

## SCREENING-LEVEL HAZARD CHARACTERIZATION

### Arylpolyolefins Category

#### SPONSORED CHEMICALS

<b>C14 – C24 Alkaryl derivatives</b>	<b>CASRN 115733-08-9</b>
<b>Polypropylene derivatives</b>	<b>CASRN 68081-77-6</b>

#### SUPPORTING CHEMICALS

<b>Benzene, C10 – C13 Alkyl derivatives</b>	<b>CASRN 67774-74-7</b>
<b>Benzene, C10 – C16 alkyl derivatives</b>	<b>CASRN 68648-87-3</b>

The High Production Volume (HPV) Challenge Program<sup>1</sup> was conceived as a voluntary initiative aimed at developing and making publicly available screening-level health and environmental effects information on chemicals manufactured in or imported into the United States in quantities greater than one million pounds per year. In the Challenge Program, producers and importers of HPV chemicals voluntarily sponsored chemicals; sponsorship entailed the identification and initial assessment of the adequacy of existing toxicity data/information, conducting new testing if adequate data did not exist, and making both new and existing data and information available to the public. Each complete data submission contains data on 18 internationally agreed to “SIDS” (Screening Information Data Set<sup>1,2</sup>) endpoints that are screening-level indicators of potential hazards (toxicity) for humans or the environment.

The Environmental Protection Agency’s Office of Pollution Prevention and Toxics (OPPT) is evaluating the data submitted in the HPV Challenge Program on approximately 1400 sponsored chemicals by developing hazard characterizations (HCs). These HCs consist of an evaluation of the quality and completeness of the data set provided in the Challenge Program submissions. They are not intended to be definitive statements regarding the possibility of unreasonable risk of injury to health or the environment.

The evaluation is performed according to established EPA guidance<sup>2,3</sup> and is based primarily on hazard data provided by sponsors; however, in preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor’s responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from one year prior to the date of the HPV Challenge submission to the present: (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, IRIS, NTP, ATSDR, IARC, EXTOXNET, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. OPPT’s focus on these specific sources is based on their being

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<sup>1</sup> U.S. EPA. High Production Volume (HPV) Challenge Program; <http://www.epa.gov/chemrtk/index.htm>.

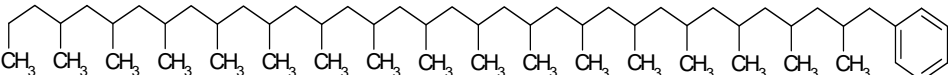
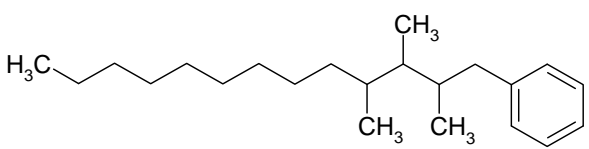
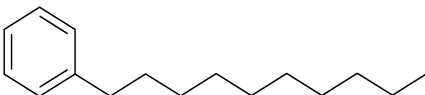
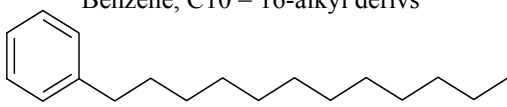
<sup>2</sup> U.S. EPA. HPV Challenge Program – Information Sources; <http://www.epa.gov/chemrtk/pubs/general/guidocs.htm>.

<sup>3</sup> U.S. EPA. Risk Assessment Guidelines; <http://cfpub.epa.gov/ncea/raf/rafguid.cfm>.

of high quality, highly relevant to hazard characterization, and publicly available.

OPPT does not develop HCs for those HPV chemicals which have already been assessed internationally through the HPV program of the Organization for Economic Cooperation and Development (OECD) and for which Screening Initial Data Set (SIDS) Initial Assessment Reports (SIAR) and SIDS Initial Assessment Profiles (SIAP) are available. These documents are presented in an international forum that involves review and endorsement by governmental authorities around the world. OPPT is an active participant in these meetings and accepts these documents as reliable screening-level hazard assessments.

These hazard characterizations are technical documents intended to inform subsequent decisions and actions by OPPT. Accordingly, the documents are not written with the goal of informing the general public. However, they do provide a vehicle for public access to a concise assessment of the raw technical data on HPV chemicals and provide information previously not readily available to the public.

