

US EPA ARCHIVE DOCUMENT



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  
WASHINGTON, D.C. 20460

OFFICE OF PREVENTION,  
PESTICIDES, AND TOXIC SUBSTANCES

DATE: May 22, 2006

**ACTION MEMORANDUM**

**SUBJECT:** Inert Ingredient Reassessment for 2,4,7,9-Tetramethyl-5-decyn-4,7-diol (CAS Reg. No. 126-86-3) and 3,6-Dimethyl-4-octyn-3,6-diol (CAS Reg. No. 78-66-0)

**FROM:** Pauline Wagner, Chief *Pauline Wagner 5/26/06*  
Inert Ingredient Assessment Branch  
Registration Division (7505P)

**TO:** Lois A. Rossi, Director  
Registration Division (7505P)

**I. FQPA REASSESSMENT ACTION**

**Action:** Reassessment of six exemptions from the requirement of a tolerance. The reassessment decision is to maintain all of the exemptions "as-is".

**Chemicals:** 2,4,7,9-Tetramethyl-5-decyn-4,7-diol (CAS Reg. No. 126-86-3)  
3,6-Dimethyl-4-octyn-3,6-diol (CAS Reg. No. 78-66-0)

Table 1. Exemptions from the Requirement of a Tolerance

CFR Citation				CAS Reg. No. 9CI Name
40 CFR §	Inert Ingredients	Limits	Uses	
180.910 <sup>a</sup>	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	Not more than 2.5% of pesticide formulation	Surfactants, related adjuvants of surfactants	126-86-3 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-
180.920 <sup>b</sup>	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	In pesticide formulations, for application to soil prior to planting or to plants before edible parts form	Surfactants, related adjuvants of surfactants	
180.930 <sup>c</sup>	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	Not more than 2.5% of pesticide formulation	Surfactants, related adjuvants of surfactants	

CFR Citation				CAS Reg. No. 9CI Name
40 CFR §	Inert Ingredients	Limits	Uses	
180.910	3,6-Dimethyl-4-octyn-3,6-diol	Not more than 2.5% of pesticide formulation	Surfactants, related adjuvants of surfactants	78-66-0 4-Octyne-3,6-diol, 3,6-dimethyl-
180.920	3,6-Dimethyl-4-octyn-3,6-diol	In pesticide formulations, for application to soil prior to planting or to plants before edible parts form	Surfactants, related adjuvants of surfactants	
180.930	3,6-Dimethyl-4-octyn-3,6-diol	Not more than 2.5% of pesticide formulation	Surfactants, related adjuvants of surfactants	

<sup>a</sup>Residues listed in 40 CFR 180.910 are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest.

<sup>b</sup>Residues listed in 40 CFR 180.920 are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only.

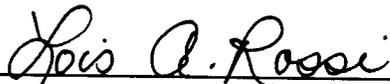
<sup>c</sup>Residues listed in 40 CFR 180.930 are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals.

**Pesticide Use:** These chemicals are used as surfactants in pesticide formulations applied to growing crops, raw agricultural commodities, and animals with use limitations of not more than 2.5% in formulation and application to soil prior to planting or to plants before the edible parts form.

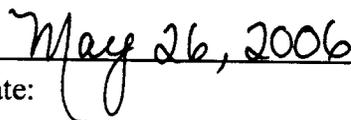
## II. MANAGEMENT CONCURRENCE

I concur with the reassessment of the three exemptions from the requirement of a tolerance for 2,4,7,9-tetramethyl-5-decyn-4,7-diol (CAS Reg. No. 126-86-3) and the three exemptions from the requirement of a tolerance for 3,6-dimethyl-4-octyn-3,6-diol (CAS Reg. No. 78-66-0).

I consider the exemptions established in 40 CFR parts 180.910, 180.920, and 180.930 to be reassessed for purposes of FFDCA's section 408(q) as of the date of my signature, below. A Federal Register Notice regarding this tolerance exemption reassessment decision will be published in the near future.



