

## SCREENING-LEVEL HAZARD CHARACTERIZATION

### SPONSORED CHEMICAL

**Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)**

### SUPPORTING CHEMICALS

**Phenyl-C10 (C10 LAB; CASRN 340017-14-3)**

**Nonylbenzene (CASRN 1081-77-2)**

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 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

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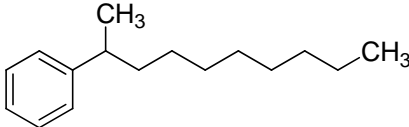
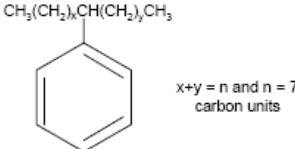
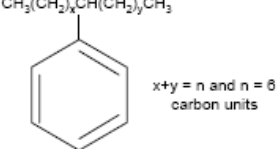
<sup>1</sup> U.S. EPA. High Production Volume (HPV) Challenge Program; <http://www.epa.gov/chemrtk/index.htm>.

<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>.

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><u>Sponsored Chemical</u> 68608-80-0</p> <p><u>Supporting Chemicals</u> 340017-14-3 1081-77-2</p>
<p><b>Chemical Abstract Index Name</b></p>	<p>Benzene, C6-12 alkyl derivs. (See Section 1) Benzene, sec-decyl- Benzene, nonyl-</p>
<p><b>Structural Formula</b></p>	<div style="text-align: center;">  <p>Benzene, C6-12 alkyl derivs. (See Section 1)</p>  <p><math>\text{CH}_3(\text{CH}_2)_x\text{CH}(\text{CH}_2)_y\text{CH}_3</math> <math>x+y = n</math> and <math>n = 7</math> carbon units</p> <p>Benzene, sec-decyl-</p>  <p><math>\text{CH}_3(\text{CH}_2)_x\text{CH}(\text{CH}_2)_y\text{CH}_3</math> <math>x+y = n</math> and <math>n = 6</math> carbon units</p> <p>Benzene, nonyl-</p> </div>
<p style="text-align: center;"><b>Summary</b></p> <p>CASRN 68608-80-0 is a liquid mixture primarily consisting of C9-C10 alkyl benzenes with low water solubility and moderate vapor pressure. It is expected to have low mobility in soil. Volatilization of CASRN 68608-80-0 is considered high based on its Henry's Law constant. The rate of hydrolysis is considered negligible. The rate of atmospheric photooxidation is considered moderate. CASRN 68608-80-0 is expected to have low persistence (P1) and high bioaccumulation potential (B3).</p> <p>The acute oral and inhalation toxicity of CASRN 68608-80-0 in rats is low. The acute dermal toxicity of CASRN 68608-80-0 in rabbits is moderate. CASRN 68608-80-0 is irritating to the skin and eyes of rabbits. Adequate data were not submitted for the repeated-dose/reproductive/development toxicity, gene mutations and chromosomal aberrations endpoints.</p> <p>The estimated 96-hour acute toxicity of CASRN 68608-80-0 to fish is 0.289 mg/L. The estimated acute toxicity for CASRN 68608-80-0 to aquatic invertebrates is 0.254 mg/L. The estimated acute toxicity of CASRN 68608-80-0 to aquatic plants is 0.443 mg/L. The estimated</p>	

21-d chronic toxicity of CASRN68608-80-0 to aquatic invertebrates is 0.047 mg/L. No experimental data are available for the acute toxicity to fish, aquatic invertebrates and aquatic plants, or for the chronic toxicity to aquatic invertebrates for CASRN 68608-80-0.

The chronic toxicity to aquatic invertebrates and repeated-dose/reproductive/developmental toxicity and gene mutations and chromosomal aberrations endpoints were identified as data gaps under the HPV Challenge Program.

