

## SCREENING-LEVEL HAZARD CHARACTERIZATION OF HIGH PRODUCTION VOLUME CHEMICALS

### CHEMICAL CATEGORY NAME

#### Dinonylnaphthalene Category

#### SPONSORED CHEMICALS

<b>Diisononylnaphthalene</b> [9 <sup>th</sup> CI Name: Naphthalene, diisononyl-]	<b>CASRN 63512-64-1</b>
<b>Dinonylnaphthalene sulfonic acid</b> [9 <sup>th</sup> CI Name: Naphthalenesulfonic acid, dinonyl-]	<b>CASRN 25322-17-2</b>
<b>Dinonylnaphthalene sulfonic acid, calcium salt</b> [9 <sup>th</sup> CI Name: Naphthalenesulfonic acid, dinonyl-, calcium salt (2:1)]	<b>CASRN 57855-77-3</b>
<b>Dinonylnaphthalene sulfonic acid, barium salt</b> [9 <sup>th</sup> CI Name: Naphthalenesulfonic acid, dinonyl-, barium salt (2:1)]	<b>CASRN 25619-56-1</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

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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>.

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, EXTOWNET, 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 may not develop HCs for those HPV chemicals which have recently been assessed and published 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. HCs may be created if new data suggest a need to update the case work where the OECD document will be used as key support documentation.

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><b><u>Subcategory I</u></b> <b>63512-64-1</b></p> <p><b><u>Subcategory II</u></b> <b>25322-17-2</b> <b>57855-77-3</b></p> <p><b><u>Subcategory II, III</u></b> <b>25619-56-1</b></p>
<p><b>Chemical Abstract Index Name</b></p>	<p><b><u>Subcategory I</u></b> <b>Diisononylnaphthalene</b></p> <p><b><u>Subcategory II</u></b> <b>Dinonylnaphthalene sulfonic acid</b> <b>Dinonylnaphthalene sulfonic acid, calcium salt</b></p> <p><b><u>Subcategory II, III</u></b> <b>Dinonylnaphthalene sulfonic acid, barium salt</b></p>
<p><b>Structural Formulae</b></p>	<p><b>See Appendix</b></p>
<p style="text-align: center;"><b>Summary</b></p> <p>The dinonylnaphthalenes are dark liquids possessing negligible vapor pressure and negligible water solubility. The dinonylnaphthalenes are expected to possess low mobility in soil. Volatilization of the dinonylnaphthalenes is low. The rate of hydrolysis is negligible for these substances. The rates of atmospheric photooxidation are expected to be rapid to moderate for all compounds in this category; however, these substances are not expected to exist in the vapor phase in the ambient atmosphere. The dinonylnaphthalenes are expected to have moderate persistence (P2) and moderate (B2) to high (B3) bioaccumulation potential.</p> <p><b>Human Health Hazard</b></p> <p><b><i>Subcategory I: Diisononylnaphthalene</i></b> Acute toxicity of diisononylnaphthalene is low for the oral and dermal routes in rats and rabbits respectively and moderate for the inhalation route in rats. Diisononylnaphthalene is irritating to rabbit skin and eyes.</p> <p>Data gaps for the repeated-dose, reproductive, developmental and genetic toxicity endpoints were identified under the HPV Challenge Program.</p> <p><b><i>Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt</i></b> Acute toxicity of dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt is low for the oral route in rats and the dermal route in rabbits. Acute inhalation</p>	

toxicity in rats is low for dinonylnaphthalene sulfonic acid and moderate for dinonylnaphthalene sulfonic acid, calcium salt. Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt are irritating to rabbit skin. Dinonylnaphthalene sulfonic acid is irritating to rabbit eyes. Dinonylnaphthalene sulfonic acid, calcium salt induced sensitization in guinea pigs. No sensitization was observed in human volunteers in a repeated insult patch sensitization test with dinonylnaphthalene sulfonic acid, calcium salt.

Data gaps for the repeated-dose, reproductive, developmental and genetic toxicity endpoints were identified under the HPV Challenge Program.

***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

Acute toxicity of dinonylnaphthalene sulfonic acid, barium salt is low by the oral route and moderate by the inhalation route in rats. Acute dermal toxicity in rabbits was low or moderate in two separate studies. Dinonylnaphthalene sulfonic acid, barium salt is irritating to rabbit skin and eyes and sensitizing to guinea pig skin. No sensitization was observed in human volunteers in a repeated insult patch sensitization test.

Data gaps for the repeated-dose, reproductive/developmental and genetic toxicity endpoints were identified under the HPV Challenge Program.

**Hazard to the Environment**

***Subcategory I: Diisononylnaphthalene***

No toxicity data were submitted for fish, aquatic invertebrates or aquatic plants. However, acute and chronic toxicity are not expected at saturation in water due to the very low estimated water solubility/dispersibility value ( $\leq 4.3 \times 10^{-7}$  mg/L).

***Subcategory II: Dinonylnaphthalene sulfonic acid, dinonylnaphthalene sulfonic acid, calcium salt, and dinonylnaphthalene sulfonic acid, barium salt***

No toxicity data were submitted for fish, aquatic invertebrates or aquatic plants. However, acute and chronic toxicity are not expected at saturation in water due to the very low estimated water solubility/dispersibility values ( $\leq 6.7 \times 10^{-5}$  mg/L).

No data gaps were identified under the HPV Challenge Program.

The sponsor, King Industries, submitted a Test Plan and Robust Summaries to EPA for the dinonylnaphthalene category on December 27, 2004. EPA posted the submission on the ChemRTK HPV Challenge website on January 19, 2005 (<http://www.epa.gov/oppt/chemrtk/pubs/summaries/dinapcat/c15766tc.htm>). EPA comments on the original submission were posted to the website on September 19, 2005. Public comments were also received and posted to the website. The sponsor submitted updated/revised documents on November 9, 2006, which were posted to the ChemRTK website on January 19, 2007. EPA comments on the revised submission were posted to the website on August 25, 2008.

