Supporting Documents for Initial Risk-Based Prioritization of High Production Volume Chemicals

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CASRN 126-86-3)
(9th CI and CA Index Name: 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-)

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BACKGROUND

Screening-level hazard, exposure and risk characterizations for high production volume chemicals (HPV) are important contributions to the chemicals cooperation work being done in North America[1] through the EPA Chemical Assessment and Management Program (ChAMP)[2]. These screening-level characterizations are developed by EPA for individual chemicals or chemical categories to support initial Risk-Based Prioritizations (RBPs) for HPV chemicals. These screening-level characterizations are technical documents intended primarily to inform the Agency's internal decision-making process. Accordingly, they are written for assessment professionals and assume a degree of technical understanding. Each of the support documents is described below.

The Risk-Based Prioritizations are found in an accompanying document and are written for a general audience. They present EPA's initial thinking regarding the potential risks presented by these chemicals and future possible actions that may be needed.

Hazard Characterizations for HPV Chemicals

EPA's screening-level hazard characterizations are based primarily on the review of the summaries of studies and other information submitted by the chemical sponsor(s) under the HPV Challenge Program[3]. These studies included in the scope of the HPV Challenge comprise the Screening Information Data Set (SIDS) of the Organization for Economic Cooperation and Development (OECD)[4], an internationally recognized battery of tests that provides the basic data necessary to make an initial evaluation of a chemical's hazards and fate. In preparing the initial hazard characterizations, EPA also consulted a variety of reliable sources[5] for additional relevant information and 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 an HPV submission, EPA also searched publicly available databases[6] for information entered from one year prior to the HPV submission through May 2008. The screening-level hazard characterization is performed according to established EPA guidance[7]. A more detailed description of the hazard characterization process is available on the EPA website[8].

With respect to chemicals for which internationally-accepted OECD SIDS Initial Assessment Profiles (SIAP) and Initial Assessment Reports (SIAR) were available, EPA did not generate its own screening-level hazard characterization, but did check for and incorporate updated information in the risk characterization.

Exposure Characterizations for HPV Chemicals

EPA recently received exposure-related data on chemicals submitted in accordance with the requirements of Inventory Update Reporting (IUR)[9]. The 2006 IUR submissions pertain to chemicals manufactured in

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[1] U.S. EPA – U.S. Commitments to North American Chemicals Cooperation: http://www.epa.gov/hpv/pubs/general/sppframework.htm.
[2] U.S. EPA – ChAMP information: http://www.epa.gov/champ/.
[3] U.S. EPA – HPV Challenge Program information: http://www.epa.gov/hpv.
[4] U.S. EPA – Technical Guidance Document, OECD SIDS Manual Sections 3.4 and 3.5: http://www.epa.gov/chemrtk/pubs/general/sidsappb.htm.
[5] U.S. EPA – Public Database Hazard Information: http://www.epa.gov/hpvis/hazardinfo.htm.
[6] U.S. EPA – Public Database Update Information: http://www.epa.gov/chemrtk/hpvis/updateinfo.htm.
[7] U.S. EPA – Risk Assessment Guidelines: http://cfpub.epa.gov/ncea/raf/rafguid.cfm.
[8] U.S. EPA – About HPV Chemical Hazard Characterizations: http://www.epa.gov/hpvis/abouthc.htm.
[9] U.S. EPA – Basic IUR Information: http://www.epa.gov/opptintr/iur/pubs/guidance/basic-information.htm.

(including imported into) the U.S. during calendar year 2005 in quantities of 25,000 pounds or more at a single site. The reports include the identity, the quantity, and the physical form of the chemical manufactured or imported, and the number of workers reasonably likely to be exposed during manufacture of the chemical. For chemicals manufactured or imported in quantities of 300,000 pounds or more at a single site, additional reported information includes: the industrial processing and uses of the chemical; the number of industrial processing sites and workers reasonably likely to be exposed to the chemical at those sites; the consumer and commercial uses of the chemical; and an indication whether the chemical was used in products intended for use by children under 14 years of age.

EPA's screening-level exposure characterizations are based largely on the information submitted under the IUR reporting, although other exposure information submitted to the Agency (for example, in HPV submissions) or readily available through a limited set of publicly accessible databases[10] was also considered. The screening-level Exposure Characterizations identify a potential (high, medium, or low) that each of five populations – the environment, the general population, workers, consumers, and children – might be exposed to the chemical. In most cases, this potential doesn't address the quantity, frequency, or duration of exposure, but refers only to the likelihood that an exposure could occur.

In many instances EPA is not able to fully disclose to the public all the IUR exposure-related data reviewed or relied upon in the development of the screening-level documents because some of the material was claimed as confidential business information (CBI) when it was submitted to the Agency. These CBI claims do limit the Agency's ability to be completely transparent in presenting some underlying exposure and use data for chemicals in public documents. EPA does consider all data, including data considered to be CBI, in the screening-level exposure and risk characterization process, and endeavors whenever possible to broadly characterize supporting materials claimed as confidential in ways that do not disclose actual CBI.