The sponsor, Huntsman Corporation, submitted a Test Plan and Robust Summaries to EPA for benzene, C6 – 12 alkyl derivatives (CASRN 68608-80-0; CA Index name: benzene, C6 – 12 alkyl derivatives) on November 23, 2001. EPA posted the submission on the ChemRTK HPV Challenge website on December 17, 2001 (<http://www.epa.gov/chemrtk/pubs/summaries/612alkde/c13311tc.htm>). EPA comments on the original submission were posted to the website on August 28, 2002. Public comments were also received and posted to the website. The sponsor updated/revised documents on March 24, 2003, which were posted to the ChemRTK website on April 22, 2003.

## **Justification for Supporting Chemicals**

The sponsor provided environmental and/or health effects data for the proposed supporting chemicals, benzene C10 – 13 alkyl derivatives (CASRN 67774-74-7), pentadecane (CASRN 629-62-9), tetradecane (CASRN 629-59-4), benzene, nonyl- (CASRN 1081-77-2), C10-linear alkylbenzene (phenyl-C10, C10-LAB; CASRN 340017-14-3) and a commercial product Alkylate 215. EPA considered data for pentadecane (CASRN 629-62-9) and tetradecane (CASRN 629-59-4) inadequate. In its comments dated August 26, 2002, EPA asked for compositional information on the sponsored substance and the proposed supporting chemicals. In the revised submission, the Sponsor included compositional information on the sponsored substance but not on the supporting chemicals. The compositional information on the sponsored substance suggests that the sponsored substance is a complex mixture. The composition of the proposed supporting chemical, CASRN 67774-74-7 was not defined; however, it has been assessed in the OECD HPV program (<http://webnet.oecd.org/hpv/UI/Search.aspx>) and a risk assessment report (RAR) is available at the following link: <http://ecb.jrc.ec.europa.eu/esis/>. The SIAP describes CASRN 67774-74-7 as a “mixture of linear alkylbenzenes” and the RAR lists several CASRNs associated with this substance and other linear alkylbenzenes. The Sponsor did not associate these CASRNs with the sponsored substance. Therefore, data for CASRN 67774-74-7 have not been included in the hazard characterization. Data submitted on the commercial product Alkylate 215 was identified by the Sponsor as both benzene, C10-16-alkyl derivs. (CASRN 68648-87-3) and benzene, C10 – 13 alkyl derivs. (CASRN 67774-74-7); both of which have been assessed in the OECD HPV program (<http://webnet.oecd.org/hpv/UI/Search.aspx>). EPA did not consider data for Alkylate 215 adequate to support the sponsored substance. Data submitted for CASRN 340017-14-3 (ecotoxicity) and CASRN 1081-77-2 (biodegradation) were considered adequate.

### **1. Chemical Identity**

#### **1.1 Identification and Purity**

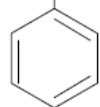
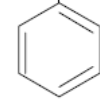
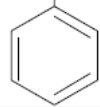


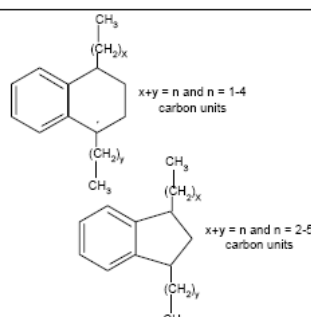
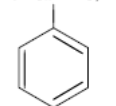
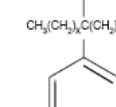
The sponsor refers to benzene, C6-12-alkyl derivs. as “Alkylate Top” which differs in composition from benzene, C6-12-alkyl derivs. Alkylate Top is the commercial product composed of both aromatic and aliphatic hydrocarbons, 48–56% C7-C10 LAB, 13–35% paraffins, 8% dialkylindanes/tetralins, and 6–22% *iso*-LAB. Benzene, C6-12-alkyl derivs. is a liquid mixture primarily consisting of C9-C10 alkyl benzenes with low water solubility and moderate vapor pressure.