<p><b>Chemical Abstract Service Registry Number (CASRN)</b></p>	<p style="text-align: center;"><b><u>Sponsored Chemicals</u></b>  <b>115733-08-9</b>  <b>68081-77-6</b></p> <p style="text-align: center;"><b><u>Supporting Chemicals</u></b>  <b>67774-74-7</b>  <b>68648-87-3</b></p>
<p><b>Chemical Abstract Index Name</b></p>	<p style="text-align: center;"><b><u>Sponsored Chemicals</u></b>  <b>Benzene, C14 – 24-branched and linear alkyl derives</b>  <b>Benzene, polypropene derives</b></p> <p style="text-align: center;"><b><u>Supporting Chemicals</u></b>  <b>Benzene, C10 – 13-alkyl derives</b>  <b>Benzene, C10 – 16-alkyl derivs</b></p>
<p><b>Structural Formula</b></p>	<p style="text-align: center;"><b><u>Sponsored Chemicals</u></b></p> <p style="text-align: center;">Representative structure for the intermediate molecular weight range benzene polypropene (C<sub>51</sub>) derivative</p>  <p style="text-align: center;">Representative structure for the C<sub>14</sub> alkyl derivative</p>  <p style="text-align: center;"><b><u>Supporting Chemicals</u></b></p> <p style="text-align: center;">Benzene, C10 – 13-alkyl derives</p>  <p style="text-align: center;">Benzene, C10 – 16-alkyl derivs</p> 

### Summary

The substances in the arylpolyolefins category are viscous liquid mixtures that have negligible to low water solubility and negligible to low vapor pressure. These substances are expected to have low mobility in soil. Volatilization is considered high; however, the low solubility and the tendency to adsorb to suspended solids and sediment may attenuate the rate of volatilization. The rate of hydrolysis is expected to be negligible. The rate of atmospheric photooxidation is considered moderate to rapid; however, these substances are not expected to exist in the vapor phase in the ambient atmosphere. CASRN 115733-08-9 is expected to be inherently biodegradable while CASRN 68081-77-6 is not expected to be biodegradable. CASRN 68081-77-6 is expected to have high persistence (P3) and low bioaccumulation potential (B1). CASRN 115733-08-9 is expected to have low persistence (P1) and high bioaccumulation potential (B3).

Acute oral toxicity and acute dermal toxicity of CASRNs 115733-08-9 and 68081-77-6 is low in rats and rabbits, respectively. Following a 4-week dietary exposure of the supporting chemical, CASRN 67774-74-7, rats showed decreased body weight at and above 125 mg/kg-day; the NOAEL for systemic toxicity is not established. The systemic toxicity assessed from the two-generation reproductive toxicity study in rats (that were dosed for 10 weeks via gavage, prior to mating) with the supporting chemical, CASRN 68648-87-3, also showed decreased body weight at 500 mg/kg-day (highest dose tested); the NOAEL for systemic toxicity is 50 mg/kg-day. In a 14-week inhalation toxicity study with the supporting chemical, CASRN 68648-87-3 in rats, a decrease in body weight was observed at and above 0.298 mg/L-day; the NOAEC for systemic toxicity is 0.102 mg/L-day. In a two-generation reproductive toxicity (gavage) study in rats with the supporting chemical, CASRN 68648-87-3, decreased pup weight gain, small litters and decreased pup survival were seen at and above 50 mg/kg-day; the NOAEL for reproductive/developmental toxicity is 5 mg/kg-day. In an oral prenatal developmental toxicity study in rats with the supporting chemical, CASRN 68648-87-3, decreased body weight was observed in dams at 500 mg/kg-day (highest dose tested); the NOAEL for maternal toxicity 125 mg/kg-day. An increased incidence of rudimentary rib structures was seen at and above 500 mg/kg-day; the NOAEL for developmental toxicity is 125 mg/kg-day. CASRN 115733-08-9 and the supporting chemical CASRN 68648-87-3, did not induce gene mutations in bacteria *in vitro* and the supporting chemical, CASRN 68648-87-3, did not induce chromosomal aberrations in rat bone marrow cells *in vivo*.

For the arylpolyolefins category members, the potential acute and chronic hazards to fish, aquatic invertebrates and aquatic plants are considered to be “no effects at saturation” based on their high log  $K_{ow}$  and low water solubility values.

No data gaps were identified under the HPV Challenge Program.