### **Category Justification**

The Dinonylnaphthalene Category is composed of diisononylnaphthalene (CASRN 63512-64-1) and three other chemicals (CASRNs 25322-17-2, 57855-77-3, 25619-56-1) produced by further reactions.

The four chemicals are placed into one category based on similar structures and physical/chemical properties. The chemical structures are all based on a naphthalene moiety bearing two nonyl groups which are assumed to be a mixture of both branched and linear forms. Dinonylnaphthalene sulfonic acid contains an additional sulfonic acid group. The calcium and barium salts contain two equivalents of the sulfonic acid and one equivalent of the respective cation.

For human health and environmental endpoints, differences in functional groups preclude read across between the members of the category. The structure and physicochemical properties of diisononylnaphthalene suggest that it will behave differently from the three sulfonic acids with regard to bioavailability. In addition, two of the three dinonylnaphthalene sulfonic acids are metal salts: calcium and barium salt. The acute oral and dermal studies indicate that dinonylnaphthalene sulfonic acid, barium salt causes significant mortality, suggesting that the barium metal may be bioavailable and toxic at high doses. Therefore, it may not represent the toxicity of the either the acid or the calcium salt.

In light of these factors, the category members have been divided into three subcategories for human health effects: Subcategory I: diisononylnaphthalene; Subcategory II: dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt and Subcategory III: dinonylnaphthalene sulfonic acid, barium salt. A read-across approach is supported among the Subcategory II members, but not between the three subcategories.

For ecological effects, the structural differences between the three sulfonic acid functional groups category members and the single non-sulfonic acid group member may produce different toxicities depending on their physical/chemical properties, and for that reason they are treated separately into two subcategories for environmental effects.

## 1. Chemical Identity

### 1.1 Identification and Purity

The members of this category are dark-colored viscous liquids (as supplied) used as additives in industrial lubricants, greases, metalworking fluids, industrial coatings, and rust preventives and are not intended to be used as stand-alone chemicals.

### 1.2 Physical-Chemical Properties

The dinonylnaphthalenes are dark liquids possessing negligible vapor pressure and negligible water solubility.

The physical-chemical properties of the dinonylnaphthalene category members are provided in Table 1. Representative structures are provided in the Appendix.

Property	Naphthalene, diisononyl-	Naphthalene sulfonic acid, dinonyl-	Naphthalene sulfonic acid, dinonyl-, barium salt (2:1)	Naphthalene sulfonic acid, dinonyl-, calcium salt (2:1)
CASRN	63512-64-1	25322-17-2	25619-56-1	57855-77-3
Molecular Weight	380.65	540.78	1056.76	959.50
Physical State	Dark-colored viscous liquid	Dark-colored viscous liquid	Dark-colored viscous liquid	Dark-colored viscous liquid
Melting Point	No data. Liquid.	No data	No data	No data
Boiling Point	Likely decomposes before boiling. >300 °C (estimated) <sup>2,3</sup>	Likely decomposes before boiling. >300 °C (estimated) <sup>2,3</sup>	Likely decomposes before boiling. >300 °C (estimated) <sup>2,3</sup>	Likely decomposes before boiling. >300 °C (estimated) <sup>2,3</sup>
Vapor Pressure	$1.9 \times 10^{-7}$ mm Hg at 25 °C (estimated) <sup>2,3</sup>	$<1.0 \times 10^{-10}$ mm Hg at 25 °C (estimated) <sup>2,3</sup>	$<1.0 \times 10^{-10}$ mm Hg at 25 °C (estimated) <sup>2,3,4</sup>	$<1.0 \times 10^{-10}$ mm Hg at 25 °C (estimated) <sup>2,3,4</sup>
Dissociation Constant (pK <sub>a</sub> )	Not applicable	0.55 (estimated) <sup>3,5</sup>	Not applicable	Not applicable
Henry's Law Constant	0.26 atm·m <sup>3</sup> /mole (estimated) <sup>2,3</sup>	$<1.0 \times 10^{-10}$ atm·m <sup>3</sup> /mole (estimated) <sup>2,3</sup>	$<1.0 \times 10^{-10}$ atm·m <sup>3</sup> /mole (estimated) <sup>2,3,4</sup>	$<1.0 \times 10^{-10}$ atm·m <sup>3</sup> /mole (estimated) <sup>2,3,4</sup>
Water Solubility	$4.3 \times 10^{-7}$ mg/L at 25 °C (estimated) <sup>2,3</sup>	$6.7 \times 10^{-5}$ mg/L at 25 °C (estimated) <sup>2,3</sup>	$1.6 \times 10^{-3}$ mg/L at 25 °C (estimated) <sup>2,3,4</sup>	$1.6 \times 10^{-3}$ mg/L at 25 °C (estimated) <sup>2,3,4</sup>
Log K <sub>ow</sub>	>10 (estimated) <sup>2,3</sup>	8.52 (estimated) <sup>2,3</sup>	6.7 (estimated) <sup>2,3,4</sup>	6.7 (estimated) <sup>2,3,4</sup>

<sup>1</sup> King Industries Revised Test Plan and Robust Summary for Dinonylnaphthalene Category. December 12, 2006. Available at: <http://www.epa.gov/chemrtk/pubs/summaries/dinapcat/c15766tc.htm> as of August 5, 2011.

<sup>2</sup> U.S. EPA. 2011. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.10. U.S. Environmental Protection Agency, Washington, DC, USA. Available online from: <http://www.epa.gov/opptintr/exposure/pubs/episutedl.htm> as of August 5, 2011.

<sup>3</sup> The estimated value is based on the representative structure shown in the Appendix.

<sup>4</sup> Estimations performed on barium and calcium salts are generally outside the estimation domain of EPIWIN.

