} values were 0.26 mg/L, 0.07 mg/L and 0.02 mg/L. This study was performed using the ISO 6341 and British standards BS 6068 (ISO 1989, BSI 1990), using five organism replicates and four aliquot replicates for a total of 20 organisms per concentration with a pH of dilution water of 7.6-8.0. It has been determined that these data are sufficiently robust to provide a good estimate of the hazard of structure 1 of HR (see robust study summary inAppendix I). In addition, due to the lack of toxicity data on structure 2 and 3 of HR, and the sufficient structural similarity between structure 1 and structures 2 and 3 of HR, the empirical toxicity data for structure 1 could be used as analogue information for the entire substance in the most conservative approach for HR.

HRPE, HRGE and HRTE

The aquatic toxicity data presented in Table 9b for Rosin, pentaerythritol ester (RPE) (CAS RN 8050-26-8) were generated using WAF method. RPE may serve as a suitable analogue for HRPE and HRGE. The difference between RPE and HRPE/HRGE is that RPE contains mainly unmodified resin acid components (i.e., with two double bonds still present such as abietic acid [structure A]) and HRGE is esterfied using a slightly different alcoholic reagent (i.e., glycerol [structure 2]b) than is used for RPE and HRPE (i.e., pentaerythritol [structure 2]c) . Overall, RPE was considered to provide an adequately similar bioavailability profile and similar mode of toxic action (ester mode of action) to HRPE and HRGE for ecotoxicity data read across purposes (see Appendix IIb).

Range-finding experiments were conducted at 0, 1, 10, 100 and 1000 mg/L where no mortality or other effects were observed for fathead minnow or *Daphnia*. The effect of filtration was tested at 1000 mg/L and the effect of lower pH (i.e., pH 6.5-6.7) at 0 and 1000 mg/L, with no effects observed for either parameter. For the green algae range-finding tests the final cell density in the unadjusted WAF prepared at 1000 mg/L was ~17 % lower than in the controls. The percentage inhibitions of final cell densities for the WAF prepared at 100 and 10 mg/L were 13% and 9%, respectively. This indicated that final cell numbers might be affected by loading rate for green algae. Thus, the definitive test was conducted at concentration gradients of 0, 125, 250, 500, 750 and 1000 mg/L with no filtration or pH adjustment, and no effects were seen in the definitive test. The definitive tests for fathead minnow and *Daphnia* were conducted with no filtering or pH adjustment at 0 mg/L and 1000 mg/L. No effects were seen at saturation in any of the toxicity experiments reported in Table 9b. The evaluation of available toxicity data for algae, aquatic invertebrates and fish indicates the potential acute hazard to these aquatic organisms is low for RPE, which, due to similar bioavailability and expected mode of action (ester), would also apply to HRPE and HRGE. The robust study summaries for the RPE WAF toxicity tests have been prepared by USEPA (2002).

Table 9b. Empirical data for aquatic toxicity for RPE (CAS No. 8050-26-8) analogue

Test organism	Type of test	Endpoint	Value (mg/L)	Reference
Green algae (*Selenastrum capriconutum*)	Acute (72 hours)	EC_{50}[1]	NES[3]	US EPA 2008b
Daphnia sp.	Acute (48 hours)	EC_{50}[1]	NES[3]	US EPA 2008b
Fathead minnow (*Pimephales promelas*)	Acute (96 hours)	LC_{50}[2]	NES[3]	US EPA 2008b

[1] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.
[2] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[3] NES – No effects observed at saturation at loadings of up to 1000 mg/L

RPE was deemed not suitable to estimate the ecotoxicity of HRTE due to large compositional differences, as RPE would be comprised mainly of tri-esters (structure 3)

and tetra-esters (structure 4), while HRTE would be comprised more of lower molecular weight di-esters (structure 1) and mono- esters (structure 2). These differences have a direct impact on bioavailability potential and suggest that RPE would be less bioavailable and likely less toxic than HRTE. RPE, however, is expected to have a similar mode of toxic action (ester mode) to HRTE. Ecotoxicity values were predicted (Table 9c) for each representative structure of HRTE.

Table 9c. Modelled data for aquatic toxicity of HRTE

Test organism	Type of test	Endpoint	Value (mg/L)	Reference
Structure 1				
Fish	Acute (96 hours)	LC_{50}[1]	0.53	ECOSAR 2000-2008[3]
			1.13	AIEPS 2003-2007
Daphnia	Acute (48 hours)	EC_{50}[2]	0.46	ECOSAR 2000-2008[3]
			2.51	AIEPS 2003-2007
Algae	Acute (96 hours)	EC_{50}[2]	0.77	ECOSAR 2000-2008[3]
			2.33	AIEPS 2003-2007
Structure 2				
Fish	Acute (96 hours)	LC_{50}[1]	2.23*	AIEPS 2003-2007
			3.58*	CPOPs 2008
Daphnia	Acute (48 hours)	EC_{50}[2]	3.71*	AIEPS 2003-2007
Algae	Acute (96 hours)	EC_{50}[2]	3.85*	AIEPS 2003-2007

[1] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[2] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.
[3] Neutral organic SAR (Baseline Toxicity).
* Exceeds water solubility of component by more than a factor of 10.

The mono-ester constituents of HRTE (i.e., structure 1) showed moderate to high potential to cause acute harm to aquatic organisms based on predicted toxicity values in Table 9c. This component of HRTE is considered in the domain of the Ecological Structure-Activity Relationship (ECOSAR) Program based on log K_{ow} and molecular weight considerations, and moderately in the domain of the Artificial Intelligence Expert Predictive System (AIEPS) based on a moderate (> 60%) compatibility with structures (28) in the AIEPS training set. The representative structure for HRTE structure 1 was out of the domain of the CPOPs (2008) model and thus no estimate is provided for this component. Due to the potential for acute toxicity ≤ 1 mg/L predicted by the ECOSAR model, it is concluded that this component has the potential to be hazardous to aquatic organisms.

The di-ester (i.e. structure 2 of HRTE) was out of the domain of the ECOSAR model, due to the large log K_{ow} (> 10) predicted for these substances. Thus, ECOSAR results for this component of HRTE were not considered reliable and were not presented here. The predicted solubility of structure 2 was very low (< $1.3x10^{-6}$ mg/L) and empirical water solubility values for the whole substance were < 1 mg/L (Table 2d). This suggests that the oligo-ester component of HRTE may not be soluble enough to become acutely

hazardous to aquatic organisms based on the aquatic toxicity estimates predicted for this component in Table 9c. This supports the notion that the likelihood of any acute effects may be very low for chemicals with such a high log K_{ow}.

The weight of evidence regarding experimental and modelled data for HR and HRTE indicates that certain components of HR (i.e. structure 1 – isopimaric acid) and HRTE (i.e., structure 1 – mono-ester) may cause acute harm to aquatic organisms at low concentrations (i.e., acute LC_{50}s are < 1.0 mg/L). The weight of evidence regarding experimental WAF ecotoxicity data for analogues of HRPE and HRGE indicates that these substances are not expected to cause acute harm to aquatic organisms at low concentrations (i.e., no effects at saturation were measured for analogue substances). In addition, the reduced bioavailability associated with a larger molecular weight, size and log K_{ow} predicted for the abundant oligo-ester (i.e., di-, tri-, and tetra-ester) components of HRPE and HRGE support these conclusions.

B - In Other Environmental Compartments

When HR, HRPE, HRGE and HRTE are released into a water body, they partition into suspended particulate matter and to bottom sediments, where sediment-dwelling organisms would be exposed to the substance. However, no appropriate environmental monitoring data or toxicity data specific to sediment-dwelling organisms are available for these substances. Although there is a large amount of information on the levels of resin acids (including minor constituents of HR) downstream from pulp/paper mill discharge points, these data were not deemed to be relevant to the sources and uses of the HR in this assessment.

For these substances, a risk quotient based on exposure in sediment pore water may be calculated based on the aquatic compartment PEC and predicted no-effect concentration (PNEC) values presented above and used for sediment-risk characterization. In the calculation, bottom sediment and its pore water are assumed to be in equilibrium with the overlying water and benthic and pelagic organisms are assumed to have similar sensitivities to the substance. Therefore the PEC and PNEC for pore water would be considered to be the same as for the aquatic compartment. This equilibrium approach would thus result in a risk quotient (PEC/PNEC) for the sediment compartment that is the same as for the aquatic compartment.

Ecological Exposure Assessment

No suitable data concerning concentrations of these substances in water in Canada have been identified. Therefore, environmental concentrations are estimated from available information, including estimated substance quantities, release rates, and size of receiving water bodies. HR and to a lesser extent HRPE, HRGE and HRTE may contain small residual amounts of unmodified resin acids (e.g., structure 1 for HR), and thus may be present in environmental media naturally at background levels and because of

environmental contamination from pulp and paper production operations. However, the quantitatively most important components of the substances considered in this assessment are not naturally occurring nor are they expected to be present in effluent from pulp and paper mills.

A – Industrial Release

The aquatic exposure of HR and HRTE are expected if the substances are released from industrial use to a wastewater treatment plant and the treatment plant discharges its effluent to a receiving water body. The concentration of the substances in the receiving water near the discharge point of the wastewater treatment plant is used as the predicted environmental concentrations (PECs) in evaluating the aquatic risk of these substances. It can be calculated using the equation

$$C_{water-ind} = \frac{1000 \times Q \times L \times (1-R)}{N \times F \times D}$$

where

$C_{water-ind}$:	aquatic concentration resulting from industrial releases, mg/L
Q:	total substance quantity used annually at an industrial site, kg/yr
L:	loss to wastewater, fraction
R:	wastewater treatment plant removal rate, fraction
N:	number of annual release days, d/yr
F:	wastewater treatment plant effluent flow, m^3/d
D:	receiving water dilution factor, dimensionless

As HR and HRTE are used industrially and are expected to be released to water, industrial release scenarios are used to estimate the aquatic concentrations of the substances with the help of Environment Canada's (2009b) Industrial Generic Exposure Tool – Aquatic (IGETA). The estimated loss to wastewater during the industrial use lifecycle for HR was 3.8% (the total value of 3.9% reported in Table 4 included consumer/commercial use as well), and for HRTE was 0.9% (the total value of 5.4% reported in Table 4 included consumer/commercial use as well). These industrial releases to wastewater result primarily from industrial application, formulation and container handling activities relating to their uses in soldering materials and adhesives. The IGETA scenario assumes that the release occurs 250 days per year, typical for small and medium-sized facilities, and is sent to a local wastewater treatment plant (WWTP) with a conservatively estimated wastewater-primary-removal efficiency of 55.7% (ASTreat 2006) for HR and 49% (SimpleTreat 1997) for HRTE.

For HR, the site-specific scenario was based on two major industrial users of the substance (i.e., accounting for over half of the total industrial use volume reported in 2006) resulting in a refined PEC of 3.3×10^{-5} mg/L (Environment Canada 2010e).

For HRTE, the total industrial use quantity of 100-1000 kg/year was assumed to be used at one site with a conservatively estimated flow of 3456 m^3 per day corresponding to the 10^{th} percentile of WWTP effluent flow rates across Canada resulting in a refined PEC of 3.3×10^{-4} mg/L (Environment Canada 2010f).

As HRPE and HRGE showed no acute effects at and well beyond saturation based on the WAF toxicity results of the analogue RPE, no industrial release scenarios were calculated for these substances.

B – Consumer Release

As HR and HRTE are found in consumer products and can be released to water, Mega Flush, Environment Canada's spreadsheet tool for estimating down-the-drain releases from consumer uses, was employed to estimate the potential substance concentration in multiple water bodies receiving sewage treatment plant effluents to which consumer products containing the substance may have been released (Environment Canada 2009c). The spreadsheet tool is designed to provide these estimates based on conservative assumptions regarding the amount of the substance used and released by consumers.

By default, we assume primary and secondary WWTP removal rates to be of 0%, consumer use of the substance to be over 365 days/year, and the flow rate at all sites to be relatively low (i.e., the tenth percentile value). These estimates are made for approximately 1000 release sites across Canada, which account for most of the major WWTPs in the country. The losses from consumer use were estimated to be 0.1% (the total value of 3.9% reported in Table 4 included industrial use as well) for HR based on its use as a colorant in paints and plastics, and 4.5% (the total value of 5.4% reported in Table 4 included industrial use as well) for HRTE based primarily on its use in depilatory waxes.

The equation and inputs used to calculate the PEC of HR and HRTE in the receiving water bodies are described in Environment Canada (2010g, 2010h). Each scenario was run assuming a total consumer use quantity of 10,000-100,000 kg/year for HR and 1,000-10,000 kg/year for HRTE (Environment Canada 2010a, 2010d).

Using this scenario, the tool estimates that the PECs in the receiving water bodies range from 1.2×10^{-5} to 3.8×10^{-8} mg/L for HR and 2.6×10^{-5} to 8.3×10^{-8} mg/L for HRTE.

As HRPE and HRGE showed no acute effects at and well beyond saturation based on the WAF toxicity results of the analogue RPE, no consumer release scenarios were calculated for these substances.

Characterization of Ecological Risk

The approach taken in this assessment was to examine the available scientific information and develop conclusions based on a weight-of-evidence approach and using precaution as required under CEPA 1999. Lines of evidence considered include results from a conservative risk quotient calculation, as well as information on the persistence, bioaccumulation, toxicity, sources and fate of the substance.

As described previously, HR, HRPE, HRGE and HRTE have relatively long half-lives in all environmental compartments. However they are also expected to have low bioaccumulation potentials.