Lois A. Rossi, Director  
Registration Division



Date:

cc: Debbie Edwards, SRRD  
Joe Nevola, SRRD



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  
WASHINGTON, D.C. 20460

OFFICE OF PREVENTION,  
PESTICIDES, AND TOXIC SUBSTANCES

May 22, 2006

**MEMORANDUM**

**SUBJECT:** Reassessment of Six Exemptions from the Requirement of a Tolerance:  
Three Exemptions for 2,4,7,9-Tetramethyl-5-decyn-4,7-diol (CAS Reg. No. 126-86-3) and Three Exemptions for 3,6-Dimethyl-4-octyn-3,6-diol (CAS Reg. No. 78-66-0)

**FROM:** Keri Grinstead  
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Registration Division (7505P)  
And  
Christina M. Jarvis  
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**TO:** Pauline Wagner, Chief  
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Registration Division (7505P)

**Background**

Attached is the science assessment for 2,4,7,9-tetramethyl-5-decyn-4,7-diol (CAS Reg. No. 126-86-3) and 3,6-dimethyl-4-octyn-3,6-diol (CAS Reg. No. 78-66-0).

This assessment summarizes available information on the use, physical/chemical properties, toxicological effects, exposure profile, environmental fate, and ecotoxicity of these chemicals. The purpose of this document is to reassess the six existing exemptions from the requirement of a tolerance for residues of these chemicals when used as inert ingredients in pesticide products as required under the Food Quality Protection Act (FQPA).

**Executive Summary**

This document evaluates 2,4,7,9-tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol; pesticide inert ingredients which each have exemptions from the requirement for a tolerance under 40 CFR 180.910, 180.920, and 180.930. An inert ingredient is defined by the U.S. Environmental Protection Agency (USEPA) as any ingredient in a pesticide product that is not intended to affect a target pest.

As inert ingredients in pesticide products, these substances are exempted from the

requirement of a tolerance under 40 CFR 180.910 when used as surfactants at not more than 2.5% in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest, under 40 CFR 180.920 when used as surfactants in pesticide formulations applied to growing crops only and limited to application to the soil prior to planting or to plants before the edible parts form, and under 40 CFR 180.930 when used as surfactants at not more than 2.5% in pesticide formulations applied to animals.

Pesticide products containing these substances as inert ingredients are used as herbicides, fungicides, and insecticides. Industrial uses of these products include use as surfactants, defoamers, and wetting agents. They are also used in consumer products such as detergents, paints, coatings, adhesives, metal working formulations, and shampoo.

2,4,7,9-Tetramethyl-5-decyn-4,7-diol is part of the Agency's High Production Volume Challenge Program and the data submitted under this program has been used as the basis of this assessment. The available data consists of acute, subchronic, and chronic studies in animals, as well as genotoxicity, reproductive, and developmental toxicity studies submitted in support of its membership in the Agency's High Production Volume Challenge Program.

There are no available applicable toxicity data for 3,6-dimethyl-4-octyn-3,6-diol; however, the Agency has determined that 2,4,7,9-tetramethyl-5-decyn-4,7-diol is a suitable analog (based on structural similarities) and its data are adequate to characterize the activity/toxicity of 3,6-dimethyl-4-octyn-3,6-diol. Based on their similar structure activity relationships (SAR), use patterns, and potential routes of exposure from their use in pesticide products, these two chemicals are being grouped together in this reassessment document.

Based on the available data, 2,4,7,9-tetramethyl-5-decyn-4,7-diol is of low to moderate acute oral and inhalation toxicity, with acute effects of greatest concern being eye and skin irritation. It is not mutagenic and no increased offspring sensitivity was observed in a one-generation reproduction study. Based on their structural similarity, the toxicity of 3,6-dimethyl-4-octyn-3,6-diol is expected to be similar to 2,4,7,9-tetramethyl-5-decyn-4,7-diol. Their use/application limitations and likely biodegradation prior to transport to a drinking water treatment facility are expected to limit exposures of concern to residues of these chemicals (from food and drinking water) when used as inert ingredients in pesticide products.

Taking into consideration available toxicity and exposure information, the Agency has determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure (dietary and non-occupational sources of exposure) to 2,4,7,9-tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol when used as inert ingredients in pesticide formulations. Therefore, it is recommended that their exemptions from the requirement of a tolerance under 40 CFR 180.910, .920, and .930 be considered reassessed as safe under section 408(q) of the Federal Food, Drug, and Cosmetic Act.