<sup>5</sup> SPARC. 2008. Online pK<sub>a</sub>/Property Calculator, w4.2.1405-s4.2.1408. University of Georgia, Athens, GA, USA. <http://archemcalc.com/sparc/?CFID=30156&CFTOKEN=90129611>

## 2. General Information on Exposure

### 2.1 Production Volume and Use Pattern

The Dinonylnaphthalene Category chemicals had an aggregated production and/or import volume in the United States between 2.5 million and 21.5 million pounds during calendar year 2005.

- CASRN 63512-64-1: 1 million to < 10 million pounds;
- CASRN 25322-17-2: 500,000 pounds to < 1 million pounds;
- CASRN 57855-77-3: 1 million to < 10 million pounds;
- CASRN 25619-56-1: < 500,000 pounds;

CASRN 63512-64-1:

Industrial processing and uses for the chemical were claimed confidential. No commercial and consumer uses were reported for the chemical.

CASRN 25322-17-2, 57855-77-3, and 25619-56-1:

Industrial processing and uses, and commercial and consumer uses for the chemicals were claimed confidential.

### 2.2 Environmental Exposure and Fate

The dinonylnaphthalenes are expected to possess low mobility in soil. No biodegradation data are available; however, the low solubility and high degree of branched alkyl structures suggests that biodegradation will be slow. Volatilization of diisononylnaphthalene is high given its estimated Henry's Law constant; however, the tendency to adsorb to soil and sediment will attenuate volatilization. Volatilization of the other dinonylnaphthalenes is low since these substances are ionic under environmental conditions. The rate of hydrolysis is negligible for these substances. The rates of atmospheric photooxidation are expected to be rapid to moderate for all compounds in this category; however, these substances are not expected to exist in the vapor phase in the ambient atmosphere. The dinonylnaphthalenes are expected to have moderate persistence (P2) and moderate (B2) to high (B3) bioaccumulation potential.

The environmental fate properties of the dinonylnaphthalene category members are provided in Table 2.

Property	Naphthalene, diisononyl-	Naphthalene sulfonic acid, dinonyl-	Naphthalene sulfonic acid, dinonyl-, barium salt (2:1)	Naphthalene sulfonic acid, dinonyl-, calcium salt (2:1)
CASRN	63512-64-1	25322-17-2	25619-56-1	57855-77-3
Photodegradation Half-life	1.5 hours (estimated) <sup>2,3</sup>	3.6 hours (estimated) <sup>2,3</sup>	3.6 hours (estimated) <sup>2,3,4</sup>	3.6 hours (estimated) <sup>2,3,4</sup>
Hydrolysis Half-life	Stable	Stable	Stable	Stable
Biodegradation	No data	No data	No data	No data
Bioaccumulation Factor	BAF = 3,911 (estimated) <sup>2,3</sup>	BAF = $3.4 \times 10^4$ (estimated) <sup>2,3</sup>	BAF = $3.4 \times 10^4$ (estimated) <sup>2,3,4</sup>	BAF = $3.4 \times 10^4$ (estimated) <sup>2,3,4</sup>
Log K <sub>oc</sub>	7.4 (estimated) <sup>2,3</sup>	6.3 (estimated) <sup>2,3</sup>	6.3 (estimated) <sup>2,3,4</sup>	6.3 (estimated) <sup>2,3,4</sup>
Fugacity (Level III Model) <sup>2,3,4</sup>				
Air (%)	0.1	0.1	<0.1	<0.1
Water (%)	13.5	5.3	1.7	1.7
Soil (%)	85.2	53.1	34.9	34.9
Sediment (%)	1.3	41.5	63.4	63.4
Persistence <sup>5</sup>	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)
Bioaccumulation <sup>5</sup>	B2 (moderate)	B3 (high)	B3 (high)	B3 (high)

<sup>1</sup> King Industries Revised Test Plan and Robust Summary for Dinonylnaphthalene Category. December 12, 2006. Available at:

<http://www.epa.gov/chemrtk/pubs/summaries/dinapcat/c15766tc.htm> as of August 5, 2011.

<sup>2</sup> U.S. EPA. 2011. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.10. U.S. Environmental Protection Agency, Washington, DC, USA. Available online from: <http://www.epa.gov/opptintr/exposure/pubs/episuitedi.htm> as of August 5, 2011.

<sup>3</sup> The estimated values are based on the representative structure shown in the Appendix.

<sup>4</sup> Estimations performed on barium and calcium salts are generally outside the estimation domain of EPIWIN.

<sup>5</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 dinonylnaphthalenes are dark liquids possessing negligible vapor pressure and negligible water solubility. The dinonylnaphthalenes are expected to possess low mobility in soil. Volatilization of the dinonylnaphthalenes is low. The rate of hydrolysis is negligible for these substances. The rates of atmospheric photooxidation are expected to be rapid to moderate for all compounds in this category; however, these substances are not expected to exist in the vapor phase in the ambient atmosphere. The dinonylnaphthalenes are expected to have moderate persistence (P2) and moderate (B2) to high (B3) bioaccumulation potential.



### **3. Human Health Hazard**

A summary of health effects data submitted for SIDS endpoints is provided in Table 3. The table also indicates where data for tested subcategory members are read-across (RA) to untested members of the subcategory.

#### ***Acute Oral Toxicity***

##### ***Subcategory I: Diisononylnaphthalene***

###### ***Diisononylnaphthalene (CASRN 63512-64-1)***

Wistar rats (10 males) were fasted and administered a single dose of 5000 mg/kg-bw undiluted diisononylnaphthalene by oral gavage and observed for 14 days following dosing. One death occurred.

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

##### ***Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt***

###### ***Dinonylnaphthalene sulfonic acid (CASRN 25322-17-2)***

Sprague-Dawley rats (5/sex) were fasted and administered a single dose of 5000 mg/kg-bw dinonylnaphthalene sulfonic acid in aliphatic hydrocarbon oil by oral gavage and observed for 14 days following dosing. One death occurred (sex not indicated).