The sponsor, the American Chemistry Council Health, Environmental and Research Task Group (HERTG), submitted a Test Plan and Robust Summaries to EPA for arylpolyolefins on December 16, 2002. EPA posted the submission on the ChemRTK HPV Challenge website on January 15, 2003 (<http://www.epa.gov/chemrtk/pubs/summaries/arylpoly/c14132tc.htm>). EPA comments on the original submission were posted to the website on May 13, 2003. Public comments were also received and posted to the website. The sponsor submitted updated/revised documents on July 14, 2003 and April 22, 2005, which were posted to the ChemRTK website on August 6, 2003 and June 3, 2005, respectively.

### **Category Justification**

The two members of the arylpolyolefins category are mixtures with components that consist of a benzene ring with one long-chain alkyl substituent group. The alkyl group is a saturated hydrocarbon chain that can vary in length and extent of branching. The alkyl group is linear or methyl branched and ranges in carbon number from C14 to approximately C82. The arylpolyolefins category is based on structural similarity, similarity of estimated physicochemical properties and similar stabilities in water, rates of photodegradation and acute mammalian toxicity values. Some differences between the two members exist relating to vapor pressure, water solubility and log  $K_{ow}$  values, but sufficient evidence shows that C14 – C24 alkaryl derivatives and polyolefin derivatives will partition similarly in the environment, undergo similar rates of photodegradation and will not be susceptible to hydrolysis. Although only limited data were available for the environmental effects endpoints, the high log  $K_{ow}$  values (> 8) and low water solubility values of the category members suggest negligible toxicity. Toxicological support for the category was limited to acute mammalian toxicity data, where both category members have low acute oral and dermal toxicity, not inducing mortality at limit doses. The category appears to be adequately supported.

### **Justification for Supporting Chemicals**

Since the sponsored chemicals do not have data for repeated-dose/reproductive/developmental toxicity and chromosomal aberrations endpoints, instead of conducting additional animal testing, data from benzene, C10 – C16 alkyl derivatives, (CASRN 68648-87-3) were used to address these endpoints. The data for CASRN 68648-87-3 were used to address the human health endpoints for benzene, C10 – C13 alkyl derivatives, (CASRN 67774-74-7) from the HPV category ‘Benzene, C6 – C12 Alkyl Derivatives’ (<http://www.epa.gov/chemrtk/pubs/summaries/612alkde/c13311tc.htm>) and are also used in the EU Risk Assessment for CASRN 67774-74-7 (<http://ecb.jrc.ec.europa.eu/existing-chemicals/>). The structure of benzene, C10 – C13 alkyl derivatives, (CASRN 67774-74-7) and benzene, C10 – C16 alkyl derivatives, (CASRN 68648-87-3) exactly parallels the compounds in the arylpolyolefins category, and their lower molecular weight strongly suggests that it will have a higher bioavailability, water solubility, and overall toxicity than the compounds in the arylpolyolefins category. Although there is some uncertainty about the appropriateness of the supporting chemicals because there was no indication whether or not the degree of branching was similar to that of the sponsored substances, the overall use of these supporting chemicals is acceptable.

For the toxicity to aquatic plants endpoint, data for the supporting chemical, C10 – C13 alkyl derivative (CASRN 67774-74-7), were provided. However, these summaries were lacking in substantial details and tested nominal concentrations well above the predicted water solubility of the test substance. Therefore, these test data are considered inadequate and were not included in the hazard characterization.

## 1. Chemical Identity

### 1.1 Identification and Purity

The chemicals are mixtures with components that consist of a benzene ring with one long-chain alkyl substituent group. The alkyl group is a saturated hydrocarbon chain that can vary in length and extent of branching. The purity of the sponsored chemicals is not included in the test plan or robust summaries. The purity of the supporting chemical CASRN 67774-74-7 is 86-99% as mentioned in the EU Risk Assessment document. (Purity is defined as the degree of the product linearity, namely the percent content of alkylates with C10-C13 linear side alkyl chains.)

### 1.2 Physical-Chemical Properties

The substances in the arylpolyolefins category are viscous liquid mixtures that possess negligible to low water solubility and negligible to low vapor pressure. The physical-chemical properties of arylpolyolefins category members are summarized in Table 1.