Risk Characterizations for HPV Chemicals

EPA combines the information from the screening-level exposure characterization with the screening-level hazard characterization to develop a qualitative screening-level risk characterization, as described in the Agency's guidance on drafting risk characterizations[11]. These screening-level risk characterizations are technical documents intended to support subsequent priority-setting decisions and actions by OPPT. The purpose of the qualitative screening-level risk characterization is two-fold: to support initial risk-based decisions to prioritize chemicals, identify potential concerns, and inform risk management options; and to identify data needs for individual chemicals or chemical categories.

These initial characterization and prioritization documents do not constitute a final Agency determination as to risk, nor do they determine whether sufficient data are available to characterize risk. Recommended actions reflect EPA's relative judgment regarding this chemical or chemical category in comparison with others evaluated under this program, as well as the uncertainties presented by gaps that may exist in the available data.

[10] U.S. EPA – Summary of Public Databases Routinely Searched: http://www.epa.gov/chemrtk/hpvis/pubdtsum.htm.
[11] U.S. EPA – Risk Characterization Program: http://www.epa.gov/osa/spc/2riskchr.htm.

QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION OF HIGH PRODUCTION VOLUME CHEMICALS

SPONSORED CHEMICAL

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS No. 126-86-3)
[9th CI Name: 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-]

September 2008

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QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION FOR 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS No. 126-86-3)

1. Physical-Chemical Properties and Environmental Fate

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is a colorless solid at room temperature with a moderate vapor pressure and high water solubility. In the environment, it is expected to partition primarily to soil and water. It is moderately mobile in soil and the rate of volatilization is considered moderate. In water, the rate of hydrolysis is considered negligible. The rate of vapor-phase photooxidation of 2,4,7,9-tetramethyl-5-decyne-4,7-diol in the ambient atmosphere is considered moderate. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol has a low potential to bioaccumulate (B1). The biodegradation rate of 2,4,7,9-tetramethyl-5-decyne-4,7-diol is slow to negligible; therefore, it is judged to have high persistence in the environment (P3).

2. Hazard Characterization

Aquatic Organism Toxicity. The acute toxicity of 2,4,7,9-tetramethyl-5-decyne-4,7-diol to fish, aquatic invertebrates and plants is low.

Human Health Toxicity. The acute toxicity of 2,4,7,9-tetramethyl-5-decyne-4,7-diol to rats exposed via oral, dermal and inhalation routes is low. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is moderately irritating to skin and highly irritating to eyes. Repeated oral exposure of rats and dogs to 2,4,7,9-tetramethyl-5-decyne-4,7-diol did not produce systemic toxicity. In an oral one-generation study in rats, there was low reproductive toxicity, and low maternal and developmental toxicity. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol did not show a potential for inducing gene mutation or chromosomal aberrations.

3. Exposure Characterization

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS# 126-86-3) has an aggregated production and/or import volume in the United States of 10 million to 50 million pounds. The industrial processing and uses reported in the Inventory Update Rule (IUR) submissions are claimed as confidential. The High Production Volume (HPV) submission for this chemical states that the chemical is used as an industrial defoaming nonionic surfactant in the coatings, ink and adhesives industries, or as a chemical intermediate. The Hazardous Substance Data Bank (HSDB) indicates that additional uses of 2,4,7,9-tetramethyl-5-decyne-4,7-diol are as a defoamer in paints and dye production, as a wetting agent in pesticide formulations, rinsing aids, and as a viscosity reducer in detergent formulations and penetrating agents.

Potential Exposures to the General Population and the Environment: Based on the information considered, i.e., the low biodegradation rate, the P3 rating, the use of this chemical in paint and adhesives, and the Agency's expert judgment, EPA identifies, for the purposes of risk-based prioritization, a high potential that the general population and the environment may be exposed. There is potential for environmental releases during manufacturing, processing, and use of this chemical. Persistence and bioaccumulation ratings for this chemical are P3 and B1. These

ratings suggest that this chemical is very persistent in the environment and is not bioaccumulative.

Potential Exposures to Workers: Based on the information considered (including IUR data, the HPV submission, and the HSDB data) and in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a high relative ranking for potential worker exposure. This relative ranking is based on the potential for significant dermal exposure and for inhalation of mists and/or particulates by a large number of workers in commercial settings, including spray application of products containing the subject substance, a relatively high number of industrial processing and uses, and a relatively high number of potentially exposed workers (> 1000 workers) at manufacturing, industrial processing and use sites.

Exposures to Consumers: EPA identifies, for the purposes of risk-based prioritization, a high potential that consumers might be exposed based on the use of products containing this chemical. Consumer uses were reported but this information was claimed to be confidential business information (CBI). There is also potential for exposure to consumers based on information from public data sources. This chemical may be used in paints, coatings, adhesives and dye production (HSDB). Depending on the consumer product, there may be dermal and/or inhalation exposures to consumers from vapors, mists, or particulates.

Exposures to Children: No uses in products intended to be used by children are reported in the IUR, nor are any found in other data sources. However, there may be potential exposure of children through the use of some consumer products, e.g., paints, adhesives. Therefore, EPA identifies, for the purposes of risk-based prioritization, a medium potential that children might be exposed.

4. Risk Characterization

The statements and rationale provided below are intended solely for the purpose of this screening-level and qualitative risk characterization and will be used for prioritizing substances for future work in the Chemical Assessment and Management Program (ChAMP).