The HR analogue, Rosin (CAS RN 65997-06-0), showed no toxicity at WAF loading rates as high as 1000 mg/L for representative fish and aquatic plants. However, an effective loading rate of 50% (EL_{50}) of 911 mg/L was found for this substance for *Daphnia sp.* (see Table 9a). Additionally, representative structure 1 for HR (isopimaric acid) showed a critical toxicity value of 0.07 mg/L which was the acute toxicity observed for *Daphnia sp.* reported by Peng and Roberts (2000). The 96-hour LC_{50} of 0.02 mg/L was not used, as this exposure period may be approaching that used for chronic toxicity of *Daphnia sp.* However, this study was not conducted as a chronic toxicity study. HRPE and HRGE analogue substance RPE (CAS RN 8050-26-8) showed no toxicity at WAF loading rates as high as 1000 mg/L for fish, aquatic invertebrate and plants representatives (see Table 9b). This result is consistent with the low environmental bioavailability, low bioaccumulation potential and large steric hindrance of the larger oligo-ester components known to make up the bulk of HRPE and HRGE.

A conservative PNEC was derived based on HR structure 1 (isopimaric acid) which showed a measured acute LC_{50} of 0.07 mg/L for *Daphnia*. This value was selected as the critical toxicity value for HR and divided by an assessment factor of 100 to account for uncertainties related to inter-species and intra-species variability in sensitivity, and extrapolation from a laboratory LC_{50} to a no-effect value in the field. This calculation resulted in a PNEC 0.0007 mg/L for HR.

For HRPE and HRGE analogue substance RPE, as no effects were seen at saturation and at the highest loading rate tested of 1000 mg/L PNEC (much greater than that expected in the environment), determination was not possible. Thus, no acute effects would be expected at saturation and no risk quotient analysis was required.

For HRTE, the PNEC was derived from the most sensitive predicted endpoint—an acute EC_{50} for *Daphnia* of 0.46 mg/L for the mono-ester component. This value was selected as the critical toxicity value, and divided by an assessment factor of 100 to account for uncertainties related to inter-species and intra-species variability in sensitivity, and extrapolation from a laboratory EC_{50} to a no-effect value in the field. This calculation resulted in a PNEC loading of 0.0046 mg/L for HRTE.

For HR, the realistic worst-case PEC for major industrial use sites was estimated to be 3.3×10^{-5} mg/L, resulting in a risk quotient of PEC/PNEC = 3.3×10^{-5} mg/L/0.0007 mg/L = 0.05, which indicates that there is no potential for harm in any sites based on industrial uses of HR in Canada. The consumer use scenario resulted in zero sites exceeding a PNEC of 0.0007 mg/L based on 10th percentile flow values for all sites and 0% wastewater removal rate, and thus there is no indication of risk from consumer use of HR in Canada.

For HRTE, a conservative PEC for industrial uses in Canada was estimated to be 3.3×10^{-4} mg/L. Thus, for industrial uses in Canada the risk quotient was PEC/PNEC = 3.3×10^{-4} mg/L/0.0046 mg/L = 0.07, which indicates that there is no potential for harm in any sites based on industrial uses of HRTE in Canada. The consumer use scenario resulted in zero sites exceeding a PNEC of 0.0046 mg/L based on 10th percentile flow values for all sites and 0% wastewater removal rate, and thus there is no indication of risk from consumer use of HRTE in Canada.

The resulting conservative loading-based risk quotients (PEC/PNEC) of <<1 for HR, HRPE, HRGE and HRTE indicate that exposure values are unlikely to be high enough to cause harm to aquatic organisms for these substances. HR, HRPE, HRGE and HRTE are thus unlikely to be causing ecological harm in Canada.

Uncertainties in Evaluation of Ecological Risk

All modelling of a substance's physical and chemical properties and P, B and iT characteristics is based on chemical structures. As these substances are UVCBs (**U**nknown or **V**ariable Composition, **C**omplex Reaction Product or **B**iological Material), it cannot be represented by a single, discrete chemical structure. Therefore, for the purposes of modelling, "representative structures" that would provide conservative estimates were identified. Given that several different representative structures may be derived for the same UVCB, it is recognized that structure-related uncertainties exist for these substances. In the production of UVCBs, including the substances in this assessment, the potential for a residual amount of components that may be highly hazardous (i.e., persistent, bioaccumulative, toxic) is possible. Due to the variability in the starting materials and reaction process, and the complexity of products that may include highly hazardous residuals there is uncertainty regarding the presence of certain components in each UVCB assessed. However, significant efforts based on available literature and expert judgment in chemistry have been made to identify major components of concern in each UVCB in order to base the assessment on a conservative estimate.

The formation of potentially hazardous metabolites (i.e., retene) has been shown for various unmodified resin acids, primarily from pulp and paper discharge. There is uncertainty, in this work regarding the extent to which components of HR and potentially HRPE, HRGE and HRTE, would degrade in the environment to form such metabolites. Base on the generally low rates of degradation predicted for the hydrogenated and esterified components in these substances, and considering that the residual amount of unmodified resin acids is expected to be low in these substances, production of these hazardous metabolites is likely minimal.

The ecotoxicity estimates for HRPE and HRGE are based on measured ecotoxicity data of close chemical analogue substances. The slight structural differences between the substances assessed and their analogues may lead to uncertainties in this read-across approach. The suitability of each analogue was judged based on key physical and

chemical parameters (i.e., log K_{ow}, water solubility, molecular weight and size), mode of toxic action, and similarity of structures.

Also, regarding ecotoxicity, based on the predicted partitioning behaviour of these substances, the significance of soil and sediment 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. For these substances, a risk quotient based on exposure in sediment pore water may be calculated based on the aquatic compartment PEC and PNEC values presented above and used for sediment risk characterization. In the calculation, bottom sediment and its pore water are assumed to be in equilibrium with the overlying water and benthic and pelagic organisms are assumed to have similar sensitivities to the substances. Therefore the PEC and PNEC for pore water would be considered to be the same as for the aquatic compartment. This equilibrium approach would thus result in a risk quotient (PEC/PNEC) for the sediment compartment that is the same as for the aquatic compartment.

The critical aquatic toxicity data considered for HRPE and HRGE were generated using the WAF method. The evaluation of available acute toxicity data for fish, aquatic invertebrates and aquatic plants indicates the acute hazard to aquatic organisms is low based on no effects observed at the water solubility limit (saturation) of RPE, an analogue substance (CAS RN 8050-26-8). While the acute testing did not show toxicity in aquatic organisms, the physical and chemical properties and fate of the substances in this category indicate they are soluble in water at concentrations that raise uncertainty regarding the potential to have chronic effects. Therefore, the chronic invertebrate toxicity test remains a source of uncertainty.

Given the use of this substance in other countries, it is possible that HR, HRPE, HRGE, and HRTE are entering the Canadian market as a component of manufactured items and consumer products. It is anticipated that even if it were possible to take these quantities into consideration the quantities of these substances released to the various environmental media (particularly water) would not be significantly different from those estimated here. It is also recognised that since the majority of these substances end up at waste disposal facilities, releases from waste disposal sites could be possible and contribute to overall environmental concentrations. However given the physical and chemical properties of these substances, such releases are expected to be minimal.

Potential to Cause Harm to Human Health

Exposure Assessment

Environmental Media

There were no empirical data identified for HR, HRPE, HRGE, or HRTE in air, water, soil or sediment in Canada or elsewhere. Environmental concentrations for HR, HRGE, HRPE and HRTE were estimated using the loss percentages predicted by the Mass Flow Tool (see Table 4) (Environment Canada 2010a, 2010b, 2010c, 2010d). The percentages were applied to the total quantity of HR, HRGE, HRPE and HRTE in Canadian commerce in 2006. The total quantities in commerce were conservatively assumed to be the maximum quantities of the in-commerce ranges: 100 000 kg for HR, 100 000 kg for HRPE, 1 000 000 kg for HRGE and 10 000 kg for HRTE (Environment Canada 2009a). The loss quantities are presented in Table 10. The following conservative assumptions were made: losses to wastewater are assumed to reach bodies of water, losses to landfills are assumed to leach into the soil and losses to recycling facilities are assumed to reach the environment (an even divide between water and soil) (Environment Canada 2010a, 2010b, 2010c, 2010d).

Table 10. Conservative estimations of losses of HR, HRPE, HRGE and HRTE at various stages of their lifecycles

	Loss quantity (kg per year)				
Type of loss	**HR**	**HRPE**	**HRGE**	**HRTE**	**Pertinent life cycle stages**
Wastewater (to water)	3900	900	24 000	540	Manufacture, industrial use, and consumer/commercial use
Landfill (to soil)	79 200	92 800	945 000	9180	Manufacture, industrial use, consumer/commercial use
Recycling (to water and soil)	14 500	2600	-	-	Manufacture, industrial use, consumer/commercial use

The estimated losses were used in ChemCAN, a Canada-specific environmental exposure model, to estimate concentrations in various environmental media (ChemCAN 2003). This model differs from the point source models used in the ecological assessment portion of this assessment, which provide estimates of exposure near release points, in that it is a regional far-field Level III fugacity model that is used to estimate average concentrations in various media to inform human exposure estimates. The PECs are presented in Table 11 and are used as surrogates for measured data in deriving intake estimates. The intake estimates for each medium, in addition to total intake for each age group, are presented in Appendices III a-d. The maximum total daily intakes are presented in Table 12 and range from 0.0029 to 0.17 µg/kg-bw per day; drinking water and soil are considered the predominant sources of estimated environmental exposure.

Table 11. Estimated concentrations of HR, HRPE, HRGE and HRTE in environmental media using ChemCAN v6.0 (ChemCAN 2003)[1]

Substance	Medium	Concentration
HR	Air[2]	0.342 ng/m^3
	Water[3]	41.4 ng/L
	Soil[3]	2179 ng/g solids
	Sediment[3]	2874 ng/g solids
HRPE	Air[2]	0.248 ng/m^3
	Water[3]	65.5 ng/L
	Soil[3]	2114 ng/g solids
	Sediment[3]	2535 ng/g solids
HRGE	Air[2]	0.238 ng/m^3
	Water[3]	1020 ng/L
	Soil[3]	16 223 ng/g solids
	Sediment[3]	18 318 ng/g solids
HRTE	Air[2]	0.180 ng/m^3
	Water[3]	17.2 ng/L
	Soil[3]	263 ng/g solids
	Sediment[3]	374 ng/g solids

[1] All modelling assumed release into the region of southern Ontario (Ontario Mixed-Wood Plain).
[2] Hydrolysis degradation half-lives were estimated using AOPWIN v1.92 (AOPWIN 2000).
[3] Due to persistence in water, soil and sediment, negligible degradation was assumed in these environmental compartments.

Table 12. Maximum upper-bounding estimates of total daily intakes of HR, HRPE, HRGE and HRTE.

Substance	Maximum total daily intake (µg/kg-bw per day)	Age group
HR	0.016	Toddler (0.5–4 yrs)
HRPE	0.017	Toddler (0.5–4 yrs)
HRGE	0.17	Formula-fed infant (0–0.5 yrs)
HRTE	0.0029	Formula-fed infant (0–0.5 yrs)

Consumer Products

Based on the physical and chemical properties of these substances, inhalation exposure is not generally expected from consumer products. In addition, based on the molecular weight and estimated log Kow of the substances, dermal absorption is also expected to be low, although no empirical dermal penetration studies were available. Empirical oral absorption data for Resin acids and Rosin acids, esters with glycerol (RGE) (CAS RN 8050-31-5) was estimated to be <5% (see section on Absorption, Distribution, Metabolism and Excretion). Exposure estimates in terms of dermal deposition were calculated below, but actual internal doses are expected to be much lower based on the properties of the substances. Material Safety Data Sheets (MSDSs) for occupational and general use products containing HR, HRPE or HRGE may include warnings for skin irritation and/or sensitization reactions as well as related first aid measures (3M Canada Company 2007, 2009; AIM 2001, 2009; Church & Dwight Co., Inc. 2008; Ciba Canada

Ltd. 2008, 2009; Henkel Canada Corporation 2010). However, there was no mention of irritation/sensitization warnings for a few of the products containing HRGE or HRPE (Bristol Myers Squibb Company 1994; 3M Canada Company 2008).

HR

In Canada, HR is present in a hot-melt adhesive available for consumers (3M Canada Company 2008). Hot-melt adhesives are solidified glues that are primarily used in glue guns for hobbyist activities such as connecting model parts or decorative flowers (RIVM 2007). Potential exposure during use of a glue gun was estimated using ConsExpo resulting in an inhalation mean event concentration and an acute dermal deposition of 0.0186 mg/m^3 and 0.141 milligrams per kilogram of body weight (mg/kg-bw) per event respectively (ConsExpo 2006) (see Appendix IV).

Hair styling products such as wax and pomade may also contain HR at a concentration of 10-30% by weight (CNS 2010). A scenario based upon hair gel in ConsExpo v4.1 resulted in a chronic dermal deposition of 1.36 mg/kg-bw per day (see Appendix IV).

HR is used as a surface treatment in pigment manufacture for a limited number of pigments (e.g., Indanthrone blue pigments) (February 2010 email from Chemical Sector Directorate, Environment Canada to Existing Substances, Risk Assessment Bureau, Health Canada; unreferenced). This treatment process may lead to the unintentional introduction of a minor amount of HR to a final manufactured product such as dry toner (2.5% by weight) or liquid paint (<0.2% by weight typically) as a residual in the pigment (Environment Canada 2009a; Ciba Canada Ltd. 2008, 2009; February 2010 email from Chemical Sector Directorate, Environment Canada to Existing Substances, Risk Assessment Bureau, Health Canada;unreferenced). This paint is used in automotive and aftermarket automotive coatings intended for industrial use (February 2010 email from Chemical Sector Directorate, Environment Canada to Existing Substances,Risk Assessment Bureau, Health Canada;unreferenced). Other uses of HR such as in solder wire and paste (AIM 2001, 2009; Henkel Canada Corporation 2010), patch sealer melt in automotive manufacturing, tackifying resin in industrial adhesives, splicing adhesives for laminating applications, powder coatings and in commercial printing and ink dispersion operations (Environment Canada 2009a) are not considered to result in significant general population exposure.