<b>Table 1. Physical-Chemical Properties of the Arylpolyolefins Category<sup>1</sup></b>		
	<b>Benzene, polypropene derivs.</b>	<b>Benzene, C14-24-branched and linear alkyl derivs.</b>
<b>Property</b>	<b>Value</b>	<b>Value</b>
CASRN	68081-77-6	115733-08-9
Molecular Weight	387–1228 (typical)	275–415 (typical)
Physical State	Viscous liquid	Viscous liquid
Melting Point	<25°C based on physical state	<25°C based on physical state
Boiling Point	>300°C (estimated) <sup>2</sup>	>300°C (estimated) <sup>2</sup>
Vapor Pressure	<1.0×10 <sup>-10</sup> mm Hg at 25°C (estimated) <sup>2</sup>	1.2×10 <sup>-4</sup> mm Hg at 25°C (estimated) <sup>2</sup>
Water Solubility	7.7×10 <sup>-22</sup> mg/L at 25°C (estimated) <sup>2</sup>	≤0.411 mg/L (measured)
Henry's Law Constant	4.2×10 <sup>6</sup> atm·m <sup>3</sup> /mole (estimated) <sup>2</sup>	1.9 atm·m <sup>3</sup> /mole (estimated) <sup>2</sup>

<b>Table 1. Physical-Chemical Properties of the Arylpolyolefins Category<sup>1</sup></b>		
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<b>Property</b>	<b>Value</b>	<b>Value</b>
CASRN	68081-77-6	115733-08-9
Log K <sub>ow</sub>	26.2 (estimated) <sup>2</sup>	9.7 (estimated) <sup>2</sup>

<sup>1</sup> American Chemistry Council, Petroleum Additives Panel. 2005. Revised Robust Summary and Test Plan for Arylpolyolefins Category Available online at <http://www.epa.gov/chemrtk/pubs/summaries/arylpoly/c14132tc.htm> as of July 7, 2010.

<sup>2</sup> U.S. EPA. 2010. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.00. U.S. Environmental Protection Agency, Washington, DC, USA. Available online at <http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm> as of July 7, 2010. Estimates run for the representative structures, as depicted in the Appendix.

## **2. General Information on Exposure**

### **2.1 Production Volume and Exposure**

The Arylpolyolefins category chemicals had an aggregated production and/or import volume in the United States between 10 million pounds and 50.5 million pounds in calendar year 2005.

- CASRN 68081-77-6: < 500,000 pounds;
- CASRN 115733-08-9 : 10 to < 50 million pounds;

CASRN 68081-77-6:

No industrial processing and uses and commercial and consumer uses were reported.

CASRN 115733-08-9:

Industrial processing and use information as well as commercial and consumer use information of the chemical are claimed confidential in the 2006 IUR.

### **2.2 Environmental Exposure and Fate**

The compounds in the arylpolyolefins category are expected to have low mobility in soil.

CASRN 115733-08-9 is inherently biodegradable (58.8% in 28 days) in a manometric respirometry test (OECD TG 301F) under aerobic conditions using an inoculum from activated sludge. CASRN 68081-77-6 is not expected to be inherently biodegradable based on their high degree of alkyl branching, high molecular weight, and low estimated water solubility.

Volatilization of the arylpolyolefins is considered high based on the estimated Henry's Law constants for representative structures for these mixtures; however, the lack of solubility and the tendency of these substances to adsorb to suspended solids and sediment may attenuate the rate of volatilization. Arylpolyolefins are not expected to undergo hydrolysis. CASRN 68081-77-6 is expected to have high persistence (P3) and low bioaccumulation potential (B1). CASRN 115733-08-9 is expected to have low persistence (P1) and high bioaccumulation potential (B3).

The environmental fate properties of arylpolyolefins category members are summarized in Table 2.

<b>Property</b>	<b>Benzene, polypropene derivs.</b>	<b>Benzene, C14-24-branched and linear alkyl derivs.</b>
	<b>Value</b>	<b>Value</b>
CASRN	68081-77-6	115733-08-9
Photodegradation Half-life	1.7 hours (estimated) <sup>2</sup>	4.8 hours (estimated) <sup>2</sup>
Hydrolysis Half-life	Stable	Stable
Biodegradation	Log BioHC Half-Life: 4.93 days <sup>2</sup>	Log BioHC Half-Life: 1.81 days <sup>2</sup> 58.8% biodegradation in 28 days (not readily biodegradable)
Bioaccumulation Factor	BAF = 0.89 (estimated) <sup>2</sup>	BAF = 7,190 (estimated) <sup>2</sup>
Log K <sub>oc</sub>	15 (estimated) <sup>2</sup>	6.2 (estimated) <sup>2</sup>
Fugacity (Level III Model) <sup>2</sup>		
Air (%)	1.0	1.2
Water (%)	96.9	27.0
Soil (%)	2.1	67.3
Sediment (%)	<0.1	4.5
Persistence <sup>3</sup>	P3 (high)	P1 (low)
Bioaccumulation <sup>3</sup>	B1 (low)	B3 (high)

<sup>1</sup> American Chemistry Council, Petroleum Additives Panel. 2005. Revised Robust Summary and Test Plan for Arylpolyolefins Category. Available online at <http://www.epa.gov/chemrtk/pubs/summaries/arylpoly/c14132tc.htm> as of July 7, 2010.