Risk Statement and Rationale

Potential Risk to Aquatic Organisms from Environmental Releases: (LOW CONCERN). EPA identifies a high potential that aquatic organisms might be exposed from environmental releases. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol has a high persistence and low bioaccumulation. These characteristics in combination with the low toxicity to fish, and aquatic invertebrates and plants indicate a low concern to aquatic organisms from environmental releases.

Potential Risk to the General Population from Environmental Releases: (LOW CONCERN). EPA identifies a high potential that the general population might be exposed from environmental releases. The potential human health hazard is expected to be low due to the lack of specific toxicity in animals following repeat exposures.

Therefore, taken together, the available information suggests a low concern for potential risk to the general population from environmental releases.

Potential Risk to Workers: (LOW CONCERN). EPA identifies a high relative ranking for potential worker exposure. The potential human health hazard is expected to be low due to the lack of specific toxicity in animals following repeated exposures. There is potential for moderate to high skin and eye irritation; however, adherence to standard good industrial hygiene practices (gloves, respirators, goggles, and other protective clothing) to prevent irritation will limit the exposure to workers. Therefore, taken together, the available information suggests a low concern for potential risks to workers.

Potential Risk to Consumers from Known Uses: (LOW CONCERN). EPA identifies a high potential that consumers might be exposed. The potential human health hazard is expected to be low due to the lack of specific toxicity in animals following repeated exposures. Therefore, taken together, the available information suggests a low concern for potential risks to consumers. However, 2,4,7,9-tetramethyl-5-decyne-4,7-diol has moderate to high potential for skin and eye irritation in animal studies; therefore, there is concern for skin and eye irritation.

Potential Risk to Children: (LOW CONCERN). EPA identifies a medium potential that children might be exposed. There are no uses in products specifically intended to be used by children. Exposure to children, however, may be expected to occur through the household use of some consumer products. The potential human health hazard is expected to be low due to low toxicity in rats following exposure during early life-stages. Therefore, taken together, the available information suggests a low concern for potential risks to children.

SCREENING-LEVEL HAZARD CHARACTERIZATION OF HIGH PRODUCTION VOLUME CHEMICALS

SPONSORED CHEMICAL

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS No. 126-86-3)
[9th CI Name: 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-]

September 2008

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SCREENING LEVEL HAZARD CHARACTERIZATION
2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS No. 126-86-3)

Introduction

The sponsor, Air Products and Chemicals, Inc., submitted a Test Plan and Robust Summaries to EPA for 2,4,7,9-tetramethyl-5-decyne-4,7-diol (CAS No. 126-86-3; 9th CI name: 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-) on December 28, 2001. EPA posted the submission on the ChemRTK HPV Challenge Website on January 31, 2002 (http://www.epa.gov/chemrtk/pubs/summaries/tetramet/c13452tc.htm). EPA comments on the original submission were posted to the website on June 19, 2002. Public comments were also received and posted to the website. The sponsor submitted updated/revised documents on August 16, 2002, which were posted to the ChemRTK website on September 24, 2002.

This screening-level hazard characterization is based primarily on the review of the test plan and robust summaries of studies submitted by the sponsor(s) under the HPV Challenge Program. 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 2001 to May 2008: the NLM databases (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, IRIS, NTP, ATSDR, EXTOXNET, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. A summary table of SIDS endpoint data with the structure(s) of the sponsored chemical(s) is included in the appendix. The screening-level hazard characterization for environmental and human health toxicity is based largely on SIDS endpoints and is described according to established EPA or OECD effect level definitions and hazard assessment practices.

Hazard Characterization

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is a colorless solid at room temperature with a moderate vapor pressure and high water solubility. In the environment, it is expected to partition primarily to soil and water. It is moderately mobile in soil and the rate of volatilization is considered moderate. In water, the rate of hydrolysis is considered negligible. The rate of vapor-phase photooxidation of 2,4,7,9-tetramethyl-5-decyne-4,7-diol in the ambient atmosphere is considered moderate. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol has a low potential to bioaccumulate (B1). The biodegradation rate of 2,4,7,9-tetramethyl-5-decyne-4,7-diol is slow to negligible; therefore, it is judged to have high persistence in the environment (P3).

The acute toxicity of 2,4,7,9-tetramethyl-5-decyne-,7-diol to fish, aquatic invertebrates and aquatic plants is low.

The acute toxicity of 2,4,7,9-tetramethyl-5-decyne-4,7-diol to rats exposed via oral, dermal and inhalation routes is low. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is moderately irritating to skin and highly irritating to eyes. Repeated oral exposure of rats and dogs to 2,4,7,9-tetramethyl-5-decyne-4,7-diol did not produce systemic toxicity. In an oral one-generation study in rats, there was low reproductive toxicity, and low maternal and developmental toxicity. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol did not show a potential for inducing gene mutation or chromosomal aberrations.

No data gaps were identified under the HPV Challenge Program.

1. Physical-Chemical Properties and Environmental Fate

The physical-chemical properties of 2,4,7,9-tetramethyl-5-decyne-,7-diol are summarized in Table 1a, while its environmental fate properties are provided in Table 1b. The structure of the compound is provided in the Appendix.