## **I. Introduction**

This report provides a qualitative assessment for 2,4,7,9-tetramethyl-5-decyn-4,7-diol, and 3,6-dimethyl-4-octyn-3,6-diol, pesticide inert ingredients with three tolerance exemptions

each (for a total of six tolerance exemptions) under 40 CFR 180.910, .920, and .930. There are no available applicable toxicity data for 3,6-dimethyl-4-octyn-3,6-diol; however, based on its structural similarities to 2,4,7,9-tetramethyl-5-decyn-4,7-diol, the data for 2,4,7,9-tetramethyl-5-decyn-4,7-diol has been determined to be adequate to characterize the activity/toxicity of 3,6-dimethyl-4-octyn-3,6-diol. Based on their similar structure activity relationships (SAR), use patterns, and potential routes of exposure from their use in pesticide products, these two chemicals are being grouped together in this reassessment document and the available data for 2,4,7,9-tetramethyl-5-decyn-4,7-diol is used as the basis of the assessment of these two chemicals.

## II. Use Information

### A. Pesticide Uses

The exemptions from the requirement of a tolerance are provided in Table 1 below.

**Table 1. Pesticide Uses**

CFR Citation				CAS Reg. No. 9CI Name
40 CFR §	Inert Ingredients	Limits	Uses	
180.910 <sup>a</sup>	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	Not more than 2.5% of pesticide formulation	Surfactants, related adjuvants of surfactants	126-86-3 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-
180.920 <sup>b</sup>	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	In pesticide formulations, for application to soil prior to planting or to plants before edible parts form	Surfactants, related adjuvants of surfactants	
180.930 <sup>c</sup>	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	Not more than 2.5% of pesticide formulation	Surfactants, related adjuvants of surfactants	
180.910	3,6-Dimethyl-4-octyn-3,6-diol	Not more than 2.5% of pesticide formulation	Surfactants, related adjuvants of surfactants	78-66-0 4-Octyne-3,6-diol, 3,6-dimethyl-
180.920	3,6-Dimethyl-4-octyn-3,6-diol	In pesticide formulations, for soil prior to planting or to plants before edible parts form	Surfactants, related adjuvants of surfactants	
180.930	3,6-Dimethyl-4-octyn-3,6-diol	Not more than 2.5% of pesticide formulation	Surfactants, related adjuvants of surfactants	

<sup>a</sup> Residues listed in 40 CFR 180.910 are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest.

<sup>b</sup> Residues listed in 40 CFR 180.920 are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only.

<sup>c</sup> Residues listed in 40 CFR 180.930 are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals.

## B. Other Uses

2,4,7,9-Tetramethyl-5-decyn-4,7-diol is used as a wetting agent, defoamer, rinse aid, viscosity reducer, and lubricity additive. Some of the consumer products it is used in include: detergents, paints, coatings, adhesives, and metal working formulations (as cited in the Hazardous Substances Data Bank (HSDB)). According to the Household Products Database (HPDB), 3,6-Dimethyl-4-octyn-3,6-diol is a component of consumer shampoo products. Neither chemical is approved for use as a food additive by the Food and Drug Administration (FDA).

## III. Physical and Chemical Properties

Some of the physical and chemical characteristics of 2,4,7,9-tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol are found in Table 2.

Table 2. Physical and Chemical Properties		
Parameter	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	3,6-Dimethyl-4-octyn-3,6-diol
CAS #	126-86-3	78-66-0
9CI Name	5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (SRS <sup>1</sup> )	4-Octyne-3,6-diol, 3,6-dimethyl- (SRS)
Molecular Formula	C <sub>14</sub> H <sub>26</sub> O <sub>2</sub> (SRS)	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub> (SRS)
Structure		
Molecular Weight	226.36 (SRS)	170.25 (SRS)
Common Names	5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-Tetramethyl decynediol Surfynol 104E (SRS)	4-Octyne-3,6-diol, 3,6-dimethyl-Surfynol 82 (SRS)
Physical State	Solid (IUCLID <sup>2</sup> 2001)	na
Melting Point	54-55°C (IUCLID 2001)	66.6°C (EPI Suite <sup>3</sup> )