HRPE

HRPE may be present in consumer products such as cosmetics and adhesives for medical bandages (Bristol Myers Squibb Company 1994; NPSS 2009; Toedt et al. 2005). Medical adhesives containing HRPE have been documented; however, the authors did not indicate the concentrations of HRPE used in these adhesives (Pereira et al. 2007).

Cosmetics containing HRPE include mascara and lipstick. Mascara may contain up to 8% of HRPE by weight (CNS 2010; Environment Canada 2009a) and may be applied daily to the eyelash area, allowing the product to potentially touch the eyelid skin surface for dermal deposition over the course of the day (16 hr) (RIVM 2006a). An upper-bounding estimate of chronic dermal exposure to mascara of 0.0282 mg/kg-bw per day was determined. Lipsticks contain between 3–10% of HRPE by weight (CNS 2010) and maximum exposure estimates include application up to 4 times daily to the lip area and ingestion from the lip area during that period of time. An upper-bounding estimate of chronic oral exposure to lipstick was determined to be 0.0564 mg/kg-bw per day. Both the dermal and oral scenarios for mascara and lipstick are presented in Appendix IV.

Other uses of HRPE such as in manufactured automotive parts, hot melt compounded sealants for the insulating glass industry and in solder wire (Environment Canada 2009a) are not considered to result in significant general population exposure.

HRGE

Consumer products containing HRGE include adhesives for laminates, used in do-it-yourself (DIY) projects (Environment Canada 2009a) and in depilatory wax for at-home hair removal (CNS 2010; Church & Dwight Co., Inc. 2008).

Hair removal products containing resins are most likely in a hot wax, wipe-off cream-based form or hair removal strips. Those containing HRGE as an ingredient together with HRTE (each at concentrations ranging from 40-50% by weight (Church & Dwight Co., Inc. 2008) are present in depilatory waxes and pre-coated strips rather than the cream-based hair removals. However, concentrations of HRPE and HRGE were reported at 10-30% by weight in the Cosmetic Notification System database (CNS 2010). The maximum concentration identified in Church & Dwight Co., Inc. (2008) of 50% by weight was used for modeling purposes as it was the most conservative value. Despite open pores from removed hair follicles, HRGE is not expected to absorb through the skin surface as described above. Assuming dermal exposure to the surface area of both legs of an adult at a frequency of 17 events per year, acute and chronic dermal deposition of 38.8 mg/kg-bw per event and 1.8 mg/kg-bw per day were determined, respectively (Appendix IV).

Adhesives used in DIY projects for laminate materials on wood, plastic or other materials may contain HRGE at a concentration ranging between 5 and 10% by weight (Environment Canada 2009a). Assuming the use for this construction glue containing 10% of HRGE twice per year, the amount of exposure is limited (Environment Canada 2009a). However, the consumer's hand may touch the adhesive during application, either from using a finger to brush the glue on a surface or from accidental contact. An upper-bounding estimate of dermal deposition to laminate adhesive of 0.353 mg/kg-bw per event was determined. The volatility of HRGE is very low, which lends to a negligible estimate of exposure from inhalation (2.86×10^{-7} mg/m^3 mean inhalation event concentration) (Appendix IV)

Other uses of HRGE such as in industrial contact adhesives (3M Company 2010a, b; 3M Canada Company 2007, 2009), industrial tackifying resin and manufactured automotive parts (Environment Canada 2009a) are not expected to result in significant general population exposure.

HRTE

HRTE is most commonly found together with HRGE in a depilatory wax, each at a concentrations ranging from 40-50% by weight (Church & Dwight Co., Inc. 2008). Using the same scenario described for HRGE, a dermal exposure scenario for the use of HRPE in depilatory wax was conducted to give acute and chronic dermal deposition of 38.8 mg/kg-bw per event and 1.8 mg/kg-bw per day respectively (Appendix IV).

Health Effects Assessment

Appendix V contains a summary of the available health effects information for HR, HRPE, and HRGE. No toxicity data were identified for HRTE.

No classifications or in-depth reviews of the health effects of HR, HRPE, HRGE and HRTE by national or international regulatory agencies were identified. However, the U.S. EPA has included HR, HRPE and HRGE in screening-level hazard characterizations as part of an initial risk-based prioritization of high production volume chemicals (US EPA 2008a, 2008b).

The results from acute oral toxicity studies indicated that the LD_{50} values in rats for HR, HRPE, and HRGE were all greater than 2000 mg/kg-bw following a single exposure (European Commission 2000a, 2000b, 2000c, 2000d; US EPA 2008a). Measured acute inhalation non-lethal concentration (LC_0) values reported in rats ranged from greater than 0.158 mg/L (> 158 mg/m^3) for HRGE to greater than 2480 ppm (> 31 000 mg/m^3) for HR (European Commission 2000a, 2000c). No acute or repeated-dose dermal studies and no repeated-dose inhalation studies were identified. No genotoxicity or reproductive/developmental toxicity studies were available for HR, HRPE, HRGE or HRTE. Thus, the following descriptions for each compound include available repeated-dose toxicity and irritation/sensitization results.

HR

In a two-year chronic/carcinogenicity study in Sprague-Dawley rats orally exposed to HR, the only effect observed was decreased body weight at the highest dose level, 1000 mg/kg-bw per day (Kay 1962a). Decreased food consumption related decrease in mean body weight and body weight gain were also reported at 1000 mg/kg-bw per day in a 90-day study in the same strain of rats. In addition, a statistically significant increase in relative organ weights, including the liver, kidney and spleen in males and the liver in females, was observed at this dose level (Calandra 1960a, 1967).

With regards to dermal sensitization, in a maximization test where guinea pigs were challenged with HR following either intradermal or epidermal induction with the same substance, a significant positive response was observed. However, no such effect was observed using Freund's complete adjuvant test in the same species (Karlberg et al. 1988). In a patch test on human patients with a known allergy to rosin, Karlberg et al. (1988) reported a marked decrease in the frequency of allergic reactions to HR at concentrations of up to 20% compared to their reactions to rosin at the same concentrations.

HRGE

In a 28-day study in which Sprague-Dawley rats were orally exposed to HRGE in feed, reduced body weight was reported only in females at 500 mg/kg-bw per day compared to controls (food consumption was unaffected). Thus, the lowest-observed-effect level (LOEL) was determined to be 500 mg/kg-bw per day. However, in a 90-day study in Sprague-Dawley rats orally exposed to HRGE in feed, no treatment related health effects were observed at doses up to 2500 mg/kg-bw per day (US EPA 2008b).

Dermal exposure of HRGE did not induce sensitization in guinea pigs or irritation in rabbits (European Commission 2000a). In a patch test involving human subjects, test material containing 10% HRGE resulted in no evidence of skin irritation or sensitization (Johnson 2004). In a few case studies, when follow up patch tests were applied to human patients with clinical symptoms of sensitization or irritation as a result of previously used HRGE-containing consumer products, positive skin sensitization reactions to 20% HRGE in petrolatum were observed (Ota et al. 2007; Foti et al. 2006; Bonamonte et al. 2001).

HRPE

No repeated-dose toxicity studies were identified for HRPE.

Some positive reactions associated with the use of HRPE-containing wound dressings have been reported. However, the authors did not indicate the concentrations of HRPE used in the adhesive portions of the wound dressings (Pereira et al. 2007; Sasseville et al. 1997; Schliz et al. 1996).

QSAR/SAR Model Results and Analogue Data

The outputs of predictive (Q)SAR models (DEREK 2008, TOPKAT 2004, CASETOX 2008 and Leadscope Model Applier 2009) on the major representative chemical structures of HR, HRPE, HRGE and HRTE were limited and gave results that were mainly negative, inconclusive, or out of the domain of applicability for the model. One SAR model, DEREK, had an alert for "plausible" peroxisome proliferation in rodents (mouse and rat) for HR, HRPE, HRGE and HRTE.

As only limited data were available with respect to the toxicity of HR, HRPE, HRGE and HRTE, and (Q)SAR model results were very limited, relevant information on potential analogues of these substances was also considered and information is summarized in Appendix VI.

Data on three analogue substances (Appendix VI) were examined to better inform the understanding of the potential health effects associated with exposure to HR, HRPE, HRGE and HRTE. Rosin (CAS RN 8050-09-7), Resin acids and Rosin acids, esters with pentaerythritol (RPE) (CAS RN 8050-26-8) and Resin acids and Rosin acids, esters with glycerol (RGE) (CAS RN 8050-31-5) were chosen as analogues for the health effects assessment based on their structural similarity and availability of toxicity studies.

Rosin (CAS RN 8050-09-7)

In a combined oral reproductive/developmental toxicity study using Rosin, no treatment-related effects on mating performance, fertility or duration of gestation were observed in Sprague-Dawley rats at doses up to 825 mg/kg-bw per day. No obvious external abnormalities were noted in the pups at any dose level. Testes and epididymides weights were similar in all groups. Litter survival, as indicated by the birth index and viability index, was similar in all groups. The reproductive/developmental effect reported was the reduction in the litter size and fetal weight as the result of reduced food intake in dams at 825 mg/kg-bw per day (Clubb and Sutherland 2002).

Similarly to that reported for HR above, in a two-year chronic/carcinogenicity study, no significant differences were observed between treated groups and controls with respect to tumour rate, haematology, urinalysis, or gross or microscopic pathology in Sprague-Dawley rats orally exposed to Rosin up to 1000 mg/kg-bw per day (US EPA 2008a). Increased relative liver weight and decreased mean body weight gain associated with a decrease in food consumption, were observed at the high dose level (1000 mg/kg-bw per day) (US EPA 2008a; Kay 1962b). Similar results were obtained in 90-day oral toxicity studies with rosin (Calandra 1960b) and HR in the same strain of rat (US EPA 2008a).

Rosin is classified by the European Union as a skin sensitizer (R43; May cause sensitisation by skin contact) (ESIS 2009). Positive sensitization reactions in human subjects were reported in patch tests with Rosin in Germany and Sweden (European Commission 2000e). Colophony (Rosin) is well recognized as a skin sensitizer and is also the third-highest cause of occupational asthma. However, the specific allergens involved particularly in occupational asthma have not been comprehensively assessed or identified (Sadhra et al. 1994)

Resin acids and Rosin acids, esters with glycerol (RGE) (CAS RN 8050-31-5)

In a 90-day study, no treatment-related effects were observed in Fischer 344 rats orally dosed up to 2500 mg/kg-bw per day of RGE (Blair 1991). However, in a 90-day study in Sprague-Dawley rats, dose-related, statistically significant increases in absolute and

relative liver weights were observed at oral doses of 1000 and 5000 mg/kg-bw per day of RGE (Mann et al.1982).

RGE was not mutagenic in the Ames test with *Salmonella typhimurium* (Jagannath 1988; Ishidate et al. 1984). Additionally, no evidence of unscheduled DNA synthesis in mammalian cells (Cifone 1988) or chromosome aberration in ovary and fibroblast cells of Chinese hamsters was observed when tested with RGE (Murli 1988; Ishidate et al. 1984).

Slight skin irritation but no eye irritation was reported with RGE when tested in rabbits. However, no dermal sensitization was found with a RGE containing product when tested in humans (no study details provided) (European Commission 2000d; Johnson 2004).

Resin acids and Rosin acids, esters with pentaerythritol (RPE) (CAS RN 8050-26-8)

In a combined oral reproductive/developmental toxicity study on RPE, no treatment related effects on mating performance, fertility or duration of gestation were observed in Sprague-Dawley rats at doses up to 1900 mg/kg-bw per day (US EPA 2008b). Additional endpoint results reported in this study were similar to those observed for Rosin (Clubb and Sutherland 2002). The NOEL for systemic and reproductive/developmental effects for RPE was greater than 1900 mg/kg-bw per day (the highest dose tested) (US EPA 2008b)

The results observed in a two-year oral rat study on RPE were similar to the results reported in two-year oral studies on HR and Rosin in rats. No obvious treatment related health effects were observed in Sprague-Dawley rats at a dose of 50 mg/kg-bw per day with respect to tumour rate, haematology, urinalysis, or gross or microscopic pathology (Kay 1962c). Similar to the results obtained in 90-day studies for HR, Rosin and RGE, significantly increased absolute and relative liver weights were also observed at the high dose (2500 mg/kg-bw per day) in a 90-day study for RPE (Calandra 1960c).

In a single-insult occlusive patch test with RPE, minimal to moderate skin irritations were observed in rabbits. However, no sign of allergic skin sensitization was detected in a maximization test in guinea pigs. RPE-induced ocular irritations were also reported in rabbits by Andersen (1998), who also showed that formulations containing 7-9.6% of RPE did not induce sensitization reactions or dermal irritations in humans in repeated-insult patch tests.

Absorption, Distribution, Metabolism and Excretion

Absorption, distribution, metabolism and excretion studies were not identified for HR, HRPE, HRGE or HRTE. Limited information on the analogue, RGE, indicated that it is very stable in the gastrointestinal tract of rats and only a minor fraction, most probably the mono-glycerol ester fraction, will undergo partial hydrolysis. Less than 1% of the dietary administered RGE was excreted either as expired carbon dioxide or in urine and most of the dose (> 95%) had been recovered in faeces (WHO 1996). Therefore, less than 5% of RGE appears to be absorbed across the gastrointestinal tract of rats. This may

explain the high LOELs observed in repeated-dose studies in rats with RGE. Due to the high LOELs observed in repeated-dose studies in rats with HRGE and HR, similar to those observed for RGE, it is expected that HRGE and HR also exhibit low absorption across the gastrointestinal tract of rats.