<sup>2</sup> U.S. EPA. 2010. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.00. U.S. Environmental Protection Agency, Washington, DC, USA. Available online at <http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm> as of July 7, 2010. Estimates run for the representative structures depicted in the Appendix.

<sup>3</sup> Federal Register. 1999. Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) pp. 60194–60204.

**Conclusion:** The substances in the arylpolyolefins category are viscous liquid mixtures that have negligible to low water solubility and negligible to low vapor pressure. These substances are expected to have low mobility in soil. Volatilization is considered high; however, the low solubility and the tendency to adsorb to suspended solids and sediment may attenuate the rate of volatilization. The rate of hydrolysis is expected to be negligible. The rate of atmospheric photooxidation is considered moderate to rapid; however, these substances are not expected to exist in the vapor phase in the ambient atmosphere. CASRN 115733-08-9 is expected to be inherently biodegradable while CASRN 68081-77-6 is not expected to be biodegradable. CASRN 68081-77-6 is expected to have high persistence (P3) and low bioaccumulation potential (B1). CASRN 115733-08-9 is expected to have low persistence (P1) and high bioaccumulation potential (B3).

### 3. Human Health Hazard

A summary of health effects data submitted for SIDS endpoints is provided in Table 3.

#### *Acute Oral Toxicity*

##### ***C14 – C24 alkaryl derivative (CASRN 115733-08-9)***

Sprague-Dawley rats (5/sex/dose) were administered CASRN 115733-08-9 in corn oil via gavage at 5000 mg/kg and observed for up to 14 days. No mortalities were observed.

**LD<sub>50</sub> > 5000 mg/kg-bw**

##### ***Polypropylene derivative (CASRN 68081-77-6)***

Sprague-Dawley rats (5/sex/dose) were administered CASRN 68081-77-6 via gavage at 5000 mg/kg and observed for up to 14 days. No mortalities were observed.

**LD<sub>50</sub> > 5000 mg/kg-bw**

#### *Acute Dermal Toxicity*

##### ***C14 – C24 alkaryl derivative (CASRN 115733-08-9)***

New Zealand White rabbits (5/sex/dose) were administered CASRN 115733-08-9 via the dermal route at 2000 mg/kg to clipped, intact skin under occlusive conditions for 24 hours and observed for up to 14 days. No mortalities were observed.

**LD<sub>50</sub> > 2000 mg/kg-bw**

##### ***Polypropylene derivative (CASRN 68081-77-6)***

New Zealand White rabbits (5/sex/dose) were administered CASRN 68081-77-6 via the dermal route at 2000 mg/kg-bw to clipped, abraded skin under semi-occlusive conditions for 24 hours and observed for up to 14 days. No mortalities were observed.

**LD<sub>50</sub> > 2000 mg/kg-bw**

#### *Repeated-Dose Toxicity*

##### ***Benzene, C10 – C13 alkyl derivative (CASRN 67774-74-7, supporting chemical)***

Rats (number, sex, strain not reported) were administered CASRN 67774-74-7 in the diet for 4 weeks at 2500 to 20,000 ppm (approximately 125 to 1000 mg/kg-day). There was a reduction in body weight and food consumption at all concentrations. No gross pathological changes were noted. Histopathology was not carried out. (Data reported in EU LAB Risk Assessment Report, June 1997)