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

###### ***Dinonylnaphthalene sulfonic acid, calcium salt (CASRN 57855-77-3)***

Sprague-Dawley rats (5/sex) were fasted and administered a single dose of 5000 mg/kg-bw dinonylnaphthalene sulfonic acid, calcium salt in oil by oral gavage and observed for 14 days following dosing. One death occurred (sex not indicated).

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

##### ***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

###### ***Dinonylnaphthalene sulfonic acid, barium salt (CASRN 25619-56-1)***

(1) Wistar rats (10 males) were fasted and administered a single dose of 5000 mg/kg-bw dinonylnaphthalene sulfonic acid, barium salt in oil by oral gavage and observed for 14 days following dosing. Seven rats died during the observation period.

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

(2) Wistar rats (5/sex/dose) were fasted and administered a single dose of 2, 3, 4, 5 or 6 ml/kg dinonylnaphthalene sulfonic acid, barium salt in oil (~1000, 1500, 2000, 2500 or 3000 mg/kg-bw; assuming density near 1 g/ml and test material is as sold: 50% by weight solution in

hydrocarbon diluents) by oral gavage and observed for 14 days following dosing. Mortality occurred in males at doses  $\geq 3$  ml/kg and in females at doses  $\geq 2$  ml/kg.

**LD<sub>50</sub> ~ 1750 mg/kg (3.5 ml/kg)**

(3) Sprague-Dawley rats (5/sex) were fasted and fed a single dose of 5000 mg/kg-bw dinonylnaphthalene sulfonic acid, barium salt in oil mixed into the diet and observed for 14 days following dosing. No mortalities were observed.

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

### *Acute Inhalation Toxicity*

#### *Subcategory I: Diisononylnaphthalene*

##### *Diisononylnaphthalene (CASRN 63512-64-1)*

Wistar rats (5/sex) were exposed whole-body to undiluted aerosolized diisononylnaphthalene at 17 mg/L for 1 hour and observed for 14 days following exposure. No mortalities were observed.

**LC<sub>50</sub> > 17 mg/L**

#### *Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt*

##### *Dinonylnaphthalene sulfonic acid (CASRN 25322-17-2)*

Wistar rats (5/sex) were exposed whole-body to aerosolized dinonylnaphthalene sulfonic acid in aliphatic hydrocarbon vehicle at 200 mg/L for 1 hour and observed for 14 days following exposure. No mortalities were observed.

**LC<sub>50</sub> > 200 mg/L**

##### *Dinonylnaphthalene sulfonic acid, calcium salt (CASRN 57855-77-3)*

Wistar rats (5/sex) were exposed whole-body to aerosolized dinonylnaphthalene sulfonic acid in oil vehicle at 18 mg/L for 1 hour and observed for 14 days following exposure. No mortalities were observed.

**LC<sub>50</sub> > 18 mg/L**

#### *Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt*

##### *Dinonylnaphthalene sulfonic acid, barium salt (CASRN 25619-56-1)*

Wistar rats (5/sex) were exposed whole-body to aerosolized diisononylnaphthalene in oil vehicle at 21 mg/L for 1 hour and observed for 14 days following exposure. No mortalities were observed.

**LC<sub>50</sub> > 21 mg/L**

### *Acute Dermal Toxicity*

#### *Subcategory I: Diisononylnaphthalene*

##### *Diisononylnaphthalene (CASRN 63512-64-1)*

New Zealand White rabbits (2 males and 3 females) were administered undiluted diisononylnaphthalene via the dermal route to abraded skin at 20,000 mg/kg-bw under semi-occluded conditions for 24 hours and observed for 14 days following dosing. No mortalities were observed.

**LD<sub>50</sub> > 20,000 mg/kg**

***Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt***

***Dinonylnaphthalene sulfonic acid (CASRN 25322-17-2)***

In two trials, New Zealand White rabbits (5 intact and 5 abraded) were administered dinonylnaphthalene sulfonic acid via the dermal route at 2000 mg/kg-bw under occluded conditions for 24 hours and observed for 14 days following dosing. One study utilized the vehicle, kerosene; the other used aliphatic hydrocarbon. No mortalities were observed.

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

***Dinonylnaphthalene sulfonic acid, calcium salt (CASRN 57855-77-3)***

New Zealand White rabbits (2 males and 3 females) were administered dinonylnaphthalene sulfonic acid, calcium salt in oil vehicle via the dermal route to abraded skin at 20,000 mg/kg-bw under semi-occluded conditions for 24 hours and observed for 14 days following dosing. No mortalities were observed.

**LD<sub>50</sub> > 20,000 mg/kg**

***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

***Dinonylnaphthalene sulfonic acid, barium salt (CASRN 25619-56-1)***

(1) New Zealand White rabbits (2 males and 3 females) were administered dinonylnaphthalene sulfonic acid, barium salt in oil vehicle via the dermal route to abraded skin at 20,000 mg/kg-bw under semi-occluded conditions for 24 hours and observed for 14 days following dosing. Mortalities were observed.

**LD<sub>50</sub> < 20,000 mg/kg**

(2) New Zealand White rabbits (2 males and 3 females) were administered dinonylnaphthalene sulfonic acid, barium salt via the dermal route to abraded skin at 2 mL/kg-bw (~ 1000 mg/kg-bw, assuming density near 1 g/mL and test material is as sold: 50% by weight solution in naphthenic diluents oil vehicle) under semi-occluded conditions for 24 hours and observed for 14 days following dosing. No mortalities were observed.

**LD<sub>50</sub> > 1000 mg/kg**

***Repeated-Dose Toxicity, Reproductive Toxicity and Developmental Toxicity***

***Subcategory I: Diisononylnaphthalene***

No data.

***Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt***

No data.

***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

No data.

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

***In vitro***

***Subcategory I: Diisononylnaphthalene***

No data.

***Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt***

No data.

***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

No data.

***Additional Information***

***Skin Irritation***

***Subcategory I: Diisononylnaphthalene***

***Diisononylnaphthalene (CASRN 63512-64-1)***

(1) New Zealand White rabbits (6 of unspecified sex) were administered undiluted diisononylnaphthalene via the dermal route to intact or abraded skin at 0.5 mL (500 mg assuming that the density of test material is near 1 g/mL) under occluded conditions for 24 hours and evaluated for skin lesions at 24 and 72 hours following dosing. No information on concentration or basis for conclusion was given. Mild irritation was noted; however, there were no mortality or clinical signs.

**Diisononylnaphthalene was mildly irritating to rabbit skin in this assay.**

(2) New Zealand White rabbits (6 males) were administered undiluted diisononylnaphthalene via the dermal route to intact or abraded skin at 0.5 mL under occluded conditions for 4 hours, at which time the test sites were washed. Evaluation for evidence of corrosion occurred at 4, 24 and 48 hours following dosing. No information on concentration or basis for conclusion was given. No evidence of corrosion was noted.

**Diisononylnaphthalene was not corrosive to rabbit skin in this assay.**

***Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt***

***Dinonylnaphthalene sulfonic acid (CASRN 25322-17-2)***

In two studies, New Zealand White rabbits (6 males) were administered 0.5 mL dinonylnaphthalene sulfonic acid in kerosene (one study) or aliphatic hydrocarbon (second study) to intact or abraded skin under occluded conditions for 24 hours and evaluated at 24 and 72 hours following dosing. No information on concentration or basis for conclusion was given. Moderate irritation was noted.

**Dinonylnaphthalene sulfonic acid was moderately irritating to rabbit skin in this assay.**

***Dinonylnaphthalene sulfonic acid, calcium salt (CASRN 57855-77-3)***

(1) New Zealand White rabbits (6 of unspecified sex) were administered 0.5 mL dinonylnaphthalene sulfonic acid, calcium salt in diluent oil to intact or abraded skin under occluded conditions for 24 hours and evaluated at 24 and 72 hours following dosing. No information on concentration or basis for conclusion was given. Moderate irritation was noted.

**Dinonylnaphthalene sulfonic acid, calcium salt was moderately irritating to rabbit skin in this assay.**

(2) New Zealand White rabbits (6 of unspecified sex) were administered undiluted dinonylnaphthalene sulfonic acid, calcium salt via the dermal route to intact or abraded skin at 0.5 mL under occluded conditions for 4 hours, at which time the test sites were washed. Evaluation for evidence of corrosion occurred at 4, 24 and 48 hours following dosing. No information on concentration or basis for conclusion was given. No evidence of corrosion was noted.

**Dinonylnaphthalene sulfonic acid, calcium salt was not corrosive to rabbit skin in this assay.**

***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

***Dinonylnaphthalene sulfonic acid, barium salt (CASRN 25619-56-1)***

(1) New Zealand White rabbits (6 of unspecified sex) were administered 0.5 mL dinonylnaphthalene sulfonic acid, barium salt in diluent oil to intact or abraded skin under occluded conditions for 24 hours and evaluated at 24 and 72 hours following dosing. No information on concentration or basis for conclusion was given. Moderate irritation was noted.

**Dinonylnaphthalene sulfonic acid, barium salt was moderately irritating to rabbit skin in this assay.**

(2) New Zealand White rabbits (6 of unspecified sex) were administered 0.5 mL dinonylnaphthalene sulfonic acid, barium salt in corn oil to intact and abraded skin under occluded conditions for 24 hours and evaluated at 24 and 72 hours following dosing. No information on concentration or basis for conclusion was given. Mild irritation was noted.

**Dinonylnaphthalene sulfonic acid, barium salt was mildly irritating to rabbit skin in this assay.**

(3) New Zealand White rabbits (6 of unspecified sex) were administered undiluted dinonylnaphthalene sulfonic acid, barium salt via the dermal route to intact and abraded skin at 0.5 mL under occluded conditions for 4 hours, at which time the test sites were washed. Evaluation for evidence of corrosion occurred at 4, 24 and 48 hours following dosing. No information on concentration or basis for conclusion was given. No evidence of corrosion was noted.

**Dinonylnaphthalene sulfonic acid, barium salt was not corrosive to rabbit skin in this assay.**

### *Eye Irritation*

#### *Subcategory I: Diisononylnaphthalene*

##### *Diisononylnaphthalene (CASRN 63512-64-1)*

New Zealand White rabbits (6, sex not specified) were administered diisononylnaphthalene instilled into one eye at 0.1 mL and not washed for 24 hours. Ocular evaluations were conducted at 24, 48 and 72 hours, and at 4, 7 and 14 days. No information on concentration or basis for conclusion was given. Mild eye irritation was noted.

**Diisononylnaphthalene was mildly irritating to rabbit eyes in this assay.**

#### *Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt*

##### *Dinonylnaphthalene sulfonic acid (CASRN 25322-17-2)*

New Zealand White rabbits (6, sex not specified) were administered 0.1 mL dinonylnaphthalene sulfonic acid in aliphatic hydrocarbon instilled into one eye and not washed for 24 hours. Ocular evaluations were conducted at 24, 48 and 72 hours, and at 4, 7 and 14 days. No information on concentration or basis for conclusion was given. Severe eye irritation was noted.

**Dinonylnaphthalene sulfonic acid was severely irritating to rabbit eyes in this assay.**

##### *Dinonylnaphthalene sulfonic acid, calcium salt (CASRN 57855-77-3)*

(1) New Zealand White rabbits (6, sex not specified) were administered 0.1 mL dinonylnaphthalene sulfonic acid, calcium salt in diluent oil instilled into one eye and not washed for 24 hours. Ocular evaluations were conducted at 24, 48 and 72 hours, and at 4, 7 and 14 days. No information on concentration or basis for conclusion was given. Eye irritation was noted.