Confidence in Toxicity Database

The confidence in the toxicity database of HR, HRPE, HRGE and HRTE is considered to be low to moderate as limited empirical data were identified. However, analogues with additional toxicity data provided results similar to those observed for HR, HRPE, HRGE and HRTE and can be used for read-across for gaps in the database.

Characterization of Risk to Human Health

Limited chronic studies for HR and selected analogues indicated no evidence of carcinogenicity in experimental animals and limited toxicological effects at 1000 mg/kg bw/day and higher. In addition, no genotoxicity studies were identified for HR, HRPE, HRGE or HRTE. The outputs of predictive (Q)SAR models for genotoxicity for HR, HRPE, HRGE and HRTE were mainly negative, inconclusive, or out of the domain of applicability. Limited *in vitro* genotoxicity data for the analogue, RGE was not suggestive of mutagenicity; however *in vivo* genotoxicity data were not identified. No reproductive/developmental toxicity studies were available for HR or its esters (HRPE, HRGE and HRTE). For the analogues, Rosin and RPE, no obvious exposure related effects were reported in adult rats or pups in combined reproductive/developmental toxicity studies. In terms of repeated-dose toxicity studies for HR, HRGE and the selected analogues, the LOEL was 500 mg/kg-bw per day based on treatment related decreased body weights in female rats in a 28-day oral study with HRGE.

The potential for exposure of the general population to HR, HRPE, HRGE and HRTE from environmental media is expected to be low. A comparison between the critical effect level for repeated dose oral exposure (500 mg/kg-bw per day) and the highest estimated maximum total daily intake from all routes of environmental exposures (0.17 µg/kg-bw/day), based on data for HRGE, results in a margin of exposure (MOE) of approximately 2 900 000. This margin is considered adequate to address uncertainties in the health effects and exposure databases.

Regarding consumer products, there is potential for low levels of daily oral and dermal exposure to HRPE from lipstick and potential for dermal exposure to HRPE from use of mascara and to HRGE and HRTE from per event consumer products (e.g., depilatory wax). Dermal exposure to HRGE and HR from occasional use (water-based adhesive, hot-melt adhesive) consumer products is expected to be low due to infrequent use. Exposure by inhalation is considered to be negligible due to the low vapour pressure of these compounds. Acute dermal deposition estimates ranged from 0.14 to 39 mg/kg-bw/day while chronic dermal deposition estimates ranged from 0.03 to 1.8 mg/kg-bw/day. Oral chronic exposure from lipstick was estimated to be

0.06 mg/kg-bw/day. These exposure estimates are several orders of magnitude lower than oral effect levels observed in experimental animals and taken together with expected low dermal absorption are not considered to be of concern for human health.

Although mixed results were obtained in sensitization and irritation studies in animals and humans, positive sensitization reactions related to the use of HRGE and HRPE containing consumer products were reported in several cases. In some cases, the authors attributed the presence of unmodified rosin residue in the consumer products to the positive sensitization reaction. In addition, allergenicity of rosin, a recognized skin sensitizer, was considerably reduced by hydrogenation according to Karlberg et al. (1988). Positive reactions appear to be associated with consumer products containing concentrations of ≥ 20% HRGE or HRPE. However, there is evidence to indicate that HR may be a possible skin sensitizer at lower concentrations. Consumer use of products containing these substances is expected to be low. For products that fall under the Controlled Products Regulations of the Hazardous Products Act, potential health effects, including sensitization, would be identified on the Material Safety Data Sheet.

Uncertainties in Evaluation of Risk to Human Health

Confidence in the environmental exposure estimates for HR, HRPE, HRGE and HRTE are low. Data in the literature were not identified for concentrations of these substances in environmental media. However, quantities in commerce for the 2006 calendar year are known, and were combined with estimated loss percentages from the Mass Flow Tool to model environmental concentrations. As the maximum values of the quantity in commerce ranges were used in the modelling, it is likely that the modeled results are conservative estimates of environmental exposure. Confidence in the consumer product exposure estimates is moderate. While exposure scenarios were readily available in ConsExpo v4.1 for the consumer products identified from literature searches, the Health Canada Cosmetic Notification System database and responses to a notice issued under section 71 of CEPA 1999, the lack of experimental physical and chemical properties as inputs for modeling detracts from the confidence in the exposure estimates.

Although structural similarity and hazard profiles provide confidence in the use of analogues (Rosin, RGE and RPE), there are uncertainties related to whether the read-across data accurately reflect the hazard of HR and its esterified derivatives, HRPE, HRGE and HRTE.

Conclusion

Based on their physical and chemical properties, on HR, HRPE and HRGE experimental biodegradation data, on analogue biodegradation data for HRTE, and on predicted data, HR, HRPE, HRGE and HRTE are expected to biodegrade slowly in the environment. In addition, new experimental data relating to bioconcentration of components of HR along with predicted bioaccumulation potential of additional components suggest that HR has a low potential to accumulate in the lipid tissues of organisms. The lower molecular weight components of HRPE, HRGE and HRTE do not show a high predicted bioaccumulation potential based on several predicted results, suggesting that metabolism will mitigate bioaccumulation potential. It has been predicted that the larger, higher molecular weight components of HRPE, HRGE and HRTE would have limited bioavailability such that significant bioaccumulation would not be expected. Thus, HR, HRPE, HRGE and HRTE do meet the persistence criterion but do not meet the bioaccumulation criterion as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Experimental toxicity data for a chemical analogue UVCB substance of HRPE and HRGE suggest that these substances would not cause acute harm to aquatic organisms including fish, daphnids and algae test species, at concentrations tested well above the solubility limits of these substances.

Experimental toxicity data for a chemical analogue UVCB substance of HR indicates that saturated solutions of the substance do not cause acute harm to test fish and algae species. However, effects were seen at the highest concentration tested for daphnids. Thus, component-based toxicity was used to determine a conservative PNEC for HR. For HR, a realistic worst-case exposure scenario was applied in which two industrial operations discharge HR into the aquatic environment. The PEC in water was many orders of magnitude below the PNECs calculated for HR.

As no suitable chemical analogue was found for HRTE, predicted component-based toxicity values were used to determine a conservative PNEC value. Then, a conservative exposure scenario was selected in which an industrial operation discharges HRTE into the aquatic environment. The PEC in water was similarly many orders of magnitude below the conservative PNECs calculated for HRTE.

Based on the information available, it is concluded that HR, HRPE, HRGE and HRTE are not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity or that constitute or may constitute a danger to the environment on which life depends.

No empirical data were identified for concentrations of these compounds in environmental media. The potential for exposure of the general population to HR, HRPE, HRGE and HRTE from environmental media is expected to be low. In addition, there is potential for low levels of exposure from the use of a limited number of consumer

products which may include lipstick, mascara, hair styling and hair removal products and consumer adhesives. Based on the physical-chemical properties of the substances, inhalation exposure is not expected from these products; however, there is potential for low levels of dermal or oral (lipstick) exposure. The health effects database for HR, HRPE, HRGE and HRTE is limited. Chronic studies for HR and selected analogues indicated no evidence of carcinogenicity in experimental animals and the available data does not indicate genotoxic potential. Positive skin sensitization reactions appear to be associated with consumer products containing concentrations of ≥ 20% HRGE or HRPE, and possibly HRTE. However, there is evidence to indicate that HR may be a possible skin sensitizer at lower concentrations. Consumer use of products containing these substances is expected to be low.

Based on comparison of the upper-bounding estimates of exposure via environmental media or consumer products for HR, HRPE, HRGE or HRTE with the oral critical effect levels observed in studies with one or more of these compounds or related analogues, a concern for human health was not identified.

Based on the information available, it is concluded that HR, HRPE, HRGE and HRTE are not entering the environment in a quantity or concentration or under conditions that constitute a danger in Canada to human life or health.

It is therefore concluded that HR, HRGE, HRPE and HRTE do not meet any of the criteria under section 64 of CEPA 1999.

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Appendix I - Robust Study Summary

Robust Study Summaries: Aquatic iT				
No	**Item**	**Weight**	**Yes/No**	**Specify**
1	Reference: Solubility and Toxicity of Resin Acids, G. Peng and J.C. Roberts, 2000, Water Research, Vol. 4, No. 10, pp. 2779-2785.			
2	Substance identity: CAS RN	n/a	N	
3	Substance identity: chemical name(s)	n/a	Y	
4	Chemical composition of the substance	2	Y	
5	Chemical purity	1	Y	Study evaluated the concentration of resin acids in standard solutions using GC-FID
6	Persistence/stability of test substance in aquatic solution reported?	1	Y	Solubility over 72 hrs was monitored by GC-FID
Method				
7	Reference	1	Y	ISO 6341 and British standard BS 6068
8	OECD, EU, national, or other standard method?	3	Y	
9	Justification of the method/protocol if not a standard method was used	2	n/a	
10	GLP (Good Laboratory Practice)	3	N	
Test organism				
11	Organism identity: name	n/a	Y	*D. Magna*
12	Latin or both Latin & common names reported?	1	Y	
13	Life cycle age / stage of test organism	1	Y	Less than 24 hours old
14	Length and/or weight	1	n/a	
15	Sex	1	n/a	
16	Number of organisms per replicate	1	Y	Five
17	Organism loading rate	1	N	
18	Food type and feeding periods during the acclimation period	1	N	
Test design / conditions				
19	Test type (acute or chronic)	n/a	Y	Acute
20	Experiment type (laboratory or field)	n/a	Y	Laboratory
21	Exposure pathways (food, water, both)	n/a	Y	Water
22	Exposure duration	n/a	Y	24 hours
23	Negative or positive controls (specify)	1	Y	Negative + dose response

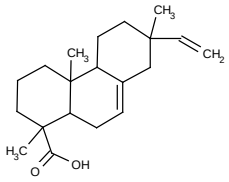
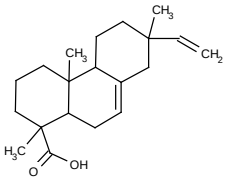
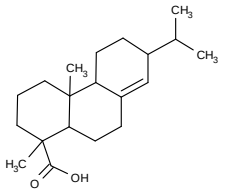
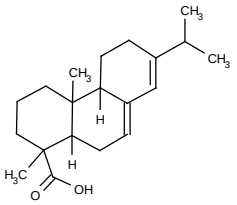
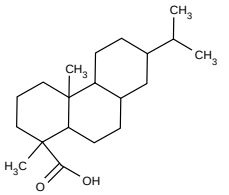
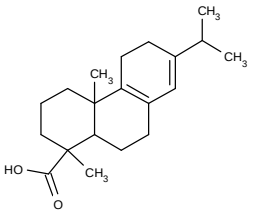
24	Number of replicates (including controls)	1	Y	Six
25	Nominal concentrations reported?	1	N	
26	Measured concentrations reported?	3	N	
27	Food type and feeding periods during the long-term tests	1	n/a	
28	Were concentrations measured periodically (especially in the chronic test)?	1	N	
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	
30	Photoperiod and light intensity	1	N	
31	Stock and test solution preparation	1	Y	
32	Was solubilizer/emulsifier used, if the chemical was poorly soluble or unstable?	1	N	
33	If solubilizer/emulsifier was used, was its concentration reported?	1	n/a	
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	1	n/a	
35	Monitoring intervals (including observations and water quality parameters) reported?	1	N	
36	Statistical methods used	1	N	
Information relevant to the data quality				
37	Was the endpoint directly caused by the chemical's toxicity, not by organism's health (e.g. when mortality in the control >10%) or physical effects (e.g. 'shading effect')?	n/a	Y	
38	Was the test organism relevant to the Canadian environment?	3	Y	
39	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
40	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2	Y	
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	Y	
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	

43	Was toxicity value below the chemical's water solubility?	3	Y	
	Results			
44	Toxicity values (specify endpoint and value)	n/a	n/a	
45	Other endpoints reported - e.g. BCF/BAF, LOEC/NOEC (specify)?	n/a	N	
46	Other adverse effects (e.g. carcinogenicity, mutagenicity) reported?	n/a	N	
47	***Score*: ... %**			***66.7***
48	***EC Reliability code*:**			***2***
49	***Reliability category (high, satisfactory, low)*:**			***Satisfactory Confidence***

Appendix IIa – Analogue Comparison of HR with Rosin for Ecological Hazard Estimation.

An analogue approach to estimate ecological hazard for HR was performed using Rosin (Chemical Abstracts Service Registry Number 8050-09-7) due to a lack of empirical data for HR. The analogue Rosin had a measured log D of 1.9 – 7.7 (pH = 2) and water solubility of 0.95 mg/L, which compared well to that of HR (log D of 2.5-7.6 and water solubility of 1.18 mg/L) (USEPA 2008a). In addition, a comparison of structural features, molecular weight and size is presented in the Table below. Overall, the bioavailability values of components in HR and Rosin are expected to be similar, thus making Rosin a good analogue for HR in this assessment.

Analogue comparison table for HR vs. Rosin.