The CA Index name of the test substance specifies that this substance contains linear alkyl chain lengths ranging from C6 to C12. The 2003 Test Plan indicates the current commercial product produced under this CA Index name contains from C7 to C10 alkyl chain lengths only. Hence, the current composition of the substance is not consistent with the specifications of the CA Index name.

The structure shown (1-methylnonylbenzene; CASRN 4537-13-7) is representative of the mixture benzene, C6-12 alkyl derivatives; the sponsor has specified that the alkyl side chain can be bonded to the benzene ring at any of the internal carbons along the chain. All estimates indicated in the data tables were performed using this structure.

The compositional information for the sponsored substance, from the revised test plan, is depicted in Table 1. In the hazard characterization, the *light sample mix* refers to the constituents of the 'relative % - light' column and the *heavy sample mix* refers to the constituents of the 'relative % - heavy' column.

**Table 1. Representative Structures of the Constituent Compounds of the Alkylate Top**

COMPOUND	Relative % - Light [Mean]	Relative % - Heavy [Mean]	REPRESENTATIVE STRUCTURE
C <sub>10</sub> -LAB	15-34 [23]	25-36 [30]	$\text{CH}_3(\text{CH}_2)_x\text{CH}(\text{CH}_2)_y\text{CH}_3$  $x+y = n$ and $n = 7$ carbon units
Sec-nonylbenzene	14-34 [24]	2-9 [8]	$\text{CH}_3(\text{CH}_2)_x\text{CH}(\text{CH}_2)_y\text{CH}_3$  $x+y = n$ and $n = 6$ carbon units
Sec-octylbenzene/ heptabenzene	7-11 [9]	8-11 [10]	$\text{CH}_3(\text{CH}_2)_x\text{CH}(\text{CH}_2)_y\text{CH}_3$  $x+y = n$ and $n = 4-5$ carbon units
n-Tetradecane	4-20 [13]	31-39 [35]	
n-Pentadecane	0.3-0.4 [0.3]	0.3-0.7 [0.5]	
Other Components (mainly dialkylindanes and dialkyltetralins)	5-12 [8]	8-9 [8]	 $x+y = n$ and $n = 1-4$ carbon units $x+y = n$ and $n = 2-5$ carbon units
Other LAB (likely mono-methyl branched [iso-LAB])	20-27 [22]	5-8 [6]	$\text{CH}_3(\text{CH}_2)_x\text{CH}(\text{CH}_2)_y\text{CH}(\text{CH}_3)\text{CH}_3$  $x+y+z = n$ and $n = 2-5$ carbon units $\text{CH}_3(\text{CH}_2)_x\text{C}(\text{CH}_3)_y\text{CH}_3$  $x+y = n$ and $n = 3-6$ carbon units

Note: Relative percent shows the range of 10 samples during light (L) and 11 samples during heavy (H) paraffin campaigns collected from September-October 2002 at the Chocolate Bayou, Texas, LAB production unit. Samples were analyzed by GC and GC/MS.

## 1.2 Physical-Chemical Properties

The physical-chemical properties of benzene, C6-12-alkyl derivs. are summarized in Table 2.

<b>Property</b>	<b>Value</b>
CASRN	68608-80-0
Molecular Weight	162.27 (C6 alkyl) to 246.43 (C12 alkyl); 204.35 (typical, C9 alkyl)
Physical State	Liquid
Melting Point	-12°C (pour point)
Boiling Point	278°C at 754 mm Hg (for typical C10 alkyl) <sup>2,3</sup>
Vapor Pressure	$1.88 \times 10^{-3}$ mm Hg at 25°C (estimated) <sup>2,4</sup>
Water Solubility	$5.7 \times 10^{-3}$ mg/L at 25°C (estimated) <sup>2,4</sup>
Dissociation Constant (pK <sub>a</sub> )	Not applicable
Henry's Law Constant	$7.6 \times 10^{-2}$ atm-m <sup>3</sup> /mole (estimated) <sup>2,5</sup>
Log K <sub>ow</sub>	7.06 (estimated) <sup>2,4</sup>

<sup>1</sup> Huntsman LLC; prepared by The Weinberg Group Inc. February 24, 2003. Revised Robust Summary for Benzene, C6-12 Alkyl Derivs.. Available online from:

<http://www.epa.gov/chemrtk/pubs/summaries/612alkde/c13311tc.htm> as of April 5, 2010.