Physical-Chemical Properties Characterization

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is a colorless solid at room temperature. It has a moderate vapor pressure and high water solubility.

Table 1a. Physical-Chemical Properties of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol[1]

Property	Value
CAS No.	126-86-3
Molecular Weight	226.36
Physical State	Colorless solid
Melting Point	54–55°C (measured)
Boiling Point	262–263°C (measured)
Vapor Pressure	0.0062–0.007 hPa at 20°C (measured)
Henry's Law Constant	8.58×10^{-7} atm-m^3/mol (estimated)[2]
Water Solubility	1.7 g/L at 20°C and pH 7.3–7.5 (measured)
Log K_{ow}	2.8 at 22°C (measured)

[1]Air Products and Chemicals, Inc. 2002. Robust Summary for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. http://www.epa.gov/chemrtk/pubs/summaries/tetramet/c13452tc.htm.

[2]US EPA. 2008. Estimation Programs Interface Suite™ for Microsoft® Windows, v 3.20. United States Environmental Protection Agency, Washington, DC, USA. http://www.epa.gov/opptintr/exposure/pubs/episuite.htm.

Environmental Fate Characterization

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is expected to partition primarily to soil and water, according to the results of a Level III fugacity model that assumes equal emission to air, water, and soil. It is moderately mobile in soil. The Henry's Law constant indicates that it is moderately volatile from moist soil and water. The rate of hydrolysis is considered negligible under environmental conditions (pH 5–9). The rate of vapor-phase photooxidation of 2,4,7,9-tetramethyl-5-decyne-4,7-diol in the ambient atmosphere is considered moderate. The estimated bioconcentration factor (BCF) of 119.9 indicates that 2,4,7,9-tetramethyl-5-decyne-4,7-diol has a low potential to bioaccumulate (B1). The rate of biodegradation of 2,4,7,9-tetramethyl-5-decyne-4,7-diol is slow to negligible based on the results of a ready biodegradation test; therefore, it is judged to have high persistence in the environment (P3).

Table 1b. Environmental Fate Characteristics of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol[1]	
Property	**Value**
Photodegradation Half-life	OH = 3.021 hours (estimated)[2] O_3 = 382 days (estimated; 7×10^{11} mol/cm^3 O_3)[2]
Aerobic Biodegradation	5% after 28 days OECD 301B Modified Strum test (not readily biodegradable); 15.7% biodegradation per day Modified SCAS test (inherently biodegradable)
Hydrolysis Half-life	Greater than one year at pH 4, pH 7, and pH 9 (measured)
Bioconcentration	BCF = 119.9 (estimated)[2,3]
Direct Photolysis	Not significant[3]
Log K_{oc}	2.41 (estimated)[2]
Fugacity (Level III Model)[2]	Air = 0.425% Water = 31.8% Soil = 67.4% Sediment = 0.383%
Persistence[4]	P3 (high)
Bioaccumulation[4]	B1 (low)

[1]Air Products and Chemicals, Inc. 2002. Robust Summary for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. http://www.epa.gov/chemrtk/pubs/summaries/tetramet/c13452tc.htm.
[2]US EPA. 2008. Estimation Programs Interface Suite™ for Microsoft® Windows, v 3.20. United States Environmental Protection Agency, Washington, DC, USA. http://www.epa.gov/opptintr/exposure/pubs/episuite.htm.
[3]Data not provided in robust summary.
[4]FR. 1999. Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) Page 60194–60204.

Conclusion: 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is a colorless solid at room temperature with a moderate vapor pressure and high water solubility. In the environment, it is expected to partition primarily to soil and water. It is moderately mobile in soil and the rate of volatilization is considered moderate. In water, the rate of hydrolysis is considered negligible. The rate of vapor-phase photooxidation of 2,4,7,9-tetramethyl-5-decyne-4,7-diol in the ambient atmosphere is considered moderate. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol has a low potential to bioaccumulate (B1). The biodegradation rate of 2,4,7,9-tetramethyl-5-decyne-4,7-diol is slow to negligible; therefore, it is judged to have high persistence in the environment (P3).

2. Environmental Effects – Aquatic Toxicity

Acute Toxicity to Fish

(1) Fathead minnows (*Pimephales promelas*) were exposed to 2,4,7,9-tetramethyl-5-decyne-4,7-diol at nominal concentrations of 0, 4, 8, 16, 32 and 64 mg/L for 96 hours under semi-static conditions. Deaths occurred within the first 24 hours of the test at the two highest concentrations.
96-h LC_{50} = 36 mg/L

(2) Carp (*Cyprinus carpio*) were exposed to 2,4,7,9-tetramethyl-5-decyne-4,7-diol at measured concentrations of 0, 10, 18, 32, 56 and 100 mg/L for 96 hours under static conditions. Deaths occurred within the first 24 hours of the test. Pigmentation and effects on swimming behavior were seen at concentrations of 18 mg/L and higher.
96-h LC_{50} = 42 mg/L

Acute Toxicity to Aquatic Invertebrates

(1) *Daphnia magna* were exposed to 2,4,7,9-tetramethyl-5-decyne-4,7-diol at nominal concentrations of 18, 32, 45, 100 and 180 mg/L for 48 hours.
48-h EC_{50} = 91 mg/L