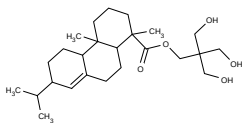
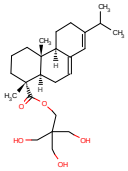
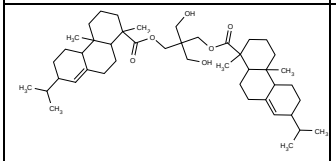
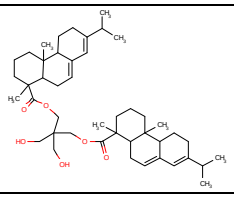
HR (CAS RN 65997-06-0)		**Rosin (CAS RN 8050-09-7)**	
Log D (pH =2)	2.5-7.6	Log D (pH =2)	1.9-7.7
Water solubility (mg/L)	1.18	Water solubility (mg/L)	0.95
Representative structures	mw* (g/mol) / size (nm)	Representative structures	mw (g/mol) / size (nm)
	302.5 / 1.15-1.43		302.5 / 1.15-1.43
	304.5 / 1.25-1.44		302.5 / 1.31-1.46
	306.5 / 1.23-1.44		302.5 / 1.29-1.46

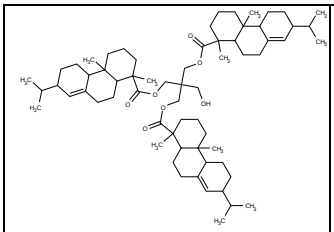
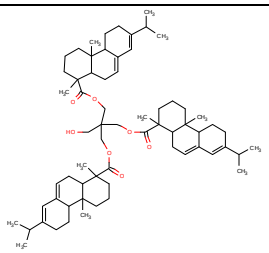
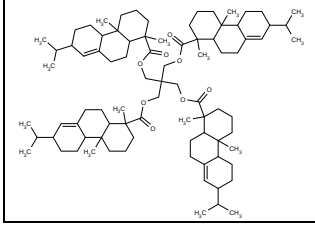
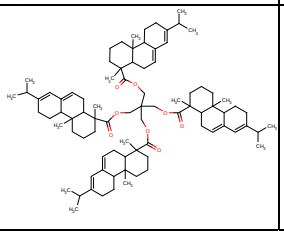
* molecular weight

Appendix IIb – Analogue Comparison of HRPE and HRGE with RPE for Ecological Hazard Estimation.

An analogue approach to estimate ecological hazard for HRPE and HRGE was performed using Resin acids and Rosin acids, esters with pentaerythritol (RPE; Chemical Abstracts Service Registry Number 8050-26-8) due to lack of empirical data for HRPE and HRGE. The analogue RPE had a measured log K_{ow} of 3.5-7.1 and water solubility of 0.38 mg/L, which compared reasonably well to that measured for HRPE and HRGE of log K_{ow} 4.6-7.3 and 4.7-5.8 and water solubility of <0.22 mg/L and 0.15 mg/L (USEPA 2008b). In addition, a comparison of structural features, molecular weight and size is presented in the analogue comparison tables. Overall, the bioavailability of components in RPE and HRPE are expected to be similar, thus making RPE a good analogue for HRPE in this assessment work. Also, the bioavailability of components in RPE and HRGE may be similar enough for the analogue approach. Both RPE and HRGE are thought to be enriched in triester components of molecular weight 951.5 g/mol (1.98-2.72) and 988.7 g/mol (2.05-2.86) and thus, serve as close analogues to be used for the purposes of this assessment. Monoester components (<500 g/mol) which would be more bioavailable than the larger components also, show similarity between RPE (analogue) and HRGE, thus further supporting the notion that both substances would have a similar bioavailability. Finally, RPE would also contain a significant amount of tetraester (>1000 g/mol) which would not be present in the HRGE. However, it is not expected that that the overall bioavailability of the RPE substance would be influenced due to the larger molecular weight and size of this component.

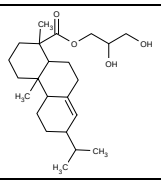
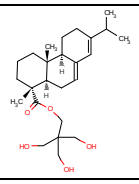
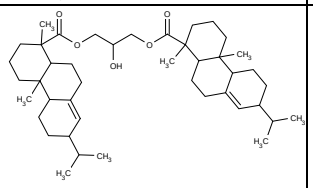
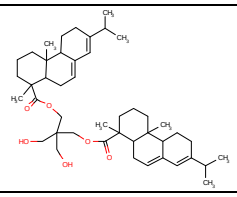
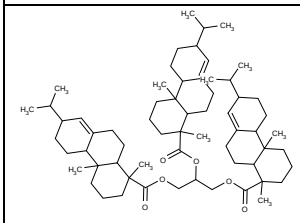
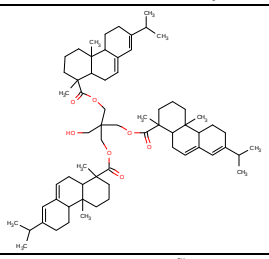
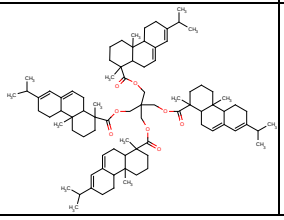
Analogue comparaison table for HRPE vs RPE

HRPE (CAS RN 64365-17-9)		**RPE (CAS RN 8050-26-8)**	
Log K_{ow}	4.6-7.3	Log K_{ow}	3.5-7.1
Water solubility (mg/L)	<0.22	Water solubility (mg/L)	0.38
Representatives structures	mw* (g/mol) / size (nm)	Representative structures	mw (g/mol) / size (nm)
	422.6 / 1.36-1.84		420.3 / 1.30-1.90
	709.1 / 1.74-3.04		704.5 / 1.73-3.01

	995.5 / 2.09-2.94		988.7 / 2.05-2.86
	1282 / 2.28-2.88		1273 / 2.21-3.03

* molecular weight

Analogue comparaison table for HRGE vs RPE

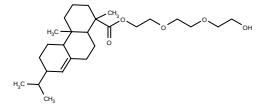
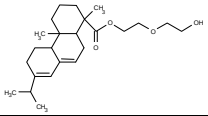
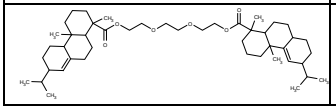
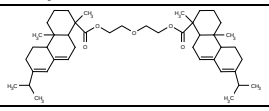
HRGE (CAS RN 65997-13-9)		**RPE (CAS RN 8050-26-8)**	
Log K_{ow}	4.7-5.8	Log K_{ow}	3.5-7.1
Water solubility (mg/L)	0.15	Water solubility (mg/L)	0.38
Representatives structures	mw* (g/mol) / size (nm)	Representative structures	mw (g/mol) / size (nm)
	378.6 / 1.27-1.90		420.3 / 1.30-1.90
	665.0 / 1.59-3.05		704.5 / 1.73-3.01
	951.5 / 1.98-2.72		988.7 / 2.05-2.86
-	-		1273 / 2.21-3.03

* molecular weight

Appendix IIc – Analogue Comparison of HRTE with RDE for Persistence Estimation

An analogue approach to estimate environmental persistence for HRTE was performed using Resin acids and Rosin acids, esters with diethylene glycol (RDE; Chemical Abstracts Service Registry Number 68153-38-8) due to lack of empirical data on the persistence of HRTE. The analogue RDE had a measured log K_{ow} of 4.0-5.8 and water solubility of <2.38 mg/L, which were some what similar to the values predicted for representatives structures of HRTE , that is log K_{ow} >5.31 and water solubility of <0.62 mg/L. In addition, a comparison of structural features and molecular weight is presented in the table below.

Analogue comparison table for HRTE vs. RDE

HRTE (CAS RN 68648-53-3)		**RDE (CAS RN 68153-38-8)**	
Log K_{ow}	≥5.31	Log K_{ow}	4.0-5.8
Water solubility (mg/L)	<0.62**	Water solubility (mg/L)	<2.38
Representatives structures	mw*(g/mol) /	Representative structures	mw (g/mol) / size (nm)
	436.6		390.4
	723.1		648.8

*molecular weight
**based on modelled data taken from Table 2d.

Appendix IIIa. Upper-Bounding Estimates of Daily Intakes of HR for Various Age Groups

Route of exposure	Estimated intake (µg/kg-bw per day) of HR by various age groups							
	0–0.5 years[1,2,3]			0.5–4 years[4]	5–11 years[5]	12–19 years[6]	20–59 years[7]	60+ years[8]
	Breast milk fed	Formula fed	Not formula fed					
Air[9]	9.6×10^{-5}	9.6×10^{-5}	9.6×10^{-5}	2.0×10^{-4}	1.6×10^{-4}	9.1×10^{-5}	7.8×10^{-5}	6.8×10^{-5}
Drinking water[10]	N/A	4.4×10^{-3}	1.6×10^{-3}	1.9×10^{-3}	1.5×10^{-3}	8.4×10^{-4}	8.8×10^{-4}	9.2×10^{-4}
Food and beverages[11]	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Soil[12]	8.7×10^{-3}	8.7×10^{-3}	8.7×10^{-3}	1.4×10^{-2}	4.6×10^{-3}	1.1×10^{-3}	9.2×10^{-4}	9.1×10^{-4}
Total intake	8.8×10^{-3}	1.3×10^{-2}	1.0×10^{-2}	1.6×10^{-2}	6.3×10^{-3}	2.0×10^{-3}	1.9×10^{-3}	1.9×10^{-3}
Maximum total intake from all routes of exposure: 1.6×10^{-2} µg/kg-bw per day								

N/A, not available

[1] No quantitative data were identified for concentrations of HR in breast milk.

[2] Assumed to weigh 7.5 kg, to breathe 2.1 m^3 of air per day, to drink 0.8 L of water per day (formula fed) or 0.3 L/day (not formula fed) and to ingest 30 mg of soil per day (Health Canada 1998).

[3] For exclusively formula-fed infants, intake from water is synonymous with intake from food. No quantitative data on concentrations of HR in drinking water or formula were identified for Canada. The concentration of HR in drinking water was estimated using ChemCAN v6.00 at 41.4 ng/L (ChemCAN 2003). For non-formula-fed infants, approximately 50% are introduced to solid foods by four months of age and 90% by six months of age (NHW 1990).

[4] Assumed to weigh 15.5 kg, to breathe 9.3 m^3 of air per day, to drink 0.7 L of water per day and to ingest 100 mg of soil per day (Health Canada 1998).

[5] Assumed to weigh 31.0 kg, to breathe 14.5 m^3 of air per day, to drink 1.1 L of water per day and to ingest 65 mg of soil per day (Health Canada 1998).

[6] Assumed to weigh 59.4 kg, to breathe 15.8 m^3 of air per day, to drink 1.2 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[7] Assumed to weigh 70.9 kg, to breathe 16.2 m^3 of air per day, to drink 1.5 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[8] Assumed to weigh 72.0 kg, to breathe 14.3 m^3 of air per day, to drink 1.6 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[9] No quantitative data were identified for concentrations of HR in air. The concentration of HR in air was estimated using ChemCAN v6.00 at 0.342 ng/m^3 (ChemCAN 2003).

[10] No quantitative data were identified for concentrations of HR in drinking water. The concentration of HR in drinking water was estimated using ChemCAN v6.00 at 41.4 ng/L (ChemCAN 2003).

[11] No quantitative data were identified for concentrations of HR in food or beverages.

[12] No quantitative data were identified for concentrations of HR in soil. The concentration of HR in soil was estimated using ChemCAN v6.00 at 2179 ng/g solids (ChemCAN 2003).

Appendix IIIb. Upper-Bounding Estimates of Daily Intakes of HRPE for Various Age Groups

Route of exposure	Estimated intake (µg/kg-bw per day) of HRPE by various age groups							
	0–0.5 years[1,2,3]			0.5–4 years[4]	5–11 years[5]	12–19 years[6]	20–59 years[7]	60+ years[8]
	Breast milk fed	Formula fed	Not formula fed					
Air[9]	6.9×10^{-5}	6.9×10^{-5}	6.9×10^{-5}	1.5×10^{-4}	1.2×10^{-4}	6.6×10^{-5}	5.7×10^{-5}	4.9×10^{-5}
Drinking water[10]	N/A	7.0×10^{-3}	2.6×10^{-3}	3.0×10^{-3}	2.3×10^{-3}	1.3×10^{-3}	1.4×10^{-3}	1.4×10^{-3}
Food and beverages[11]	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Soil[12]	8.4×10^{-3}	8.4×10^{-3}	8.4×10^{-3}	1.4×10^{-2}	4.4×10^{-3}	1.1×10^{-3}	8.9×10^{-4}	8.8×10^{-4}
Total intake	8.5×10^{-3}	1.5×10^{-2}	1.1×10^{-2}	1.7×10^{-2}	6.8×10^{-3}	2.5×10^{-3}	2.3×10^{-3}	9.4×10^{-4}
Maximum total intake from all routes of exposure: 1.7×10^{-2} µg/kg-bw per day								

N/A, not available

[1] No quantitative data were identified for concentrations of HRPE in breast milk.

[2] Assumed to weigh 7.5 kg, to breathe 2.1 m^3 of air per day, to drink 0.8 L of water per day (formula fed) or 0.3 L/day (not formula fed) and to ingest 30 mg of soil per day (Health Canada 1998).

[3] For exclusively formula-fed infants, intake from water is synonymous with intake from food. No quantitative data on concentrations of HR in drinking water or formula were identified for Canada. The concentration of HRPE in drinking water was estimated using ChemCAN v6.00 at 65.5 ng/L (ChemCAN 2003). For non-formula-fed infants, approximately 50% are introduced to solid foods by four months of age and 90% by six months of age (NHW 1990).

[4] Assumed to weigh 15.5 kg, to breathe 9.3 m^3 of air per day, to drink 0.7 L of water per day and to ingest 100 mg of soil per day (Health Canada 1998).