<sup>2</sup> Supporting chemical, benzene, (1-methylnonyl)- (CASRN 4537-13-7) data presented is representative of the mixture C6-12 alkyl mixture. Its structure, the experimental log K<sub>ow</sub>, boiling point, vapor pressure, and water solubility were used for all estimations. The structure is provided in the Appendix.

<sup>3</sup> Lynch, E. R., McCall, E. B. 1960. Syntheses of some monoalkylbenzenes. J. Chem. Soc. 1254–1262.

<sup>4</sup> Sherblom, P. M., Gschwend, P. M., Eganhouse, R. P. 1992. Aqueous solubilities, vapor pressures and 1-octanol/water partition coefficients for C9-C14 linear alkylbenzenes. J. Chem. Eng. Data 37(4):394–399. Additional reported measured log K<sub>ow</sub> values: benzene, 1-methyldecyl- (7.63; CASRN 4536-88-3, not on TSCA); Benzene, 1-methylundecyl- (8.19; CASRN 2719-61-1, not on TSCA).

<sup>5</sup> U.S. EPA. 2010. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.00. U.S. Environmental Protection Agency, Washington, DC, USA. Available online from:

<http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm> as of April 5, 2010.

## 2. General Information on Exposure

### 2.1 Production Volume and Use Pattern

According to the 2006 IUR submissions, CASRN 68608-80-0 had an aggregated production and/or import volume in the United States between 1 and 10 million pounds.

Non-confidential information in the IUR indicated that the industrial processing and uses of the chemical include fuels. Non-confidential commercial and consumer uses of this chemical include “other”.

## 2.2 Environmental Exposure and Fate

The environmental fate properties of benzene, C6-12-alkyl derivs. are summarized in Table 3.

Benzene, C6-12-alkyl derivs. is expected to have a low mobility in soil. The sponsor cites two biodegradation studies for a representative compound benzene, nonyl- (CASRN 1081-77-2). Benzene, nonyl- was found to be degraded 72% in 8 days using a method with enriched sediment medium (MLP of  $1 \times 10^8$  cells/g of sediment). Another study using shake flasks of enriched seawater, indicated 65% degradation after 10 days with a pure culture of *alcaligenes sp.* PHY12 originating from a bacterial community isolated from seafoam. Pure cultures of *Nocardia amarae* MB-11 bacteria isolated from soil were capable of degrading various isomers of C10-C14 linear alkylbenzenes. The extent of degradation was 57–70% within 6 days and chain length had little impact on the extent of biodegradation. The molecular structure of benzene, C6-12-alkyl derivs. and a weight of evidence from these studies suggest that benzene, nonyl- is representative of benzene, C6-12-alkyl derivs. and will consequently experience biodegradation under exposure to most microbial communities. The rate of hydrolysis is expected to be negligible under environmental pH and temperature. The rate of volatilization is considered high based on its Henry's Law constant. Benzene, C6-12-alkyl derivs. is expected to have low persistence (P1) and high bioaccumulation potential (B3).

<b>Property</b>	<b>Value</b>
Photodegradation Half-life	7.6 hours (estimated) <sup>2,3</sup>
Hydrolysis Half-life	Stable
Biodegradation	65% in 10 days (pure culture study) <sup>1,4</sup> ; 72% after 8 days (microbial enriched sediment study) <sup>1,5</sup> ; 57-70% in 6 days (pure culture study) <sup>3,6</sup>
Bioaccumulation Factor	BAF = $1.1 \times 10^4$ (estimated) <sup>2,7</sup>
Log Koc	4.7 (estimated) <sup>2,3</sup>
Fugacity (Level III Model) <sup>2,7</sup>	
Air (%)	1.3
Water (%)	18.0
Soil (%)	64.8
Sediment (%)	15.9
Persistence <sup>8</sup>	P1 (low)
Bioaccumulation <sup>8</sup>	B3 (high)