(2) *D. magna* were exposed to 2,4,7,9-tetramethyl-5-decyne-4,7-diol at measured concentrations of 0, 62.5, 125, 250, 500 and 1000 mg/L for 48 hours.
48-h EC_{50} = 88 mg/L

Toxicity to Aquatic Plants

Green algae (*Pseudokirchneriella subcapitata*) cultures were exposed to 2,4,7,9-tetramethyl-5-decyne-4,7-diol at measured concentrations ranging from 1 to 100 mg/L for 72 hours.
96-h EC_{50} (biomass) = 15 mg/L
96-h EC_{50} (growth) = 82 mg/L

Conclusion: The acute toxicity of 2,4,7,9-tetramethyl-5-decyne-4,7-diol to fish, aquatic invertebrates and aquatic plants is low.

3. Human Health Effects

Acute Oral Toxicity

Sprague-Dawley rats were orally administered 2,4,7,9-tetramethyl-5-decyne-4,7-diol as a 5% solution in hydrous alcohol. No effects on mortality, clinical signs, body weight or changes during necropsy were seen.
LD_{50} > 500 mg/kg-bw

Acute Inhalation Toxicity

Rats were exposed to aerosolized 2,4,7,9-tetramethyl-5-decyne-4,7-diol via whole-body inhalation for 1 hour at a concentration of greater than 20 mg/L. No mortality was seen. Ocular and nasal irritation and decreased spontaneous activity were noted immediately following the exposure. All animals returned to normal within 3 hours. No changes were noted during necropsy of randomly selected test animals.
LC_{50} > 20 mg/L

Acute Dermal Toxicity

(1) An acute dermal toxicity test was conducted in rats. No study details were provided in the robust summary.
LD_{50} (rat) > 2000 mg/kg-bw

(2) New Zealand rabbits were dermally exposed to 1000 mg/kg-bw 2,4,7,9-tetramethyl-5-decyne-4,7-diol for 24 hours and the rabbits were observed for 14 days post-dose.
LD_{50} (rabbit) > 1000 mg/kg-bw

Repeated-Dose Toxicity

(1) Beagle dogs (4/sex/dose) were administered the test substance orally in gelatin capsules at doses of 0, 200, 250 or 300 mg/kg-bw/day for 91 days. There were no effects on food consumption, body weight, clinical chemistry, hematology and urinalysis parameters, gross pathology or histology. Mean liver weights and liver-to-body weight ratios were higher in all treated groups compared to the control group.
NOAEL = 300 mg/kg-bw/day

(2) In a 28-day dietary study, Long-Evans rats, 6 animals/dose/group, were administered the test substance at 625, 1250, 2500 or 5000 ppm (corresponding to approximately 31.25, 62.5, 125 or 250 mg/kg-bw/day). There were no effects on mortality, body weight, or gross necropsy observations. No histopathology data were provided.
NOAEL ~ 250 mg/kg-bw/day)

Reproductive/Developmental Toxicity

In a one-generation reproduction study, 10 male and 20 female Sprague-Dawley rats were administered 2,4,7,9-tetramethyl-5-decyne-4,7-diol at 0, 500, 1000 or 2000 mg/kg-bw/day via the diet. Parental animals (F_0) were fed

their respective diets from the start of cohabitation until their scheduled sacrifice, males following the 20th day of breeding and females when their litters were weaned at 21 days of age. Dosing of the offspring (F_{1a}) continued for 91 days after weaning. The parental (F_0) females showed decreased body weight and lactation indices in the high dose group and normal histology of reproductive organs. Fertility, viability and gestation indices were not affected by treatment. The offspring (F_{1a}) showed a significant decrease in body weight gain in both sexes at the mid- and high dose groups, and in the low-dose males during the first 8 weeks. A marked increase in absolute and relative liver weights in the mid- and high-dose groups was also seen with corresponding histopathology showing mild to moderate centrilobular cloudy swelling of hepatocytes.
LOAEL (parental systemic toxicity) = 2000 mg/kg-bw/day (based on decreased body weight of females)
NOAEL (parental systemic toxicity) = 1000 mg/kg-bw/day
LOAEL (reproductive/developmental toxicity) = 1000 mg/kg-bw/day (decreased body weight gain in both sexes of pups, increased liver weights and associated histopathology in pups)
NOAEL (reproductive/developmental toxicity) = 500 mg/kg-bw/day

Genetic Toxicity – Gene Mutation

In vitro
Mutagenic activity for 2,4,7,9-tetramethyl-5-decyne-4,7-diol was investigated in a Reverse Mutation Assay in *Salmonella typhimurium* strains TA98, TA100, TA1535, and TA1537 and *Escherichia coli* strain WP2(uvrA) at 10, 50, 100, 500, 1000 and 5000 µg/plate, in the presence and absence of metabolic activation. No information on positive or negative controls was provided in the robust summary. Cytotoxicity was noted at dose levels of 1000 and 5000 µg/plate. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol treatment did not result in an increase in revertant colonies in any of the strains tested.
2,4,7,9-Tetramethyl-5-decyne-4,7-diol was not mutagenic in this assay.