[5] Assumed to weigh 31.0 kg, to breathe 14.5 m^3 of air per day, to drink 1.1 L of water per day and to ingest 65 mg of soil per day (Health Canada 1998).

[6] Assumed to weigh 59.4 kg, to breathe 15.8 m^3 of air per day, to drink 1.2 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[7] Assumed to weigh 70.9 kg, to breathe 16.2 m^3 of air per day, to drink 1.5 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[8] Assumed to weigh 72.0 kg, to breathe 14.3 m^3 of air per day, to drink 1.6 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[9] No quantitative data were identified for concentrations of HRPE in air. The concentration of HRPE in air was estimated using ChemCAN v6.00 at 0.248 ng/m^3 (ChemCAN 2003).

[10] No quantitative data were identified for concentrations of HRPE in drinking water. The concentration of HRPE in drinking water was estimated using ChemCAN v6.00 at 65.5 ng/L (ChemCAN 2003).

[11] No quantitative data were identified for concentrations of HRPE in food or beverages.

[12] No quantitative data were identified for concentrations of HRPE soil. The concentration of HRPE in soil was estimated using ChemCAN v6.00 at 2114 ng/g solids (ChemCAN 2003).

Appendix IIIc. Upper-Bounding Estimates of Daily Intakes of HRGE for Various Age Groups.

Route of exposure	Estimated intake (µg/kg-bw per day) of HRGE by various age groups							
	0–0.5 years[1,2,3]			0.5–4 years[4]	5–11 years[5]	12–19 years[6]	20–59 years[7]	60+ years[8]
	Breast milk fed	Formula fed	Not formula fed					
Air[9]	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Drinking water[10]	N/A	0.11	0.04	0.05	0.04	0.02	0.02	0.02
Food and beverages[11]	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Soil[12]	0.06	0.06	0.06	0.10	0.03	0.01	0.01	0.01
Total intake	0.06	0.17	0.11	0.15	0.07	0.03	0.03	0.03
Maximum total intake from all routes of exposure: 0.17 µg/kg-bw per day								

N/A, not available

[1] No quantitative data were identified for concentrations of HRGE in breast milk.

[2] Assumed to weigh 7.5 kg, to breathe 2.1 m^3 of air per day, to drink 0.8 L of water per day (formula fed) or 0.3 L/day (not formula fed) and to ingest 30 mg of soil per day (Health Canada 1998).

[3] For exclusively formula-fed infants, intake from water is synonymous with intake from food. No quantitative data on concentrations of HRGE in drinking water or formula were identified for Canada. The concentration of HRGE in drinking water was estimated using ChemCAN v6.00 at 1.020 µg/L (ChemCAN 2003). For non-formula-fed infants, approximately 50% are introduced to solid foods by four months of age and 90% by six months of age (NHW 1990).

[4] Assumed to weigh 15.5 kg, to breathe 9.3 m^3 of air per day, to drink 0.7 L of water per day and to ingest 100 mg of soil per day (Health Canada 1998).

[5] Assumed to weigh 31.0 kg, to breathe 14.5 m^3 of air per day, to drink 1.1 L of water per day and to ingest 65 mg of soil per day (Health Canada 1998).

[6] Assumed to weigh 59.4 kg, to breathe 15.8 m^3 of air per day, to drink 1.2 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[7] Assumed to weigh 70.9 kg, to breathe 16.2 m^3 of air per day, to drink 1.5 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[8] Assumed to weigh 72.0 kg, to breathe 14.3 m^3 of air per day, to drink 1.6 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[9] No quantitative data were identified for concentrations of HRGE in air. The concentration of HRGE in air was estimated using ChemCAN v6.00 at 0.238 ng/m^3 (ChemCAN 2003).

[10] No quantitative data were identified for concentrations of HRGE in drinking water. The concentration of HRGE in drinking water was estimated using ChemCAN v6.00 at 1.02 µg/L (ChemCAN 2003).

[11] No quantitative data were identified for concentrations of HRGE in food or beverages.

[12] No quantitative data were identified for concentrations of HRGE in soil. The concentration of HRGE in soil was estimated using ChemCAN v6.00 at 16.223 µg/g solids (ChemCAN 2003).

Appendix IIId. Upper-Bounding Estimates of Daily Intakes of HRTE for Various Age Groups

Route of exposure	Estimated intake (µg/kg-bw per day) of HRTE by various age groups							
	0–0.5 years[1,2,3]			0.5–4 years[4]	5–11 years[5]	12–19 years[6]	20–59 years[7]	60+ years[8]
	Breast milk fed	Formula fed	Not formula fed					
Air[9]	5.0×10^{-5}	5.0×10^{-5}	5.0×10^{-5}	1.1×10^{-4}	8.4×10^{-5}	4.8×10^{-5}	4.1×10^{-5}	3.6×10^{-5}
Drinking water[10]	N/A	1.8×10^{-3}	6.9×10^{-4}	7.8×10^{-4}	6.1×10^{-4}	3.5×10^{-4}	3.6×10^{-4}	3.8×10^{-4}
Food and beverages[11]	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Soil[12]	1.0×10^{-3}	1.0×10^{-3}	1.0×10^{-3}	1.7×10^{-3}	5.5×10^{-4}	1.3×10^{-4}	1.1×10^{-4}	1.1×10^{-4}
Total intake	1.1×10^{-3}	2.9×10^{-3}	1.8×10^{-3}	2.6×10^{-3}	1.2×10^{-3}	5.3×10^{-4}	5.1×10^{-4}	5.3×10^{-4}
Maximum total intake from all routes of exposure: 2.9×10^{-3} µg/kg-bw per day								

N/A, not available

[1] No quantitative data were identified for concentrations of HRTE in breast milk.

[2] Assumed to weigh 7.5 kg, to breathe 2.1 m^3 of air per day, to drink 0.8 L of water per day (formula fed) or 0.3 L/day (not formula fed) and to ingest 30 mg of soil per day (Health Canada 1998).

[3] For exclusively formula-fed infants, intake from water is synonymous with intake from food. No quantitative data on concentrations of HRTE in drinking water or formula were identified for Canada. The concentration of HRTE in water was estimated using ChemCAN v6.00 at 17.2 ng/L (ChemCAN 2003). For non-formula-fed infants, approximately 50% are introduced to solid foods by four months of age and 90% by six months of age (NHW 1990).

[4] Assumed to weigh 15.5 kg, to breathe 9.3 m^3 of air per day, to drink 0.7 L of water per day and to ingest 100 mg of soil per day (Health Canada 1998).

[5] Assumed to weigh 31.0 kg, to breathe 14.5 m^3 of air per day, to drink 1.1 L of water per day and to ingest 65 mg of soil per day (Health Canada 1998).

[6] Assumed to weigh 59.4 kg, to breathe 15.8 m^3 of air per day, to drink 1.2 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[7] Assumed to weigh 70.9 kg, to breathe 16.2 m^3 of air per day, to drink 1.5 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[8] Assumed to weigh 72.0 kg, to breathe 14.3 m^3 of air per day, to drink 1.6 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[9] No quantitative data were identified for concentrations of nitromethane in air. The concentration of HRTE in air was estimated using ChemCAN v6.00 at 0.180 ng/m^3 (ChemCAN 2003).

[10] No quantitative data were identified for concentrations of HRTE in drinking water. The concentration of HRTE in water was estimated using ChemCAN v6.00 at 17.2 ng/L (ChemCAN 2003).

[11] No quantitative data were identified for concentrations of HRTE in food or beverages.

[12] No quantitative data were identified for concentrations of HRTE in soil. The concentration of HRTE in soil was estimated using ChemCAN v6.00 at 263 ng/g solids (ChemCAN 2003).

Appendix IV: Upper-Bounding Exposure Estimates for HR, HRPE, HRGE and HRTE for Consumer Product Scenarios using ConsExpo v4.1 (ConsExpo 2006)

Substance	Consumer product	Assumptions[1]	Exposure estimate
HRGE & HRTE	Depilatory wax (used to remove hair)	Common assumptions: - frequency of use: 17/yr (RIVM 2006a) - product amount: 5.5 g (RIVM 2006a) - exposure duration: 15 min (RIVM 2006a) - surface area of legs (adult): 0.560 m^2 (RIVM 2006b) HRGE assumption: - weight fraction: 0.5 (Church & Dwight Co., Inc. 2008) HRTE assumption: - weight fraction: 0.5 (Church & Dwight Co., Inc. 2008)	HRGE: - acute dermal deposition 38.8 mg/kg-bw per event - chronic dermal deposition 1.8 mg/kg-bw per day HRTE: - acute dermal deposition 38.8 mg/kg-bw per event - chronic dermal deposition 1.8 mg/kg-bw per day
HRGE	Water-based adhesive (used to connect laminate to furniture)	The scenario assumptions are based on a ConsExpo default scenario for bottled glue – moderate size surfaces (construction uses) (RIVM 2007) The dermal scenario used uptake by diffusion: - maximum weight fraction: 0.1 (Environment Canada 2010a) - product amount used: 250 g - frequency of use: 2/yr - dermal absorption: 100% - exposure duration: 30 min - product amount on skin: 0.25 g - exposed area: 215 cm^2	- acute dermal deposition 0.353 mg/kg-bw per event
HRPE	Lipstick	- maximum weight fraction: 0.1 (CNS 2010) - frequency of use: 1460/yr - amount ingested: 0.01 g (RIVM 2006a uptake fraction: 1	- oral chronic dose 0.0564 mg/kg bw per day
HR	Hair wax/pomade	The scenario assumptions are based on a ConsExpo default scenario for hair gel (RIVM 2006a) - maximum weight fraction: 0.30 (CNS	- chronic dermal deposition 1.36 mg/kg-bw per

		2010) - exposed area: 580 cm^2 (RIVM 2006a) - applied amount: 0.3 g (RIVM 2006a) - exposure frequency: 358/yr (RIVM 2006a)	day
HRPE	Mascara	- maximum weight fraction: 0.08 (Environment Canada 2010a) - exposed area: 1.6 cm^2 (RIVM 2006a) - applied amount: 0.025 g (RIVM 2006a) - exposure duration: 960 min (RIVM 2006a)	- chronic dermal deposition 0.0282 mg/kg-bw per day
HR	Hot melt adhesive	The inhalation component of the scenario assumes instantaneous release (due to the high temperature of application, ~150-180°C) (RIVM 2007): - maximum weight fraction: 0.1 (3M Canada Company 2008) - frequency of use: 12/yr - exposure duration: 25 min - room volume: 20 m^3 - ventilation rate: 0.6/hr - applied amount: 65 g - uptake fraction: 1 The dermal scenario used uptake by diffusion: - exposed area: 43 cm^2 - amount on skin: 0.1 g - exposure duration: 25 min	- mean inhalation event concentration: 0.0186 mg/m^3 - acute dermal deposition: 0.141 mg/kg-bw per event

[1]Adult body weight and inhalation rate were assumed to be 70.9 kg and 16.2 m^3 per day respectively (Health Canada 1998).

Appendix V: Summary of Health Effects Information for HR (CAS RN 65997-06-0), HRGE (CAS RN 65997-13-9) and HRPE (CAS RN 64365-17-9).

Endpoint	**Lowest effect levels[1]/Results**		
Laboratory animals and *in vitro*			
	HR CAS RN (65997-06-0)	**HRGE (CAS RN 65997-13-9)**	**HRPE (CAS RN 64365-17-9)**
Acute toxicity	**Oral LD_{50}** (rat) > 2000 mg/kg-bw (European Commission 2000c) **Inhalation LC_0 (non-lethal concentration)** (rat) > 2480 ppm (31 000 mg/m^3) (European Commission 2000c) No dermal studies identified.	**Oral LD_{50}** (rat) > 2000 mg/kg-bw (European Commission 2000a) **Inhalation LC_0 (non-lethal concentration)** (rat) > 0.158 mg/l (6 hours exposure) (European Commission 2000a) No dermal studies identified.	**Oral LD_{50}** (rat) > 2000 mg/kg-bw (European Commission 2000b) No dermal nor inhalation studies identified.
Short-term repeated-dose toxicity	No data identified.	**(Lowest) Oral LOEL** = 500 mg/kg-bw per day (1.0%) based on reduced body weight in females when both sexes of Sprague-Dawley rats (10 per sex per group) were exposed to 0, 0.2 or 1.0% (equivalent to 0, 100 or 500 mg/kg-bw per day, respectively) of HRGE in diet for 28 days. No weight changes were reported in males. Food consumption and gross and microscopic pathology were unaffected by treatment. (US EPA 2008a). No other studies identified.	No data identified.

Sub-chronic toxicity	**(Lowest) Oral LOEL** = 1000 mg/kg-bw per day (1%) based on decreased mean body weight and body weight gain (food consumption related) in weanling Sprague-Dawley rats (10 per sex per group) exposed to hydrogenated rosin at 0, 0.01, 0.05, 0.2, 1 or 5% (approximately 0, 10, 50, 200, 1000 or 5000 mg/kg-bw per day respectively) in diet for 90 days. A statistically significant increase in absolute liver weight and relative weights of liver, kidney, spleen in males, and liver in females at 1000 mg/kg-bw per day of HR were observed but were not considered to be toxicologically significant according by the author. All high dose animals died between days 4 and 12 (author claimed that the death was related to starvation associated with food refusal) (Calandra 1960a). No other studies identified.	**Highest Oral NOEL** =2500 mg/kg-bw per day (5%) based on no treatment-related effects in Sprague Dawley rats (20 to 25 per sex per group) treated with 0, 0.2, 1.0 or 5.0% of HRGE in diet (equivalent to 0, 100, 500 or 2500 mg/kg bw per day, respectively) for 90 days. Parameters measured were body weight, food consumption, haematology, clinical chemistry, urinalysis, ophthalmology, fecal parameters, organ weights and gross and microscopic pathology in all dose groups (US EPA 2008a). No treatment-related effects were also reported in another 90-day study on the same strain of rats (both sexes) treated with HRGE in diet at 0, 2000, 5000, or 10000 ppm for 90 days (equivalent to 0, 100, 250 or 500 mg/kg-bw per day, respectively) (Laveglia 1987). Other study identified: Calandra 1967.	No data identified.
Chronic toxicity/ carcinogenicity	Both sexes of Sprague-Dawley rats (30 per sex per group) were exposed to dietary concentrations of 0, 0.05, 0.2 or 1% of HR (equivalent to 0, 0, 50, 200, or 1000 mg/kg-bw per day, respectively) for two years. No evidence of carcinogenicity was noted at any dose level. No effects on haematology, urinalysis, organ weights, and gross and microscopic pathology were reported.	No data identified.	No data identified.