**LOAEL = 125 mg/kg-day** (based on decreased body weight)

**NOAEL = Not established**

***Benzene, C10 – C16 alkyl derivative (CASRN 68648-87-3, supporting chemical)***

Sprague-Dawley rats (15/sex/concentration) were administered CASRN 68648-87-3 via whole-body inhalation at 0, 102, 298, or 580 mg/m<sup>3</sup> (0.102, 0.298 or 0.580 mg/L-day, respectively) 6 hours/day, 5 days/week for approximately 14 weeks. Hypoactivity, irritation of the eyes and /or nose and respiratory difficulties were observed at 0.580 mg/L-day; some of these signs were also seen at 0.298 mg/L-day during the exposure periods. Discharges or secretion from the nose mouth and eyes, hypoactivity, inflammation around mouth, redness around the ears and integumentary conditions were seen during non-exposure periods. Decreases in mean body weights were seen at 0.298 and 0.580 mg/L-day. An increase in liver weights and increased serum levels of hepatic enzymes (alkaline phosphatase, SGOT, LDH and SGPT) were seen in females at 0.580 mg/L-day, no gross or histopathological changes were seen. A sub-acute multifocal inflammation of the alveoli was observed in animals at 0.580 mg/L-day. (Data reported in EU LAB Risk Assessment Report, June 1997)

**LOAEC = 0.298 mg/L-day** (based on decreased body weight)

**NOAEC = 0.102 mg/L-day**

***Reproductive Toxicity***

***Benzene, C10 – C16 alkyl derivative (CASRN 68648-87-3, supporting chemical)***

In a two-generation reproductive toxicity study, CD rats (30/sex/dose) were administered CASRN 68648-87-3 in corn oil via gavage at 0, 5, 50 or 500 mg/kg-day for about 10 weeks before mating. All adult rats were observed for mortality and clinical signs of toxicity, detailed physical examination, body weight, food consumption, complete gross postmortem examination. Pituitary glands, testes and epididymis, prostate and seminal vesicles, vagina, uterus, ovaries and gross lesions were examined microscopically for the control and high-dose animals. Gross lesions were examined for low and mid-dose animals. There was no treatment-related effect on mortality. Females were dosed during mating, gestation and lactation for a total of 127 days of treatment. After weaning, F1 generation animals (30/sex/dose) were dosed for an 11-week pre-mating period. Dosing of F1 females continued through mating, gestation and lactation. F2 pups were euthanized on day 13 of gestation. Mean body weight of males at 500 mg/kg-day was statistically significantly ( $p < 0.01$ ) and consistently below control weights. At 500 mg/kg-day, females also had significantly decreased body weights. No treatment-related adverse effects were seen during gross and histopathological examination. Reproductive effects at the high-dose included small litter size, fewer live pups and decreased pup survival. The pup viability index at birth and survival during the lactation period were significantly reduced at 50 and 500 mg/kg-day. (Data reported in EU LAB Risk Assessment Report, June 1997; Robinson and Schroeder, 1992)

**LOAEL (systemic toxicity) = 500 mg/kg-day** (based on decreased body weight)

**NOAEL (systemic toxicity) = 50 mg/kg-day**

**LOAEL (reproductive/developmental toxicity) = 50 mg/kg-day** (based on decreased pup weight gain, small litters, fewer live pups and decreased pup survival)

**NOAEL (reproductive/developmental toxicity) = 5 mg/kg-day**

### ***Developmental Toxicity***

#### ***Benzene, C10 – C16 alkyl derivative (CASRN 68648-87-3, Supporting Chemical)***

In a prenatal developmental toxicity study, 24 mated females were given CASRN 68648-87-3 at doses of 0, 125, 500 and 2000 mg/kg-day via gavage from 6 to 15 of gestation. Dams were terminated at gestation day 20 and fetuses were examined for external soft tissue and skeletal defects. The only effects noted at 125 mg/kg-day was a slight decrease in maternal weight gain, which was not statistically significant. The decreases in maternal weight gain were significant at 500 and 2000 mg/kg-day; however, compensatory increases in weight gain occurred during the post-treatment period. Ossification variations and delayed ossification were increased significantly at 2000 mg/kg-day (79.7% of fetuses with variations and delayed ossification versus 57.3% in the control group). Although not statistically significant, rudimentary rib structures were notably increased at 500 mg/kg-day compared to the control group (in 48 fetuses in 18 litters with rudimentary ribs versus 20 fetuses in 14 litters in the control group). There were no significant differences between control and treated groups in the number of fetuses with soft tissue malformations and variations. (Robinson and Schroeder, 1992)

**LOAEL (maternal toxicity) = 500 mg/kg-day** (based on decreased body weight gain)

**NOAEL (maternal toxicity) = 125 mg/kg-day**

**LOAEL (developmental toxicity) = 500 mg/kg-day** (based on delayed ossification and ossification variation)

**NOAEL (developmental toxicity) = 125 mg/kg-day**

### ***Genetic Toxicity – Gene Mutation***

#### ***In vitro***

##### ***C14 – C24 alkaryl derivative (CASRN 115733-08-9)***

*Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537 and TA1538 were exposed to CASRN 115733-08-9 at 0 (vehicle control), 0.025, 0.075, 0.25, 0.75 or 2.5 mg/plate in the presence and absence of metabolic activation. Positive controls were tested concurrently and produced an appropriate response. The cytotoxic concentration was not provided.