**Dinonylnaphthalene sulfonic acid, calcium salt was irritating to rabbit eyes in this assay.**

(2) New Zealand White rabbits (3/sex) were administered 0.1 mL dinonylnaphthalene sulfonic acid, calcium salt in light mineral oil instilled into one eye. Eyes were examined at 1, 24, 48 and 72 hours and at 7 and 10 days following exposure and scored according to Draize. Corneal ulcerations were observed with 2% sodium fluorescein at 24 hours. Moderate to severe conjunctivitis and corneal opacities were also noted. All effects diminished over the course of the study.

**Dinonylnaphthalene sulfonic acid, calcium salt was irritating to rabbit eyes in this assay.**

***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

***Dinonylnaphthalene sulfonic acid, barium salt (CASRN 25619-56-1)***

(1) New Zealand White rabbits (6, sex not specified) were administered 0.1 mL dinonylnaphthalene sulfonic acid, barium salt in diluent oil instilled into one eye and not washed for 24 hours. Ocular evaluations were conducted at 24, 48 and 72 hours, and at 4, 7 and 14 days. No information on concentration or basis for conclusion was given. Severe eye irritation was noted.

**Dinonylnaphthalene sulfonic acid, barium salt was severely irritating to rabbit eyes in this assay.**

(2) New Zealand White rabbits (6, sex not specified) were administered 0.1 mL dinonylnaphthalene sulfonic acid, barium salt in corn oil instilled into one eye and not washed for 24 hours. Ocular evaluations were conducted at 24, 48 and 72 hours, and at 6 and 7 days. No information on concentration or basis for conclusion was given. Eye irritation was minimal.

**Dinonylnaphthalene sulfonic acid, barium salt was mildly irritating to rabbit eyes in this assay.**

(3) New Zealand White rabbits (3/sex) were administered 0.1 mL dinonylnaphthalene sulfonic acid, barium salt in light mineral oil instilled into one eye. Eyes were examined at 1, 24, 48 and 72 hours and at 7 and 10 days following exposure and scored according to Draize. Moderate to severe conjunctivitis were noted in all animals and corneal opacities were noted in four animals. Corneal ulcerations were observed with 2% sodium fluorescein at 24 hours in two rabbits. All effects diminished over the course of the study.

**Dinonylnaphthalene sulfonic acid, barium salt was moderately to severely irritating to rabbit eyes in this assay.**

***Sensitization***

***Subcategory I: Diisononylnaphthalene***

No data are available.

***Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt***

***Dinonylnaphthalene sulfonic acid, calcium salt (CASRN 57855-77-3)***

(1) Volunteers (104 total) were administered dinonylnaphthalene sulfonic acid, calcium salt in a repeated insult patch test/sensitization test as nine consecutive occlusive applications of the test compound (concentration not specified) administered every 48 hours over a 3-week period. The challenge phase was initiated 17 days following the ninth induction exposure at 0, 5 and 10% in mineral oil to previously unexposed sites. One individual exhibited a reaction suggestive of contact sensitization at the 96-hour observation. This subject was re-challenged with 0, 5, and 10% test material w/w in mineral oil and the vehicle (100% mineral oil) alone. No reactions indicative of contact sensitization were observed in the second challenge.

**Dinonylnaphthalene sulfonic acid, calcium salt was not sensitizing to human skin in this assay.**

(2) Ten male Hartley guinea pigs were administered dinonylnaphthalene sulfonic acid, calcium salt (50% in mineral oil; 0.4 ml per test site) in a Buehler Guinea Pig Sensitization Test. Three 6-hour induction exposures were conducted over 3 weeks. Following a 14-day rest, a challenge dose of the same concentration was applied to a naïve site and scored for sensitization (erythema and edema) at 24 hours. Ten positive control animals were treated with 0.08% dinitrochlorobenzene and five negative control animals were treated with the test material at the challenge only. One animal in the negative controls, showed mild erythema at 24 and 48 hours and minimal sensitization after the challenge. All test animals and five additional naïve controls were rested for an additional 7 days and re-challenged with the same concentration. The naïve controls showed no response on re-challenge. Five of 10 treated guinea pigs exhibited minimal to mild sensitization following the first challenge; 7 of 10 treated guinea pigs showed mild sensitization after the re-challenge. Summarized from TSCATS (OTS0000821).

**Dinonylnaphthalene sulfonic acid, calcium salt was sensitizing to guinea pig skin in this assay.**

***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

***Dinonylnaphthalene sulfonic acid, barium salt (CASRN 25619-56-1)***

(1) Volunteers (103/group) were administered dinonylnaphthalene sulfonic acid, barium salt in a repeated insult patch test/sensitization test as nine consecutive occlusive applications of the test compound (concentration not specified) administered every 48 hours over a 3-week period. The challenge phase was initiated 17 days following the ninth induction exposure at 0, 5 and 10% in mineral oil to previously unexposed sites. One individual exhibited a reaction suggestive of sensitization at 48 and 96 hours after challenge. Upon rechallenge, the subject showed irritation to the test compound in 10% w/w mineral oil at 96 hours, but not sensitization.