	(Lowest) Oral LOEL for non-neoplastic effects = 1000 mg/kg-bw per day (1%) based on the decreased weight gain in both sexes at the interim sacrifice (12 months) (the only effect observed in this study, the reliability of this unaudited IBT study is questionable according to US EPA 2008b) (Kay 1962a). No other studies identified.		
Sensitization	In a maximization test, female Dunkin-Hartley guinea pigs (15-21/ treated group, 15-20/control group) were challenged with 10, 3, or 1% of HR for 24 hours following the induction of Rosin or HR (5% intradermally and 25% epidermally). A significant response was found at the high concentration with the hydrogenated rosin induction groups. However, no such effect was found with the Rosin induction groups. In Freund's complete adjuvant test, no significant response was observed in female Dunkin-Hartley guinea pigs challenged with 10, 3, 1, or 0.3% of HR following induction of three intradermal injections of a 5% solution of HR (Karlberg et al. 1988).	No sensitization noticed in guinea pigs in a maximization test (no study details provided) (European Commission 2000a).	No data identified.
Irritation	No skin irritation noticed in rabbits (no study details provided) (European Commission 2000a).	No data identified.	No data identified.

Human			
	HR CAS RN 65997-06-0	**HRGE CAS RN 65997-13-9**	**HRPE CAS RN 64365-17-9**
Sensitization	In a patch test, Rosin or HR was applied to 11 human subjects with known sensitivity to Rosin (sex and age not identified) at concentrations of 0.001%, 0.01, 0.1, 1, 10, and 20%. Fewer reactions to HR than to Rosin were observed. No patient was found to react to the hydrogenated rosin without reacting to the unmodified rosin at the same concentration. Although the positive reactions were observed in 1 or 2 subjects at 0.001% to 0.1% HR, 5 out of 11 subjects showed positive reactions at 1% and 10% concentrations. At 20% HR, only 7 subjects were tested and 3 out of 7 subjects showed positive reactions compared to all 7 subjects who showed positive reactions to 20% Rosin (Karlberg et al. 1988).	In a patch test, 51 subjects of both sexes (ages 17-75 years old) were exposed to 0.2 mL of the test material containing 20% Hydrogenated Purified Ester Gum-2-Octyldodecyl Myristate and 80% petrolatum (effective concentration of HRGE in the test material was 10%). No evidence of skin irritation or sensitization was noted in any of the subjects (Johnson 2004). In three follow up patch tests, HRGE 20% in petrolatum was applied to human patients with clinical symptoms of sensitization or irritation as a result of previously used HRGE containing consumer products. Positive skin sensitization reactions were observed (Ota et al. 2007; Foti et al. 2006; Bonamonte et al. 2001).	In three follow up patch tests, an unspecified amount of HRPE was applied to human patients with clinical symptoms of sensitization or irritation as a result of previously using HRPE containing wound dressings (contain approximately up 20% of HRPE used as adhesive in final products). Positive skin sensitization reactions were observed (Pereira et al. 2007; Sasseville et al. 1997; Schliz et al. 1996).

[1] LC_{50}, median lethal concentration; LD_{50}, median lethal dose; LOAEL/LOAEC, lowest-observed-adverse-effect level/concentration; LOEL/LOEC, lowest-observed-effect level/concentration; NOAEL/NOAEC, no-observed-adverse-effect level/concentration

Appendix VI: Summary of Health Effects Information for Analogues Rosin (CAS RN 8050-09-7), Resin acids and Rosin acids, esters with glycerol (RGE) (CAS RN 8050-31-5) and Resin acids and Rosin acids, esters with pentaerythritol (RPE) (CAS RN 8050-26-8)

Endpoint	**Lowest effect levels[1]/Results**		
Laboratory animals and *in vitro*			
	Rosin (CAS RN 8050-09-7)	**Resin acids and Rosin acids, esters with glycerol (RGE) (CAS RN 8050-31-5)**	**Resin acids and Rosin acids, esters with pentaerythritol (RPE) (CAS RN 8050-26-8)**
Acute toxicity	**Lowest Oral LD_{50}** (mouse, guinea pig) = 4100- 4600 mg/kg-bw (US EPA 2008b). Other Oral LD_{50} (rat) = 7600 - 8400 mg/kg-bw (US EPA 2008b) No dermal nor inhalation studies identified.	**Oral LD_{50}** (rat) > 2000 mg/kg-bw (European Commission 2000d) No dermal nor inhalation studies identified.	**Oral LD_{50}** (rat) > 2000 mg/kg-bw (US EPA 2008b) No dermal nor inhalation studies identified.
Sub-chronic toxicity	**(Lowest) Oral LOEL =** 1000 mg/kg-bw per day based on reduced body weight and increased relative organ (liver, kidney and spleen) weights observed in five separate 90-day studies in Sprague-Dawley rats (10 per sex per group) exposed to 0, 0.01, 0.05, 0.2, 1.0 or 5.0% (equivalent to 0, 10, 50, 200, 1000 or 5000 mg/kg-bw per day, respectively) of Rosin in diet. No treatment-related effects on haematology or urinalysis parameters were reported in any	**(Lowest) Oral LOEL =** 1000 mg/kg-bw per day based on dose-related, statistically significant increases in relative liver weights in mid- and high-dose males of Sprague-Dawley rats (15 per sex per group) exposed to RGE in diet at 0, 0.2, 1, or 5% (equivalent to 0, 200, 1 000, or 5 000 mg/kg-bw per day respectively) for 90 days. Other effects observed were statistically significant increases in relative liver weights in high-dose females, statistically significantly decreased food consumption in high-dose males and females, and very slight periportal hepatocytic vacuolation in high-dose females (Mann et al. 1982).	**(Lowest) Oral LOAEL** = 2500 mg/kg-bw per day) based on a significant increase in absolute and relative liver weights in the high-dose Sprague Dawley rats observed in both sexes of (10 per sex per dose group) exposed to RPE at 0.01, 0.05, 0.2, 1, and 5% in diet (equivalent to 0, 5, 25, 100, 500 and 2500 mg/kg-bw per day respectively) for 90 days. Not treatment related effect on body weight, body weight gain, clinical signs, haematology, urinalysis, or gross pathology were reported (Calandra 1960c).

	study. At necropsy, no treatment-related changes were noted. An increase in absolute liver weights was reported in three of the five studies: relative organ weights were reported as "altered" in two studies and increases in relative organ weights (liver, kidney and/ or spleen) were reported in three studies. (Calandra 1960b). No other studies identified.	Other studies: Blari 1991. No dermal nor inhalation studies identified.	
Chronic toxicity/ carcinogenicity	Both sexes of Sprague-Dawley rats (30 per sex per dose) were exposed to dietary concentrations of 0, 0.05 or 1% of Rosin (equivalent to 0, 50 or 1000 mg/kg-bw per day, respectively) for two years. No evidence of carcinogenicity was noted at any dose level. **(Lowest) Oral LOEL for non-neoplastic effects** = 1000 mg/kg-bw per day (1%) based on decreased mean body weight and body weight gain (associated with decreased food consumption); and increased relative liver weight were observed in high dose groups **(**US EPA 2008b; Kay 1962b). No other studies identified.	No data identified.	Both sexes of Sprague-Dawley rats (30 per sex per group) were exposed to RPE in the diet at 0 or 0.05% (equivalent to 0 or 50 mg/kg-bw per day) for two years. Treatment did not affect body weight, body weight gain, food consumption, food utilization, haematology, urinalysis, gross pathology, organ weights or microscopic pathology. The number of tumour bearing animals was 0 males and 5 females in the first control group; 0 males and 9 females in the second control group; and 2 males and 7 females in the 0.05% group. In all groups, the tumours were primarily subcutaneous fibroadenomas or adenofibromas. No other treatment-related effects were reported (Kay 1962c).

Genotoxicity and related endpoints: ***in vitro***	No data identified.	**Gene mutation** **Negative**: *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537 and TA1538 at 2.5 to 500 µg/plate with or without metabolic activation (Jagannath 1988); strains TA92, TA94, TA98, TA100, TA1535 and TA1537 at 10 000 µg/plate with or without metabolic activation (Ishidate et al. 1984). **Chromosome aberration** **Negative:** Chinese hamster ovary (CHO) cells at 50.7- 507 µg/mL or 127-507 µg/ml with or without metabolic activation (Murli 1988). Fibroblast of Chinese hamster at 8000 µg/ml (Ishidate et al. 1984). **Unscheduled DNA synthesis** **Negative**: Rat primary hepatocyte at 5.08-102 µg/mL (Cifone 1988).	No data identified.
Reproductive/ developmental toxicity	Sprague-Dawley rats (10 per sex per group) were administered Rosin via diet at 0, 1000, 3000 or 10 000 ppm (equivalent to 0, 105, 275 or 825 mg/kg-bw per day, respectively; males dosed for at least four weeks, starting from two weeks prior to mating while the females dosed from two weeks prior to mating until at least day four of lactation). **(Lowest) LOEL for reproductive/developmental toxicity** = 825 mg/kg-bw per day (10 000 ppm) based on reduced mean litter and pup weight (considered as a secondary effect to	**No data identified.**	Sprague-Dawley rats (10 per sex per group) were administered RPE via diet at 0, 1000, 5000 and 20 000 ppm (equivalent to 0, 95, 475 or 1900 mg/kg-bw per day respectively; males dosed for at least four weeks, starting from two weeks prior to mating while the females dosed from two weeks prior to mating until at least day four of lactation). A slightly lower male fertility index in mid- and high-dose groups was reported (within the historical background range). There was no obvious effect of treatment at any dose level on mean number of live pups and implants compared with control. Mean litter and pup weights were slightly lower than control over day 1 to 4 of lactation in all treated groups without clear dose relationship, although weight gain from days 1to 4 was comparable with controls. No treatment related abnormalities noted among pups, no obvious effect of treatment on epididymis or testes

	reduced food intake and subsequent body weight loss in dams). There were no effects of treatment on mating performance, fertility or duration of gestation. **(Lowest) LOEL for systemic toxicity** = 275 mg/kg-bw per day (3 000 ppm) based on slightly reduced body-weight gain in males. Other effects observed at the high dose was a treatment related decreased body weight gain in both sexes associated with decreased food consumption in the first few weeks of treatment (Clubb and Sutherland 2002). No other studies identified.		weights in any treatment group and no histology or necropsy findings that could be attributed to treatment at any dose level. There were no obvious effects of treatment with RPE noted at any of the dose levels. The NOEL for systemic and reproductive/developmental effects for RPE was greater than 1900 mg/kg-bw per day (20 000 ppm) (US EPA 2008a)
Sensitization	Several resin acid and related products were tested in guinea pigs. Ambiguous or positive sensitization reactions were reported (European Commission 2000e).	No sensitization noticed in guinea pigs in a maximization test (no study details provided) (European Commission 2000d).	In a maximization test, female Dunkin-Hartley guinea pigs (10-15 per group) were challenged with 15% of RPE following the intradermal induction with 5% of the same substance. No sign of allergic skin sensitization were detected (Andersen 1998).
Irritation	Slight skin and eye irritation noticed in rats (no study details provided) (European Commission 2000e).	Slight skin irritation noticed in rabbits (no study details provided) (European Commission 2000d). In an ocular irritation test, Purified Ester Gum-2-Octyldodecyl Myristate (contains 50% RGE and 50% octyldodecyl myristate) was evaluated using	In a Draize test, 10% of RPE was instilled into the conjunctival sac of the eye of rabbits. No ocular irritation was observed (Andersen 1998). In a single insult occlusive patch test, RPE was tested on the skin of rabbits (strain and sex not specified).

		six New Zealand white rabbits. The test substance was instilled (0.1 ml) into the conjunctival sac of one eye of each animal. No ocular irritating reaction was reported (Johnson 2004).	Minimal irritation was observed at a dose level of 25% of RPE. Moderate reactions were observed with a mascara (containing 9.2% of RPE) and an eyeliner (containing 7% of RPE) (Andersen 1998).
Human			
	Rosin (CAS RN 8050-09-7)	**Resin acids and Rosin acids, esters with glycerol (RGE) (CAS RN 8050-31-5)**	**Resin acids and Rosin acids, esters with pentaerythritol (RPE) (CAS RN 8050-26-8)**
Sensitization/ Irritation	Positive sensitization reactions in human subjects were reported in patch tests with Rosin in Germany and Sweden. Several Rosin containing consumer products or Rosin related products used occupationally, were associated with dermal or inhalation allergic reactions (European Commission 2000e). Colophony (Rosin) is well recognized as a skin sensitizer and is also the third-highest cause of occupational asthma. However, the specific allergens involved particularly in occupational asthma have not been comprehensively assessed or identified (Sadhra et al. 1994)	No dermal sensitization was found with a RGE related product when tested in human (no study details provided) (European Commission 2000d).	In a repeated insult patch test, an eyeliner containing 0.1 mL of 7% of RPE was applied to 50 human subjects (both sexes). No sensitization reactions were observed. A mascara and an eyeshadow (containing 9.6% and 9.2% of RPE, respectively) were also tested on human subjects. No sensitization reactions or dermal irritation were observed (Andersen 1998).