Genetic Toxicity – Chromosomal Aberrations

In vitro
An *in vitro* cytogenetic assay was performed using Chinese Hamster Ovary cells exposed to 2,4,7,9-tetramethyl-5-decyne-4,7-diol concentrations of 19.5, 39.1, 78.1-78.3, 156.3, 312.5, 1250 and 3500 µg/mL, in the presence and absence of metabolic activation. Cytotoxicity was evident at 312.5 µg/mL and higher. There was no statistically significant increase in the number of cells with structural aberrations at the three non-cytotoxic concentrations, with and without metabolic activation (39.1, 78.1-78.3 and 156.3 µg/mL). The mitotic index was comparable to that for the control.
2,4,7,9-Tetramethyl-5-decyne-4,7-diol did not induce chromosomal aberrations at non-cytotoxic concentrations.

Additional Information

Skin Irritation

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was mildly irritating when applied to rabbit's intact skin as a paste under semi-occlusive conditions. When melted and applied to the rabbit's intact skin for 4 hours under semi-occlusive conditions, 2,4,7,9-tetramethyl-5-decyne-4,7-diol was moderately irritating.

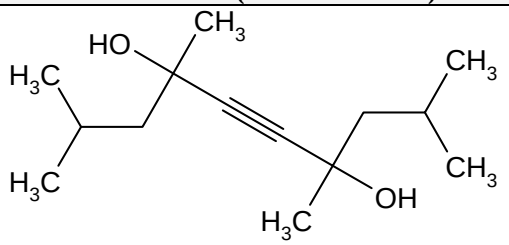
Eye Irritation

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was highly irritating to rabbit eyes. In unwashed eyes, corneal opacity (persisted to day 21), iritis (cleared by day 7) and conjunctival irritation (cleared by day 14) were seen. In the washed eyes, corneal opacity cleared by day 14, iritis by day 7 and conjunctival irritation by day 14.

Conclusion: The acute toxicity of 2,4,7,9-tetramethyl-5-decyne-4,7-diol to rats exposed via oral, dermal and inhalation routes is low. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is moderately irritating to skin and highly irritating to eyes. Repeated oral exposure of rats and dogs to 2,4,7,9-tetramethyl-5-decyne-4,7-diol did not produce systemic toxicity. In an oral one-generation study in rats, there was low reproductive toxicity, and low maternal and

developmental toxicity. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol did not show a potential for inducing gene mutation or chromosomal aberrations.

APPENDIX

Summary Table of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program	
Endpoints	**SPONSORED CHEMICAL 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS No. 126-86-3)**
Structure	
Summary of Environmental Effects – Aquatic Toxicity Data	
Fish **96-h LC_{50} (mg/L)**	36 - 42
Aquatic Invertebrates **48-h EC_{50} (mg/L)**	88 - 91
Aquatic Plants **72-h EC_{50} (mg/L)** **(growth)** **(biomass)**	 15 82
Summary of Human Health Data	
Acute Oral Toxicity **LD_{50} (mg/kg-bw)**	> 500
Acute Dermal Toxicity **LD_{50} (mg/kg-bw)**	> 1000 (rabbits) to > 2000 (rats)
Acute Inhalation Toxicity **LC_{50} (mg/L/6h/day)**	> 20
Repeated-Dose Toxicity **NOAEL (mg/kg-bw/day)**	NOAEL = 5000 ppm (250 mg/kg, rat) NOAEL = 300 mg/kg (dog)
Reproductive/ Developmental Toxicity **NOAEL/LOAEL (mg/kg-bw/day)** **(parental systemic toxicity)** **(reproductive/developmental toxicity)**	 LOAEL = 2000 NOAEL = 1000 LOAEL = 1000 NOAEL = 500
Genetic Toxicity – Gene Mutation ***In vitro***	Negative
Genetic Toxicity – Chromosomal Aberrations ***In vitro***	Negative
Additional Information **Skin irritation** **Eye irritation**	 Moderately irritating Highly irritating

Screening Level Exposure Characterization for HPV Challenge Chemical

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS No. 126-86-3) [9th CI Name: 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-]

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Screening Level Exposure Characterization
5, Decyne-4, 7-Diol, 2,4,7,9-Tetramethyl- (CAS # 126-86-3)

Non-CBI Executive Summary

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS# 126-86-3) has an aggregated production and/or import volume in the United States of 10 million to 50 million pounds.[12] The industrial processing and uses reported in the Inventory Update Rule (IUR) submissions are claimed as confidential. The High Production Volume (HPV) submission for this chemical states that the chemical is used as an industrial defoaming nonionic surfactant in the coatings, ink and adhesives industries, or as a chemical intermediate.[13] The Hazardous Substance Data Bank (HSDB) indicates that additional uses of 2,4,7,9-tetramethyl-5-decyne-4,7-diol are as a defoamer in paints, coatings, adhesives and dye production, as a wetting agent in pesticide formulations, rinsing aids, a viscosity reducer, in detergent formulations and penetrating agents.[14]

Potential Exposures to the General Population and the Environment: Based on the information considered, i.e., the low biodegradation rate, the P3 rating, the use of this chemical in paint and adhesives, and the Agency's expert judgment, EPA identifies, for purposes of risk-based prioritization, that the potential for exposure to the general population and the environment is high. There is potential for environmental releases during manufacturing, processing, and use of this chemical. Persistence and bioaccumulation ratings for this chemical are P3 and B1. These ratings suggest that this chemical is very persistent in the environment and is not bioaccumulative.