**Dinonylnaphthalene sulfonic acid, barium salt was not sensitizing to human skin in this assay.**

(2) Hartley guinea pigs (ten of mixed sex) were administered dinonylnaphthalene sulfonic acid, barium salt at a minimally irritating concentration (75% by weight in corn oil from an original 50:50 solution with mineral oil) in a Buehler Guinea Pig Sensitization Test. Three 6-hour induction exposures were conducted over 3 weeks, followed by a 14-day rest, then a challenge dose on an unexposed site. Irritation and sensitization was scored at 24 and 48 hours after challenge. Ten positive control animals were treated with dinitrochlorobenzene (DNCB; 0.08% in 80% ethanol for induction and 0.15% in acetone at challenge) and ten naïve control animals were treated with the test material (6% by weight in corn oil) at the challenge only. One of the positive control animals died of an undetermined cause and the remainder showed mild to severe sensitization. The negative controls showed negative or minimal response. Four of 10 treated guinea pigs exhibited a mild to moderate sensitization response. Summarized from TSCATS (OTS0000821-1).

**Dinonylnaphthalene sulfonic acid, barium salt was sensitizing to guinea pig skin in this assay.**



**Conclusion:**

***Subcategory I: Diisononylnaphthalene***

Acute toxicity of diisononylnaphthalene is low for the oral and dermal routes in rats and rabbits respectively and moderate for the inhalation route in rats. Diisononylnaphthalene is irritating to rabbit skin and eyes.

***Subcategory II: Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt***

Acute toxicity of dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt is low for the oral route in rats and the dermal route in rabbits. Acute inhalation toxicity in rats is low for dinonylnaphthalene sulfonic acid and moderate for dinonylnaphthalene sulfonic acid, calcium salt. Dinonylnaphthalene sulfonic acid and dinonylnaphthalene sulfonic acid, calcium salt are irritating to rabbit skin. Dinonylnaphthalene sulfonic acid is irritating to rabbit eyes. Dinonylnaphthalene sulfonic acid, calcium salt induced sensitization in guinea pigs. No sensitization was observed in human volunteers in a repeated insult patch sensitization test with dinonylnaphthalene sulfonic acid, calcium salt.

***Subcategory III: Dinonylnaphthalene sulfonic acid, barium salt***

Acute toxicity of dinonylnaphthalene sulfonic acid, barium salt is low by the oral route and moderate by the inhalation route in rats. Acute dermal toxicity in rabbits was low or moderate in two separate studies. Dinonylnaphthalene sulfonic acid, barium salt is irritating to rabbit skin and eyes and sensitizing to guinea pig skin. No sensitization was observed in human volunteers in a repeated insult patch sensitization test.

<b>Table 3. Summary of the Screening Information Data Set under the U.S. HPV Challenge Program – Human Health Data</b>				
<b>Endpoints</b>	<b>Subcategory I</b>	<b>Subcategory II</b>		<b>Subcategory III</b>
	<b>SPONSORED CHEMICAL Diisononylnaphthalene  (63512-64-1)</b>	<b>SPONSORED CHEMICAL Dinonylnaphthalene sulfonic acid  (25322-17-2)</b>	<b>SPONSORED CHEMICAL Dinonylnaphthalene sulfonic acid, calcium salt (57855-77-3)</b>	<b>SPONSORED CHEMICAL Dinonylnaphthalene sulfonic acid, barium salt (25619-56-1)</b>
<b>Acute Oral Toxicity LD<sub>50</sub> (mg/kg-bw)</b>	> 5000	> 5000	> 5000	1750
<b>Acute Inhalation Toxicity LC<sub>50</sub> (mg/L)</b>	> 17	> 200	> 18	> 21
<b>Acute Dermal Toxicity LD<sub>50</sub> (mg/kg-bw)</b>	> 20,000	> 2000	> 20,000	> 1000; < 20,000
<b>Repeated-Dose Toxicity NOAEL/LOAEL</b>	No Data.	No Data.	No Data.	No Data.
<b>Reproductive Toxicity NOAEL/LOAEL</b>	No Data.	No Data.	No Data.	No Data.

<b>Table 3. Summary of the Screening Information Data Set under the U.S. HPV Challenge Program – Human Health Data</b>				
<b>Endpoints</b>	<b>Subcategory I</b>	<b>Subcategory II</b>		<b>Subcategory III</b>
	<b>SPONSORED CHEMICAL</b> Diisononylnaphthalene  (63512-64-1)	<b>SPONSORED CHEMICAL</b> Dinonylnaphthalene sulfonic acid  (25322-17-2)	<b>SPONSORED CHEMICAL</b> Dinonylnaphthalene sulfonic acid, calcium salt (57855-77-3)	<b>SPONSORED CHEMICAL</b> Dinonylnaphthalene sulfonic acid, barium salt (25619-56-1)
<b>Developmental Toxicity</b> <b>NOAEL/LOAEL</b>	No Data.	No Data.	No Data.	No Data.
<b>Genetic Toxicity – Gene Mutation</b> <i>In vitro</i>	No Data.	No Data.	No Data.	No Data.
<b>Genetic Toxicity – Chromosomal Aberrations</b> <i>In vitro</i>	No Data.	No Data.	No Data.	No Data.
<b>Additional Information</b> <b>Skin Irritation</b>	<b>Mildly irritating</b>	<b>Moderately irritating</b>	<b>Moderately irritating</b>	<b>Moderately irritating</b>
<b>Eye irritation</b>	<b>Mildly irritating</b>	<b>Severely irritating</b>	<b>Irritating</b>	<b>Severely irritating</b>
<b>Sensitization</b>	–	–	<b>Sensitizing</b>	<b>Sensitizing</b>

Measured data in bold text; (RA) = Read Across; – indicates that endpoint was not evaluated 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 and Aquatic Invertebrates and Toxicity to Aquatic Plants***

No data were submitted for members of the dinonylnaphthalene category.

**Conclusion:**

***Subcategory I: Diisononylnaphthalene***

No toxicity data were submitted for fish, aquatic invertebrates or aquatic plants. However, acute and chronic toxicity are not expected at saturation in water due to the very low estimated water solubility/dispersibility value ( $\leq 4.3 \times 10^{-7}$  mg/L).