**CASRN 115733-08-9 was not mutagenic in this assay.**

##### ***Benzene, C10 – C16 alkyl derivative (CASRN 68648-87-3, Supporting Chemical)***

*Salmonella typhimurium* strains TA98, TA100, TA1535 and TA1537 were exposed to CASRN 68648-87-3 at 0 (vehicle control), 0.10, 40, 200, 1000, 3000 or 10,000 µg/plate in the presence and absence of metabolic activation. Positive controls were tested concurrently and produced an appropriate response. No cytotoxicity was seen. (Robinson and Nair, 1992)

**CASRN 68648-87-3 was not mutagenic in this assay.**

### ***Genetic Toxicity – Chromosomal Aberrations***

#### ***In vivo***

##### ***Benzene, C10 – C16 alkyl derivative (CASRN 68648-87-3, Supporting Chemical)***

Male and female Sprague-Dawley rats (18 – 24/dose) were administered benzene, CASRN 68648-87-3 in corn oil via gavage at 0 (vehicle control), 1200, 4000 or

12,700 mg/kg-bw. At 6, 12, 24 and 48 hour after treatment 6 animals/sex/dose were euthanized and bone marrow cells were evaluated for chromosomal aberrations. Two hours before termination, colchicine was given to all animals by intra-peritoneal injection to arrest cells in metaphase. The mean mitotic indices, mean chromosome numbers, percentage aberrant cells and the mean number of aberrations per cell for each group were compared. Positive controls were tested concurrently and produced an appropriate response. Marked decreases in body weight occurred at the high-dose level. Both mean chromosome numbers and mean mitotic indices were similar in test and vehicle control groups. No statistically significant increases in chromosomal aberrations or gaps were seen in the treated groups at any of the sampling times. (Robinson and Nair, 1992)

**CASRN 68648-87-3 did not induce chromosomal aberrations in this assay.**

**Conclusion:** Acute oral toxicity and acute dermal toxicity of CASRNs 115733-08-9 and 68081-77-6 is low in rats and rabbits, respectively. Following a 4-week dietary exposure of the supporting chemical, CASRN 67774-74-7, rats showed decreased body weight at and above 125 mg/kg-day; the NOAEL for systemic toxicity is not established. The systemic toxicity assessed from the two-generation reproductive toxicity study in rats (that were dosed for 10 weeks via gavage, prior to mating) with the supporting chemical, CASRN 68648-87-3, also showed decreased body weight at 500 mg/kg-day (highest dose tested); the NOAEL for systemic toxicity is 50 mg/kg-day. In a 14-week inhalation toxicity study with the supporting chemical, CASRN 68648-87-3 in rats, a decrease in body weight was observed at and above 0.298 mg/L-day; the NOAEC for systemic toxicity is 0.102 mg/L-day. In a two-generation reproductive toxicity (gavage) study in rats with the supporting chemical, CASRN 68648-87-3, decreased pup weight gain, small litters and decreased pup survival were seen at and above 50 mg/kg-day; the NOAEL for reproductive/developmental toxicity is 5 mg/kg-day. In an oral prenatal developmental toxicity study in rats with the supporting chemical, CASRN 68648-87-3, decreased body weight was observed in dams at 500 mg/kg-day (highest dose tested); the NOAEL for maternal toxicity 125 mg/kg-day. An increased incidence of rudimentary rib structures was seen at and above 500 mg/kg-day; the NOAEL for developmental toxicity is 125 mg/kg-day. CASRN 115733-08-9 and the supporting chemical CASRN 68648-87-3, did not induce gene mutations in bacteria *in vitro* and the supporting chemical, CASRN 68648-87-3, did not induce chromosomal aberrations in rat bone marrow cells *in vivo*.