**Table 3. Environmental Fate Characteristics of Benzene, C6-12-Alkyl Derivs.<sup>1</sup>**

Property	Value
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<sup>1</sup>Huntsman LLC; prepared by The Weinberg Group Inc. Feb 24, 2003. Revised Robust Summary for Benzene, C6-12 Alkyl Derivs.. Available online from: <http://www.epa.gov/chemrtk/pubs/summaries/612alkde/c13311tc.htm> as of April 5, 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 from: <http://www.epa.gov/opptintr/exposure/pubs/episuite.html> as of April 5, 2010.

<sup>3</sup>Bhatia, M., Singh, H. D. 1996. Biodegradation of commercial linear alkyl benzenes by *Nocardia amarae*. J. Biosci. 21(4):487–496.

<sup>4</sup>Supporting chemical, benzene, nonyl- (CASRN 1081-77-2) biodegradation study is listed by the sponsor and cited in: Rotani, J. F., Bonin, R., Giusti, G. 1987. Mechanistic study of interactions between photo-oxidation and biodegradation of n-nonylbenzene in seawater. Mar. Chem. 22:1–12.

<sup>5</sup>Supporting chemical, benzene, nonyl- (CASRN 1081-77-2) biodegradation study is listed by the sponsor and cited in: Azoulay, E., Colin, M., Dubreuil, J., Dou, H., Mille, G, Giusti, G. 1983. Relationship between hydrocarbons and bacterial activity in Mediterranean sediments: Part 2- hydrocarbon degrading activity of bacteria from sediments. Mar. Environ. Res. 9:19-36.

<sup>6</sup>Data obtained on linear alkyl benzenes consisting of chain lengths of C10-C14.

<sup>7</sup>Supporting chemical, benzene, (1-methylnonyl)- (CASRN 4537-13-7) data presented is representative of the mixture C6-12 alkyl mixture. Its structure, the experimental log  $K_{ow}$ , boiling point, vapor pressure, and water solubility were used for all estimations.

<sup>8</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:** Benzene, C6-12-alkyl derivs. is a liquid mixture primarily consisting of C9-C10 alkyl benzenes with low water solubility and moderate vapor pressure. It is expected to have low mobility in soil. Volatilization of benzene, C6-12-alkyl derivs. is considered high based on its Henry’s Law constant. The rate of hydrolysis is considered negligible. The rate of atmospheric photooxidation is considered moderate. Benzene, C6-12-alkyl derivs. is expected to have low persistence (P1) and high bioaccumulation potential (B3).

### 3. Human Health Hazard

The human health hazard properties of benzene, C6-12-alkyl derivs. are summarized in Table 4.

#### *Acute Oral Toxicity*

##### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

Sprague-Dawley rats (2 males and 3 females) were administered 10,000 mg/kg bw undiluted benzene, C6 – 12 alkyl derivative (*light* sample mix) via oral route and observed for 14 days. There were no mortalities.

**LD<sub>50</sub> > 10,000 mg/kg-bw**

#### *Acute Dermal Toxicity*

##### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

(1) Four New Zealand albino rabbits of both sexes were administered 3160, 5010 or 7940 mg/kg undiluted benzene, C6 – 12 alkyl derivative (*light and heavy* sample mix) via the dermal route (conditions not stated) for 24 hours and observed for 14 days. Rabbits exposed to 7940 mg/kg died on days 2 (female) and 10 (male), respectively. Animals at the 3160 and 5010 mg/kg survived.

**LD<sub>50</sub> = 5010 – 7940 mg/kg**

(2) Four New Zealand albino rabbits of both sexes were administered 1260, 2000, 3160 or 5010 mg/kg undiluted benzene, C6 – 12 alkyl derivative (*light* sample mix) via the dermal route

(conditions not stated) for 24 hours and observed for 14 days. Animals at exposed to 3160 and 5010 mg/kg died. Animals exposed up to 2000 mg/kg survived.