Potential Exposures to Workers: Based on the information considered (including IUR data, the HPV submission, and the HSDB data) and in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a high relative ranking for the potential worker exposure. This relative ranking is based on the potential for significant dermal exposure and for inhalation of mists and/or particulates by a large number of workers in commercial settings, including spray application of products containing the subject substance, a relatively high number of industrial processing and uses, and a relatively high number of potentially exposed workers (> 1000 workers) at manufacturing, industrial processing and use sites.

Exposures to Consumers: EPA identifies, for the purposes of risk-based prioritization, that the potential for exposures to consumers based on the use of products containing this chemical is high. Consumer uses were reported but this information was claimed to be confidential business information (CBI).

[12] USEPA, 2006 Partial Updating of TSCA Chemical Inventory
[13] USEPA, 2001. IUCLID Data Set. Accessed, 5/14/08. http://www.epa.gov/chemrtk/pubs/summaries/tetramet/c13452rs.pdf
[14] HSDB, 2008. Hazardous Substances Data Bank. Accessed, 5/14/08, CHEMICAL 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol. http://toxnet.nlm.nih.gov/

There is also potential for exposure to consumers based on information from public data sources. This chemical may be used in paints, coatings, adhesives and dye production (HSDB).

Depending on the consumer product, there may be dermal and/or inhalation exposures to consumers from vapors, mists, or particulates.

Exposures to Children: No uses in products intended to be used by children are reported in the IUR, nor are any found in other data sources. However, there may be potential exposure of children through the use of some consumer products, e.g., paints, adhesives. Therefore, EPA identifies, for the purposes of risk-based prioritization, that the potential for exposure to children is medium.

Volume and Use Information

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS# 126-86-3) has an aggregated production and/or import volume in the United States of 10 million to 50 million pounds (IUR).[15] The companies and sites that manufactured and/or imported this chemical are claimed confidential in the IUR submissions. Persons submitting IUR information for 2005 asserted that some or all of the information was confidential. Data and information that are confidential have been excluded from this summary. According to the IUR submissions, the industrial processing and uses, and commercial/consumer uses are claimed confidential.

The HPV submission for this chemical states that the chemical is mostly used as an industrial defoaming nonionic surfactant for predominantly waterborne applications in the coatings, ink, and adhesive industries. It is generally used at low levels, typically 0.1 – 0.5%. In the coatings industry, it is used in waterborne architectural, industrial maintenance, general industrial, wood, plastic, concrete and paper coatings. In the ink industry, it is used in water-based printing inks, overprint varnish systems, lithographic fountain solutions, and pigment grinding applications. In the adhesives industry, it is used as a component of pressure sensitive adhesives, plywood adhesives, and laminating adhesives. Other uses include industrial cleaners, agriculture, latex dipping, emulsion polymerization, foundry and metalworking fluids, and chemical processing.

In addition to the use as a surfactant, the HPV submission also states that it is used as a chemical intermediate and is converted into a polyethylene glycol ether surfactant, also for use in industrial applications.[16]

The HSDB indicates that additional uses of 2,4,7,9-tetramethyl-5-decyne-4,7-diol is as defoamer in paints, coatings, adhesives and dye production, as a wetting agent in pesticide formulations, rinsing aids, a viscosity reducer, in detergent formulations and penetrating agents.[17]

[15] USEPA, 2006 Partial Updating of TSCA Chemical Inventory
[16] Air Products and Chemicals, Inc. 2002. Robust Summary for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. http://www.epa.gov/chemrtk/pubs/summaries/tetramet/c13452tc.htm.
[17] HSDB, 2008. Hazardous Substances Data Bank. Accessed 5/14/08, http://toxnet.nlm.nih.gov/.

Exposures to Workers

Based on the information considered (including IUR data, the HPV submission, and HSDB data) and in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a high relative ranking for potential worker exposure. This relative ranking is based on the potential for significant dermal exposure and for inhalation of mists and/or particulates by a large number of workers in commercial settings including spray application of products containing the subject substance, a relatively large number of industrial processing and uses, and a relatively high number of potentially exposed workers (> 1000 workers) at manufacturing, industrial processing and use sites. The following is a summary of relevant information affecting occupational exposure.

Summary of Parameters affecting Worker Exposure

Parameter	
Volume*	10 million to 50 million pounds
Physical Form(s)*	CBI
Vapor Pressure	0.00465-0.00525 torr at 20°C (measured)
Concentration*	CBI
Number of Industrial Workers*	> 1000 (including those in manufacturing, processing and use)
Uses	surfactant mostly in the coatings, ink, adhesives.
Key MSDS Info	same as in section below

* Non-confidential IUR data are included in this summary

Based on IUR data, the maximum total number of workers reasonably likely to be exposed to this chemical during manufacturing and industrial processing and use may be 1,000 or greater. This estimate does not include potentially exposed commercial workers. The National Occupational Exposure Survey (NOES), conducted from 1981 to 1983, estimated a total of 66,526 workers potentially exposed to this chemical.[18] Differences between numbers of workers estimated by IUR submitters and by the NOES are attributable to many factors, including time, scope, and method of the estimates. For example, NOES estimates are for all workplaces while IUR data are for industrial workplaces only, and NOES used a survey and extrapolation method while IUR submitters simply provide their best estimates based on available information for the specific reporting year.

