

## SCREENING-LEVEL HAZARD CHARACTERIZATION

### 2, 4-Pentanedione (CASRN 123-54-6)

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 or OECD HPV 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 presented in an international forum that involves review and endorsement by governmental

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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>.

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><b>123-54-6</b></p>
<p><b>Chemical Abstract Index Name</b></p>	<p><b>Acetylacetone; acetyl-propanone-2; 2,4-dioxopentane</b></p>
<p><b>Structural Formula</b></p>	
<p style="text-align: center;"><b>Summary</b></p> <p>CASRN 123-54-6 is a colorless to slightly yellowish liquid with high water solubility and high vapor pressure. It is expected to have high mobility in soil. CASRN 123-54-6 achieved 79-88% of its theoretical biochemical oxygen demand (BOD) over a 28 day incubation period and is considered readily biodegradable. The rate of volatilization is considered moderate. The rate of hydrolysis is considered negligible. The rate of atmospheric photooxidation is negligible. An estimated bioaccumulation factor of 1.0 suggests bioconcentration is low. CASRN 123-54-6 is expected to have low persistence (P1) and low bioaccumulation potential (B1).</p> <p>The acute toxicity of CASRN 123-54-6 to rats is low via the oral route and moderate via the dermal and inhalation routes. CASRN 123-54-6 is mildly irritating to the rabbit eye. In a 14-week repeated-dose inhalation toxicity study in rats, mortality in 30/30 females and 10/30 males at 2711 mg/L was observed. At 1217 mg/L, slight decreases in body weight gain (5% lower than controls) were observed in females, and minor alterations in hematology and in serum and urine analyses were observed in both sexes. The NOAEC for systemic toxicity is 417 mg/L. There are no specific reproductive toxicity studies for this chemical. However, no treatment-related histological or organ weight changes were observed in reproductive organs examined from the 14-week repeated-dose inhalation study in rats. The NOAEC for reproductive toxicity in rats is 2711 mg/L. A prenatal developmental toxicity study in rats exposed via vapor inhalation to CASRN 123-54-6 observed a significant reduction in maternal body weight gain at 1668 mg/L, the highest dose tested. The NOAEC for maternal toxicity is 834 mg/L. Signs of developmental toxicity consist of reduced fetal weights and reduced fetal ossification at 834 mg/L. The NOAEC for developmental toxicity is 209 mg/L. Equivocal results are observed on reproductive and gestational parameters in a dominant lethal assay. CASRN 123-54-6 is not mutagenic in bacterial cells, but induced chromosomal aberrations in mammalian cells <i>in vitro</i>. CASRN 123-54-6 does not induce micronuclei <i>in vivo</i>.</p> <p>The 96-hour LC<sub>50</sub> of CASRN 123-54-6 to fish is 60.1 mg/L. For a 48-hour static test in closed system for aquatic invertebrates of this chemical, the EC<sub>50</sub> is 34.4 mg/L. The 24-hour EC<sub>50</sub> value for aquatic plants exposed to this chemical is &gt;300mg/L, this value is supported by the ECOSAR 96-hour EC<sub>50</sub> algal value of 10.8 mg/L.</p>	

No data gaps were identified for SIDS endpoints.

The sponsor country, Germany, presented the SIDS documents at the OECD SIAM 13 during November 2001. The SIAR, SIAP and Dossier was finalized by OECD and published by UNEP in April 2004 (<http://www.chem.unep.ch/irptc/sids/OECDSEDS/PENTANEDIONE.pdf>). This hazard characterization includes EPA review of the SIDS documents and any relevant studies obtained through literature search.

## 1. Chemical Identity

### 1.1 Identification and Purity

See identification and purity information at:

<http://www.chem.unep.ch/irptc/sids/OECDSEDS/PENTANEDIONE.pdf>.

### 1.2 Physical-Chemical Properties

See physical-chemical properties at:

<http://www.chem.unep.ch/irptc/sids/OECDSEDS/PENTANEDIONE.pdf>.

## 2. General Information on Exposure

### 2.1 Production Volume and Use Pattern

CASRN 123-54-6 had an aggregated production and/or import volume in the United States between 1 and 10 million pounds during calendar year 2005.

Non-confidential information in the IUR indicated that the industrial processing and uses of the chemical include intermediates, solvents (which become part of product formulation or mixture), and solvents (for chemical manufacture and processing and are not part of product at greater than 1% by weight). Non-confidential commercial and consumer uses of this chemical include paints and coating, and other.

### 2.2 Environmental Exposure and Fate

See environmental exposure and fate data at:

<http://www.chem.unep.ch/irptc/sids/OECDSEDS/PENTANEDIONE.pdf>.

## 3. Human Health Hazard

See human health hazard data at:

<http://www.chem.unep.ch/irptc/sids/OECDSEDS/PENTANEDIONE.pdf>.

4. **Hazard to the Environment**

See environmental hazard data at:

<http://www.chem.unep.ch/irptc/sids/OECDSIDS/PENTANEDIONE.pdf>.