**LD<sub>50</sub> = 2000 - 3160 mg/kg**

(3) Seven New Zealand albino rabbits of both sexes were administered 794, 1000, 1260, 2000, 3160 or 5010 mg/kg undiluted benzene, C6 – 12 alkyl derivative (*heavy* sample mix) via the dermal route (conditions not stated) for 24 hours and observed for 14 days. Animals exposed to doses of 2000 mg/kg and greater died. Animals exposed up to 1260 mg/kg survived.

**LD<sub>50</sub> = 1260 - 2000 mg/kg**

### ***Acute Inhalation Toxicity***

#### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

In four acute inhalation toxicity studies, six male Sprague-Dawley rats were exposed to benzene C6 – 12 alkyl derivatives (*light* sample mix) vapor at 0.34, 0.3, 0.55 or 0.9 mg/L for 6 hours and observed for 14 days. There were no mortalities.

**LC<sub>50</sub> > 0.9 mg/L**

### ***Repeated-Dose/Reproductive/ Developmental Toxicity***

Adequate data were not submitted for these endpoints.

### ***Genetic Toxicity – Gene Mutation and Chromosomal Aberrations***

Adequate data were not submitted for these endpoints.

### ***Additional Information***

#### ***Skin Irritation***

##### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

Six New Zealand albino rabbits were treated with 0.5 mL undiluted CASRN 68608-80-0 (*light* sample mix) on the skin (conditions not stated) for 24 hours. At 24 and 72 hours, severe irritation was observed. There was a severe defatting effect and skin sloughing off in 14-21 days. (OTS0546131; <http://www.srcinc.com/what-we-do/databaseforms.aspx?id=384>)

**CASRN 68608-80-0 was severely irritating to rabbit skin.**

#### ***Eye Irritation***

##### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

Six New Zealand albino rabbits were treated with 0.1 mL undiluted CASRN 68608-80-0 (*light* sample mix) in the eye (conditions not stated) for 24 hours and observed at 10 minutes and at 1, 24, 48-72 and 120 hours. At 10 minutes and 1 hour there was slight erythema and copious discharge. At 24 hours, there was dullness of the cornea and slight erythema and discharge. At 48-72 hours there was slight improvement and no effects observed at 120 hours.

(OTS0546131; <http://www.srcinc.com/what-we-do/databaseforms.aspx?id=384>)

**CASRN 68608-80-0 was slightly irritating to rabbit eye.**

**Conclusion:** The acute oral and inhalation toxicity of CASRN 68608-80-0 in rats is low. The acute dermal toxicity of CASRN 68608-80-0 in rabbits is moderate. CASRN 68608-80-0 is irritating to the skin and eyes of rabbits. Adequate data were not submitted for the repeated-dose/reproductive/development toxicity, gene mutations and chromosomal aberrations endpoints.

<b>Table 4. Summary of the Screening Information Dataset as Submitted under the U.S. HPV Challenge Program: Human Health Data</b>	
<b>Endpoints</b>	<b>SPONSORED CHEMICAL Benzene, C6 – 12 Alkyl Derivatives (68608-80-0)</b>
<b>Acute Oral Toxicity LD<sub>50</sub> (mg/kg-bw)</b>	<b>&gt; 10,000</b>
<b>Acute Dermal Toxicity LD<sub>50</sub> (mg/kg)</b>	<b>1260-7940</b>
<b>Acute Inhalation Toxicity LC<sub>50</sub> (mg/L)</b>	<b>&gt;0.9</b>
<b>Repeated-Dose Toxicity NOAEL/LOAEL Oral (mg/kg-bw/day)</b>	Data Gap
<b>Reproductive Toxicity NOAEL/LOAEL Oral (mg/kg-bw/day)</b>	Data Gap
<b>Developmental Toxicity NOAEL/LOAL Oral (mg/kg-bw/day)</b>	Data Gap
<b>Genetic Toxicity – Gene Mutation <i>In vitro</i></b>	Data Gap
<b>Genetic Toxicity – Chromosomal Aberrations <i>In vitro</i></b>	Data Gap
<b>Additional Information Skin Irritation Eye Irritation</b>	Slightly irritating Strong irritant

#### 4. Hazard to the Environment

The environmental hazard properties of benzene, C6-12-alkyl derivs. are summarized in Table 5.