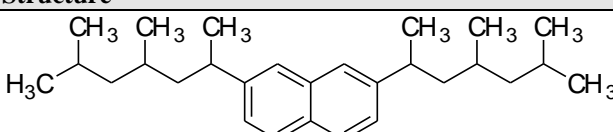
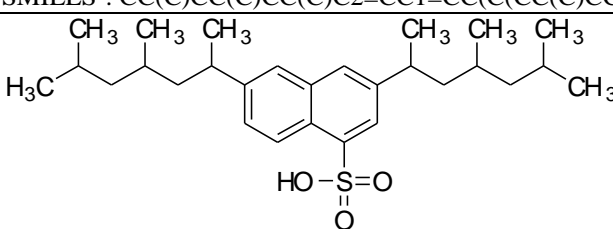
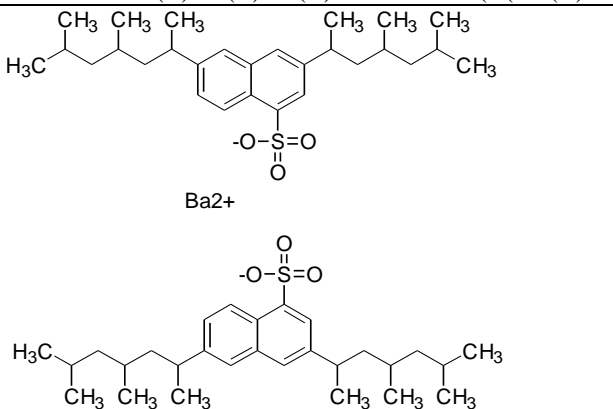
***Subcategory II: Dinonylnaphthalene sulfonic acid, dinonylnaphthalene sulfonic acid, calcium salt, and dinonylnaphthalene sulfonic acid, barium salt***

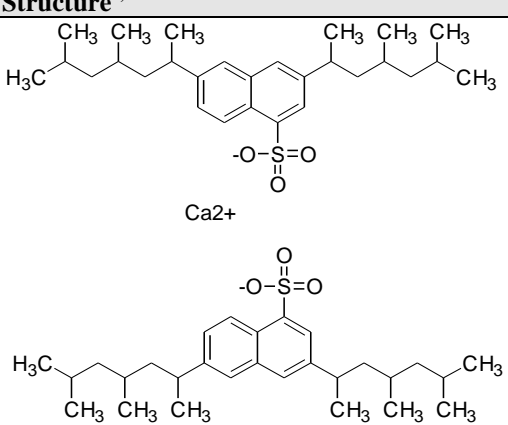
No toxicity data were submitted for fish, aquatic invertebrates or aquatic plants. However, acute and chronic toxicity are not expected at saturation in water due to the very low estimated water solubility/dispersibility values ( $\leq 6.7 \times 10^{-5}$  mg/L).

Table 4. Summary of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program – Aquatic Toxicity Data				
	Subcategory I	Subcategory II		
Endpoints	SPONSORED CHEMICAL Diisononylnaphthalene  (63512-64-1)	SPONSORED CHEMICAL Dinonylnaphthalene sulfonic acid  (25322-17-2)	SPONSORED CHEMICAL Dinonylnaphthalene sulfonic acid, calcium salt (57855-77-3)	SPONSORED CHEMICAL Dinonylnaphthalene sulfonic acid, barium salt (25619-56-1)
Fish 96-h LC <sub>50</sub> (mg/L)	NES	NES		
Aquatic Invertebrates 48-h EC <sub>50</sub> (mg/L)				
Aquatic Plants 72-h EC <sub>50</sub> (mg/L)				
Chronic Toxicity to Fish 21-d EC <sub>50</sub> (mg/L)				
Chronic Toxicity to Invertebrates 21-d EC <sub>50</sub> (mg/L)				

NES = No effects at saturation (water solubility/dispersibility limit).

**APPENDIX**

Sponsored Chemicals		
Chemical Name	CASRN	Structure <sup>1,2</sup>
Naphthalene, diisononyl-	63512-64-1	 <p>Representative structure SMILES<sup>3</sup>: <chem>CC(C)CC(C)CC(C)C2=CC=CC=C2C=C1=CC(C)CC(C)CC(C)C=C1</chem></p>
Naphthalene sulfonic acid, dinonyl-	25322-17-2	 <p>Representative structure SMILES<sup>3</sup>: <chem>CC(C)CC(C)CC(C)C2=CC=CC=C2C=C1=CC(C)CC(C)CC(C)C=C1C(S(=O)(O)=O)=C2</chem></p>
Naphthalene sulfonic acid, dinonyl-, barium salt (2:1)	25619-56-1	 <p>Representative structure SMILES<sup>3</sup>: <chem>CC(C)CC(C)CC(C)C2=CC=CC=C2C=C1=CC(C)CC(C)CC(C)C=C1C(S(=O)(O[Na])=O)=C2</chem></p>

Sponsored Chemicals		
Chemical Name	CASRN	Structure <sup>1,2</sup>
Naphthalene sulfonic acid, dinonyl-, calcium salt (2:1)	57855-77-3	 <p>Representative structure SMILES<sup>3</sup>: <chem>CC(C)CC(C)CC(C)C2=CC1=CC(C(CC(C)CC(C)C)C)=CC=C1C(S(=O)(ONa)=O)=C2</chem></p>

1. These substances are a mixture of various isomers. In order not to divulge confidential business information (CBI), EPA assumes that the sponsored substance includes both branched and unbranched (linear) alkyl groups.
2. Although the common names imply isononyl alkyl chains, the isononyl group is, in fact, a highly branched structure. The isononyl alkyl chain is derived from “nonene” which is actually a propylene trimer (i.e. tripropylene).
3. The SMILES notation used for the estimations was for a single naphthalene sulfonic acid sodium salt since this substance is expected to dissociate in solution to the anion of naphthalene sulfonic acid, dinonyl- and the free metal.