**Table 3. Summary of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program – Human Health Data**

Endpoints	SPONSORED CHEMICAL C14 – C24 Alkaryl derivative (115733-08-9)	SPONSORED CHEMICAL Polypropylene derivative (68081-77-6)	SUPPORTING CHEMICAL Benzene, C10 – C13 alkyl derivatives (67774-74-7)	SUPPORTING CHEMICAL Benzene, C10 – C16 alkyl derivatives (68648-87-3)
Acute Oral Toxicity LD <sub>50</sub> (mg/kg)	> 5000	> 5000	–	–
Acute Dermal Toxicity LD <sub>50</sub> (mg/kg)	> 2000	> 2000	–	–
Repeated-Dose Toxicity NOAEL/LOAEL Oral (mg/kg-day)	No Data (4-weeks) NOAEL = Not established LOAEL = 125 (RA)	No Data (4-weeks) NOAEL = Not established LOAEL = 125 (RA)	(4-weeks) <b>NOAEL = Not established</b> <b>LOAEL = 125</b>	–
Repeated-Dose Toxicity NOAEC/LOAEC Inhalation (mg/L-day)	No Data NOAEC = 0.102 LOAEC = 0.298 (RA)	No Data NOAEC = 0.102 LOAEC = 0.298 (RA)	–	<b>NOAEC = 0.102</b> <b>LOAEC = 0.298</b>
Reproductive Toxicity NOAEL/LOAEL Oral (mg/kg-day) Systemic Toxicity  Reproductive Toxicity	No Data NOAEL = 50 LOAEL = 500  NOAEL = 5 LOAEL = 50 (RA)	No Data NOAEL = 50 LOAEL = 500  NOAEL = 5 LOAEL = 50 (RA)	–	<b>NOAEL = 50</b> <b>LOAEL = 500</b>  <b>NOAEL = 5</b> <b>LOAEL = 50</b>
Developmental Toxicity NOAEL/LOAL Oral (mg/kg-day) Maternal/Developmental Toxicity	No Data NOAEL = 125 LOAEL = 500 (RA)	No Data NOAEL = 125 LOAEL = 500 (RA)	–	<b>NOAEL = 125</b> <b>LOAEL = 500</b>
Genetic Toxicity – Gene Mutation <i>In vitro</i>	<b>Negative</b>	No Data Negative (RA)	–	<b>Negative</b>
Genetic Toxicity – Chromosomal Aberrations <i>In vivo</i>	No Data Negative (RA)	No Data Negative (RA)	–	<b>Negative</b>

Measured data in bold text; (RA) = Read Across; – indicates that endpoint was not addressed for this substance.

#### 4. Hazard to the Environment

A summary of aquatic toxicity data submitted for SIDS endpoints is provided in Table 4.

##### ***Acute Toxicity to Fish, Acute Toxicity to Aquatic Invertebrates & Toxicity to Aquatic Plants***

There was no adequate test data to address these endpoints. However, the potential acute and chronic hazards of the arylpolyolefins category members to fish, aquatic invertebrates and aquatic plants are considered to be “no effects at saturation” based on the high log K<sub>ow</sub> and low water solubility values.

**Conclusion:** For the arylpolyolefins category members, the potential acute and chronic hazards to fish, aquatic invertebrates and aquatic plants are considered to be “no effects at saturation” based on the high log K<sub>ow</sub> and low water solubility values.

<b>Table 4. Summary of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program – Aquatic Toxicity Data</b>		
<b>Endpoints</b>	<b>SPONSORED CHEMICALS</b>	
	<b>C14 – C24 Alkaryl derivative (115733-08-9)</b>	<b>Polypropylene derivative (68081-77-6)</b>
<b>Fish</b>		
<b>96-h LC<sub>50</sub> (mg/L)</b>	NES	NES
<b>Aquatic Invertebrates</b>		
<b>48-h EC<sub>50</sub> (mg/L)</b>	NES	NES
<b>Aquatic Plants</b>		
<b>72-h EC<sub>50</sub> (mg/L)</b>		
<b>Growth rate</b>	NES	NES
<b>Biomass</b>		

NES = no effects at saturation (water solubility limit)

#### 5. References

1. European Union Risk Assessment Report; 1997, CAS No. 67774-74-7, Volume 3.
2. E.C. Robinson and R.E. Schroeder; *Reproductive and Developmental Toxicity of a Linear Alkylbenzene Mixture in Rats*. *Fundamental and Applied Toxicology* 18, 549-556 (1992)
2. E.C. Robinson and R.S. Nair; *The Genotoxic Potential of Linear lkyllbenzene Mixtures in a Short-Term Test Battery*. *Fundamental and Applied Toxicology* 18, 540-548 (1992)