##### *Acute Toxicity to Fish*

###### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

No adequate data were available.

ECOSAR v. 1.00a was used to estimate acute toxicity to CASRN 68608-80-0

**96-hour LC<sub>50</sub> = 0.289 mg/L (ECOSAR v. 1.00a)**

##### *Acute Toxicity to Aquatic Invertebrates*

###### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

No adequate data were available.

ECOSAR v. 1.00a was used to estimate acute toxicity to CASRN 68608-80-0

**48-hour EC<sub>50</sub> = 0.254 mg/L**

###### ***Phenyl-C10 (C10 LAB) (CASRN 340017-14-3, supporting chemical)***

*Daphnia magna* were exposed to phenyl-C10 (C10 LAB) at nominal concentrations of 0.1, 0.05, 0.025 or 0.0125 mg/L under unspecified conditions for 48 hours.

**48-h EC<sub>50</sub> = No effects at saturation**

##### *Toxicity to Aquatic Plants*

###### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

No adequate data were available.

ECOSAR v. 1.00a was used to estimate acute toxicity to CASRN 68608-80-0

**96-hour EC<sub>50</sub> = 0.443 mg/L (ECOSAR v. 1.00a)**

##### *Chronic Toxicity to Aquatic Invertebrates*

###### ***Benzene, C6 – 12 Alkyl Derivatives (CASRN 68608-80-0)***

No adequate data were available.

ECOSAR v. 1.00a was used to estimate chronic toxicity to CASRN 68608-80-0

**21-d LC<sub>50</sub> = 0.047 mg/L**

**Conclusion:** The estimated 96-hour acute toxicity to fish from CASRN 68608-80-0 is 0.289 mg/L. The estimated acute toxicity for CASRN 68608-80-0 to aquatic invertebrates is 0.254 mg/L. The estimated acute toxicity of CASRN 68608-80-0 to aquatic plants is 0.443 mg/L. The estimated 21-d chronic toxicity of CASRN 68608-80-0 to aquatic invertebrates is 0.047 mg/L. No experimental data are available for the acute toxicity to fish, aquatic invertebrates and aquatic plants, or for the chronic toxicity to aquatic invertebrates for CASRN 68608-80-0. The chronic toxicity to aquatic invertebrates for the sponsored chemical, CASRN 68608-80-0, is considered a data gap under the HPV Challenge Program.

<b>Table 5. Summary of the Screening Information Dataset as Submitted under the U.S. HPV Challenge Program: Aquatic Toxicity Data</b>		
<b>Endpoints</b>	<b>Benzene, C6 – 12 Alkyl Derivatives (68608-80-0)</b>	<b>Phenyl-C10 (C10 LAB) (340017-14-3)</b>
<b>Fish</b> <b>96-h LC<sub>50</sub> (mg/L)</b>	0.289 (e)	–
<b>Aquatic Invertebrates</b> <b>48-h EC<sub>50</sub> (mg/L)</b>	–	<b>NES</b>
<b>Aquatic Plants</b> <b>72-h EC<sub>50</sub> (mg/L)</b>	0.443 (e)	–
<b>Chronic Toxicity to Aquatic Invertebrates</b> <b>21-d LC<sub>50</sub> (mg/L)</b>	Data Gap 0.047 (e)	-

Measured data in bold ; (e) estimated; – indicates that endpoint was not addressed for this chemical; NES = no effects at saturation