	In a patch test, Rosin was applied to 11 human subjects with known sensitivity to Rosin (sex and age not identified) at concentrations of 0.001, 0.01, 0.1, 1, 10, and 20% in petrolatum. Positive reactions appeared at 0.001% and 0.01% in two test subjects and 9 of 11 test subjects reported positive reaction at 0.1% and 1% and all 11 test subject reacted to 10% of Rosin. Only 7 subjects were tested at 20% of Rosin, but all showed positive reactions (Karlberg et al. 1988).		

[1] LC_{50}, median lethal concentration; LD_{50}, median lethal dose; LOAEL/LOAEC, lowest-observed-adverse-effect level/concentration; LOEL/LOEC, lowest-observed-effect level/concentration NOAEL/NOAEC, no-observed-adverse-effect level/concentration

Appendix VIIa – PBT Model Inputs Summary Table for HR

	Phys-Chem/Fate	**Fate**	**Fate**	**Fate**	**PBT Profiling**	**Ecotoxicity**
Model Input Parameters	EPIWIN Suite (all models, including: AOPWIN, PCKOCWIN, BCFBAF BIOWIN and ECOSAR)	ASTreat	EQC	Arnot-Gobas BCF/BAF Model	Canadian-POPs (including: Catabol, BCF Mitigating Factors Mode)	Artificial Intelligence Expert System (AIEPS)/TOPKAT
SMILES Code	CC1(CCC2C(C1)=CCC1C2(C)CCCC1(C)C(O)=O)C=C	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)C1	-	CC1(CCC2C(C1)=CCC1C2(C)CCCC1(C)C(O)=O)C=C	CC1(CCC2C(C1)=CCC1C2(C)CCCC1(C)C(O)=O)C=C	CC1(CCC2C(C1)=CCC1C2(C)CCCC1(C)C(O)=O)C=C
	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)=C1	-	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)=C1
	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)C1	-	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(O)=O)C1
Molecular weight (g/mol)	302.5, 304.5, 306.5	306.5	302.5, 304.5, 306.5			
Melting point (ºC)			160, 147, 142			
Boiling point (ºC)						
Data temperature (ºC)			20			
Density (kg/m^3)		$1.2x10^{-3}$				
Vapour pressure (Pa)			$7.54x10^{-5}$, $1.05x10^{-4}$			

			$1.5x10^{-4}$			
Henry's Law constant (dimensionless)		$3.2x10^{-4}$				
Log K_{aw} (Air-water partition coefficient; dimensionless)						
Log K_{ow} (Octanol-water partition coefficient; dimensionless)			5.5, 6.0, 6.3	5.5, 6.0, 6.3	5.5, 6.0, 6.3	
K_{ow} (Octanol-water partition coefficient; dimensionless)						
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)						
Water solubility (mg/L)		0.06	2.42, 2.69, 2.00			
Log K_{oa} (Octanol-air partition coefficient; dimensionless)						
Soil-water partition coefficient (L/kg)[1]						
Sediment-water partition coefficient (L/kg)[1]						

Suspended particles-water partition coefficient (L/kg)[1]		96694				
Fish-water partition coefficient (L/kg)[2]						
Aerosol-water partition coefficient; dimensionless[3]						
Vegetation-water partition coefficient; dimensionless[1]						
Enthalpy (K_{ow})						
Enthalpy (K_{aw})						
Half-life in air (days)			1.00E+11[5]			
Half-life in water (days)			1.00E+11[5]			
Half-life in sediment (days)			1.00E+11[5]			
Half-life in soil (days)			1.00E+11[5]			
Half-life in vegetation (days)[4]						
Metabolic rate constant (1/days)						
Biodegradation rate constant (1/days)		1.37				
Biodegradation half-life in primary clarifier						

($t_{1/2-p}$) (hr)						
Biodegradation half-life in aeration vessel ($t_{1/2-s}$) (hr)						
Biodegradation half-life in settling tank ($t_{1/2-s}$) (hr)						

[1] derived from log K_{oc}
[2] derived from BCF data
[3] default value
[4] derived from half-life in water
[5]Negligible (default value)

Appendix VIIb – PBT Model Inputs Summary Table for HRPE

	Phys-Chem/Fate	**Fate**	**Fate**	**PBT Profiling**	**Ecotoxicity**
Model Input Parameters	EPIWIN Suite (all models, including: AOPWIN, PCKOCWIN, BCFBAF BIOWIN and ECOSAR)	EQC	Arnot-Gobas BCF/BAF Model	Canadian-POPs (including: Catabol, BCF Mitigating Factors Model)	Artificial Intelligence Expert System (AIEPS)/ TOPKAT
SMILES Code	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)CO)=C1	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)CO)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)CO)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)CO)=C1
	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(CO)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1
	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(CO)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1
	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1
Molecular weight (g/mol)	422.6, 709.1, 995.5, 1282	422.6, 709.1, 995.5, 1282			
Melting point (ºC)		223, 309, 350, 350			

Boiling point (ºC)					
Data temperature (ºC)		20			
Density (kg/m^3)					
Vapour pressure (Pa)		$3.32x10^{-4}$, $1.33x10^{-15}$, $3.35x10^{-25}$, $1.85x10^{-26}$			
Henry's Law constant (Pa·m^3/mol)					
Log K_{aw} (Air-water partition coefficient; dimensionless)					
Log K_{ow} (Octanol-water partition coefficient; dimensionless)		5.70, 12.2, 19.2, 27.7	5.70, 12.2, 19.2, 27.7	5.70, 12.2, 19.2, 27.7	
K_{ow} (Octanol-water partition coefficient; dimensionless)					
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)					
Water solubility (mg/L)		8.52, $4.17x10^{-6}$, $9.97x10^{-7}$, $1.28x10^{-6}$			
Log K_{oa}					

(Octanol-air partition coefficient; dimensionless)					
Soil-water partition coefficient (L/kg)[1]					
Sediment-water partition coefficient (L/kg)[1]					
Suspended particles-water partition coefficient (L/kg)[1]					
Fish-water partition coefficient (L/kg)[2]					
Aerosol-water partition coefficient; dimensionless[3]					
Vegetation-water partition coefficient; dimensionless[1]					
Enthalpy (K_{ow})					
Enthalpy (K_{aw})					
Half-life in air (days)		1.00E+11[5]			
Half-life in water (days)		1.00E+11[5]			

Half-life in sediment (days)		1.00E+11[5]			
Half-life in soil (days)		1.00E+11[5]			
Half-life in vegetation (days)[4]					
Metabolic rate constant (1/days)					
Biodegradation rate constant (1/days) or (1/hr) -specify					
Biodegradation half-life in primary clarifier ($t_{1/2-p}$) (hr)					
Biodegradation half-life in aeration vessel ($t_{1/2-s}$) (hr)					
Biodegradation half-life in settling tank ($t_{1/2-s}$) (hr)					

[1] Derived from log K_{oc}
[2] Derived from BCF data
[3] Default value
[4] Derived from half-life in water
[5]Negligible (default value)

Appendix VIIc – PBT Model Inputs Summary Table for HRGE

	Phys-Chem/Fate	Fate	Fate	PBT Profiling	Ecotoxicity
Model Input Parameters	EPIWIN Suite (all models, including: AOPWIN, PCKOCWIN, BCFBAF, BIOWIN and ECOSAR)	EQC	Arnot-Gobas BCF/BAF Model	Canadian-POPs (including: Catabol, BCF Mitigating Factors Model)	Artificial Intelligence Expert System (AIEPS)/ TOPKAT
SMILES Code	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)CO)=C1	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)CO)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)CO)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)CO)=C1
	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(O)COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1
	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)OC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)OC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)OC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCC(COC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)OC(=O)C2(C)CCCC3(C)C4CCC(C=C4CCC23)C(C)C)=C1
Molecular weight (g/mol)	378.6, 665.0, 951.5	378.6, 665.0, 951.5			
Melting point (ºC)					
Boiling point (ºC)					
Data temperature (ºC)		20			
Density (kg/m^3)					
Vapour pressure (Pa)		4.03×10^{-9}, 1.54×10^{-15}, 4.76×10^{-19}			

Henry's Law constant ($Pa \cdot m^3/mol$)					
Log K_{aw} (Air-water partition coefficient; dimensionless)					
Log K_{ow} (Octanol-water partition coefficient; dimensionless)		5.23, 12.3, 19.7	5.23, 12.3, 19.7	5.23, 12.3, 19.7	
K_{ow} (Octanol-water partition coefficient; dimensionless)					
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)					
Water solubility (mg/L)		2.54, 1.30×10^{-6}, 9.51×10^{-7}			
Log K_{oa} (Octanol-air partition coefficient; dimensionless)					
Soil-water partition coefficient (L/kg)[1]					
Sediment-water partition					

coefficient (L/kg)[1]					
Suspended particles-water partition coefficient (L/kg)[1]					
Fish-water partition coefficient (L/kg)[2]					
Aerosol-water partition coefficient; dimensionless[3]					
Vegetation-water partition coefficient; dimensionless[1]					
Enthalpy (K_{ow})					
Enthalpy (K_{aw})					
Half-life in air (days)		1.00E+11[5]			
Half-life in water (days)		1.00E+11[5]			
Half-life in sediment (days)		1.00E+11[5]			
Half-life in soil (days)		1.00E+11[5]			
Half-life in vegetation (days)[4]					
Metabolic rate constant (1/days)					

Biodegradation rate constant (1/days) or (1/hr) -specify					
Biodegradation half-life in primary clarifier ($t_{1/2-p}$) (hr)					
Biodegradation half-life in aeration vessel ($t_{1/2-s}$) (hr)					
Biodegradation half-life in settling tank ($t_{1/2-s}$) (hr)					

[1] Derived from log K_{oc}
[2] Derived from BCF data
[3] Default value
[4] Derived from half-life in water
[5] Negligible (default value)

Appendix VIId – PBT Model Inputs Summary Table for HRTE

	Phys-Chem/Fate	**Fate**	**Fate**	**Fate**	**PBT Profiling**	**Ecotoxicity**
Model Input Parameters	EPIWIN Suite (all models, including: AOPWIN, PCKOCWIN, BCFBAF BIOWIN and ECOSAR)	SimpleTreat	EQC	Arnot-Gobas BCF/BAF Model	Canadian-POPs (including: Catabol, BCF Mitigating Factors Model)	Artificial Intelligence Expert System (AIEPS)/ TOPKAT
SMILES Code	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=

	(=O)OCCOCCOCCO)=C1	(=O)OCCOCCOCCO)C1		(=O)OCCOCCOCCO)=C1	(=O)OCCOCCOCCO)=C1	O)OCCOCCOCCO)=C1
	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCCOCCOCCOC(=O)C2(C)CCCC3(C)C2CCC2CCC(C=C32)C(C)C)=C1	-	-	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCCOCCOCCOC(=O)C2(C)CCCC3(C)C2CCC2CCC(C=C32)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCCOCCOCCOC(=O)C2(C)CCCC3(C)C2CCC2CCC(C=C32)C(C)C)=C1	CC(C)C1CCC2C(CCC3C2(C)CCCC3(C)C(=O)OCCOCCOCCOC(=O)C2(C)CCCC3(C)C2CCC2CCC(C=C32)C(C)C)=C1
Molecular weight (g/mol)	436.6, 723.1	438.65	436.6, 723.1			
Melting point (ºC)			201, 291			
Boiling point (ºC)						
Data temperature (ºC)			20			
Density (kg/m^3)						
Vapour pressure (Pa)			$1.09x10^{-9}$, $1.84x10^{-13}$			
Henry's Law constant (Pa·m^3/mol)		$2.9x10^{-6}$				
Log K_{aw} (Air-water partition coefficient; dimensionless)						
Log K_{ow} (Octanol-water partition coefficient; dimensionless)		5.4	5.31, 12.8	5.31, 12.8	5.31, 12.8	
K_{ow} (Octanol-water partition		251189				

coefficient; dimensionless)						
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)						
Water solubility (mg/L)			$7.23x10^{-7}$			
Log K_{oa} (Octanol-air partition coefficient; dimensionless)						
Soil-water partition coefficient (L/kg)[1]						
Sediment-water partition coefficient (L/kg)[1]						
Suspended particles-water partition coefficient (L/kg)[1]		18707				
Fish-water partition coefficient (L/kg)[2]						
Aerosol-water partition coefficient; dimensionless[3]						

Vegetation-water partition coefficient; dimensionless[1]						
Enthalpy (K_{ow})						
Enthalpy (K_{aw})						
Half-life in air (days)			1.00E+11[5]			
Half-life in water (days)			1.00E+11[5]			
Half-life in sediment (days)			1.00E+11[5]			
Half-life in soil (days)			1.00E+11[5]			
Half-life in vegetation (days)[4]						
Metabolic rate constant (1/days)						
Biodegradation rate constant (1/hr)		0.007				
Biodegradation half-life in primary clarifier ($t_{1/2-p}$) (hr)						
Biodegradation half-life in aeration vessel ($t_{1/2-s}$) (hr)						
Biodegradation half-life in settling tank ($t_{1/2-s}$) (hr)						

[1] Derived from log K_{oc}
[2] Derived from BCF data
[3] Default value
[4] Derived from half-life in water
[5]Negligible (default value)