Based on IUR data, the physical form of this chemical is claimed confidential. Also, the maximum concentration is claimed confidential

This chemical does not have OSHA Permissible Exposure Limits (PELs).[19]

[18] NIOSH, 1983. National Occupational Exposure Survey (NOES, 1981-1983). Accessed, 5/14/08. http://www.cdc.gov/noes/noes2/x9984occ.html

[19] NIOSH, 1988. OSHA PEL Project Documentation. http://www.cdc.gov/niosh/pel88/npelcas.html, Accessed, 5/19/08.

Environmental Releases

Environmental releases may impact general population and environmental exposures. Factors affecting releases include volumes produced, processed and used; numbers of sites; and, processes of manufacture, processing, and use.

Based on IUR data, there are a relatively high number of industrial sites using the chemicals. The number of commercial sites that may use the chemical in pure form or as part of a mixture was claimed to be confidential information.

The chemical is not on the Toxics Release Inventory.[20] No additional data on releases were available from other sources.

Based on the uses in the HPV submission it is expected that there will be releases to various media (air, land, and water). The actual percentages and quantities of the releases of this chemical are not known.

Exposures to the General Population and the Environment

Based on the information under the release section above, it is likely that there would be some releases to water and/or air during manufacturing, processing, and use. A search of additional relevant databases did not provide any further information on releases of this chemical. EPA identifies, for the purposes of risk-based prioritization, that the potential for environmental release and subsequent exposure to the general population and the environment is likely. The IUR ranking for general population and the environment is high due to the likelihood that there will be exposure to this chemical based on public data sources that indicate this chemical is used in consumer products such as architectural coatings and adhesives and therefore, it is likely that there will be potential for environmental release and subsequent exposure to the general population and the environment.

Persistence and bioaccumulation ratings for this chemical are P3 and B1. These ratings suggest that this chemical is very persistent in the environment and is not bioaccumulative. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is a colorless solid at room temperature with a moderate vapor pressure and high water solubility. In the environment, it is expected to partition primarily to soil and water. It is moderately mobile in soil and the rate of volatilization is considered moderate. In water, the rate of hydrolysis is considered negligible. The rate of vapor-phase photooxidation of 2,4,7,9-tetramethyl-5-decyne-4,7-diol in the ambient atmosphere is considered moderate. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol has a low potential to bioaccumulate (B1). The biodegradation rate of 2,4,7,9-tetramethyl-5-decyne-4,7-diol is slow to negligible; therefore, it is judged to have high persistence in the environment (P3).

Based on the totality of the information considered, i.e., the low biodegradation rate, the P3 rating, the use of this chemical in paint and adhesives, and the Agency's expert judgment, EPA

[20] USEPA, 2006. Toxic Release Inventory. Accessed, 5/14/08. http://www.epa.gov/tri/

identifies, for purposes of risk-based prioritization, a high potential that the general population and the environment might be exposed.

Exposures to Consumers

Consumer uses are included in IUR data, and all of these are claimed confidential (Table 2). There is also potential for exposure to consumers based on information from public data sources. This chemical may be used in paints, coatings, adhesives and dye production.[21] Potential exposure to consumers and children is likely from this airborne chemical when contained in a consumer product.

Depending on the consumer product, there may be dermal and/or inhalation exposures to consumers from vapors, mists, or particulates. EPA identifies, for the purposes of risk-based prioritization, a high potential that consumers might be exposed from products containing this chemical based on IUR data and information from public data sources that indicate this chemical is contained in a consumer product.

Exposures to Children

No uses in products intended to be used by children were reported in the IUR, nor were any found in other data sources. However, there may be potential exposure of children through the use of some consumer products, e.g., paints, adhesives, etc. Therefore, EPA identifies, for the purposes of risk-based prioritization, a medium potential that children might be exposed.

[21] HSDB, 2008. Hazardous Substances Data Bank. Accessed, 5/14/08, CHEMICAL 5, Decyne-4, 7-diol, 2,4,7,9-tetramethyl-. http://toxnet.nlm.nih.gov/.

Non Confidential IUR Data Summary: 5, Decyne-4, 7-Diol, 2,4,7,9-Tetramethyl- (CAS # 126-86-3)

Manufacturing/ Import Information

Production (including import volume):	10 million to 50 million pounds
List of non-CBI companies/ sites:	Confidential
Maximum number of exposed workers:	1,000 or greater (including those in manufacturing, processing and use)
Highest non-CBI maximum concentration:	Confidential
Non-CBI physical forms:	Confidential

Table 1
Industrial Processing and Use Information
Reported in 2006 IUR

Processing Activity	Industrial Sector	Function in Ind. Sector
Claimed as CBI		

Table 2
Commercial/Consumer Uses
Reported in 2006 IUR

Commercial/ Consumer Product Category Description	Highest maximum concentration range	Use in Children's Products
Claimed as CBI	Confidential	Confidential