<b>Table 2. Physical and Chemical Properties</b>		
<b>Parameter</b>	<b>2,4,7,9-Tetramethyl-5-decyn-4,7-diol</b>	<b>3,6-Dimethyl-4-octyn-3,6-diol</b>
<b>Boiling Point</b>	262-263°C (IUCLID 2001)	254.4°C (EPI Suite)
<b>Water Solubility</b>	1.7 g/l @ 20°C (IUCLID 2001)	1.8 g/l @ 25°C (EPI Suite)
<b>Vapor Pressure</b>	0.0062-0.007 hPa @ 20°C (IUCLID 2001)	0.0008 hPa @ 20°C (EPI Suite)
<b>log Kow</b>	2.8 (IUCLID 2001)	1.79 estimated (EPI Suite)
<b>Henry's Law Constant</b>	2.091E-07 atm·m <sup>3</sup> /mole estimated (EPIWIN)	7.413E-008 atm·m <sup>3</sup> /mole estimated (EPI Suite)

<sup>1</sup>SRS – Environmental Protection Agency's Substance Registry System, <http://www.epa.gov/srs>

<sup>2</sup>IUCLID - International Uniform Chemical Information Database is a database of existing chemicals that is being compiled by the European Chemicals Bureau (ECB). IUCLID is the basic tool for data collection and evaluation within the EU-Risk Assessment Programme; it has been accepted by the OECD as the data exchange tool under the OECD Existing Chemicals Programme.

<sup>3</sup>The EPI (Estimation Programs Interface) Suite™ is a Windows® based suite of physical/chemical property and environmental fate estimation models developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). EPI Suite™ uses a single input to run the following estimation models: KOWWIN™, AOPWIN™, HENRYWIN™, MPBPWIN™, BIOWIN™, PCKOCWIN™, WSKOWWIN™, BCFWIN™, HYDROWIN™, and STPWIN™, WVOLWIN™, and LEV3EPI™. EPI Suite™ was previously called EPIWIN.

(<http://www.epa.gov/opptintr/exposure/docs/episuite.htm>)

na – not available

#### IV. Hazard Assessment

2,4,7,9-Tetramethyl-5-decyn-4,7-diol, and 3,6-dimethyl-4-octyn-3,6-diol are being evaluated as part of the US EPA's tolerance reassessment process of inert ingredients. No information was found to indicate that these substances have been the subject of previous hazard or risk assessments by the US EPA.

2,4,7,9-Tetramethyl-5-decyn-4,7-diol is sponsored under EPA's High Production Volume (HPV) Challenge Program (<http://www.epa.gov/chemrtk/volchall.htm>). The goal of the HPV program is to collect and make publicly available a complete set of baseline health and environmental effects data on those chemicals that are manufactured in, or imported into, the United States in amounts equal to or exceeding one million pounds per year. Industry sponsors volunteer to evaluate the adequacy of existing data and to conduct tests where needed to fill the gaps in the data, and EPA (and the public) has an opportunity to review and comment on the sponsors' robust summary report. A robust summary has been submitted for 2,4,7,9-tetramethyl-5-decyn-4,7-diol. This data set represents the primary source of information for 2,4,7,9-tetramethyl-5-decyn-4,7-diol, and also for 3,6-dimethyl-4-octyn-3,6-diol, based on their structural similarity.

There are no applicable toxicity data available for 3,6-dimethyl-4-octyn-3,6-diol; however, the Agency has determined that 2,4,7,9-tetramethyl-5-decyn-4,7-diol is a suitable analog based on their similar structures, use patterns and limitations, and potential routes of exposure when used as inert ingredients in pesticide products. Therefore, the available data for 2,4,7,9-tetramethyl-5-decyn-4,7-diol is being used as the basis for the assessment of both chemicals.

## A. Hazard Profile

The available toxicity data base for 2,4,7,9-tetramethyl-5-decyn-4,7-diol consists of acute, subchronic, and chronic studies in animals, as well as genotoxicity, developmental, and reproductive toxicity studies. No relevant neurotoxicity data have been identified for 2,4,7,9-tetramethyl-5-decyn-4,7-diol, nor have any carcinogenicity data been identified. Neurological disturbances, however, were only reported in high-dosed dogs in a 130 day study.

2,4,7,9-Tetramethyl-5-decyn-4,7-diol is of low to moderate acute toxicity via the oral route of exposure, with the acute effects of greatest concern being eye and skin irritation (IUCLID 2001).

Available toxicity data are summarized in the following section.

## B. Toxicological Data

### Acute Toxicity

2,4,7,9-Tetramethyl-5-decyn-4,7-diol: Available data on acute toxicity are summarized in Table 3.

**Table 3. Summary of Acute Toxicity**

Parameter	2,4,7,9-Tetramethyl-5-decyn-4,7-diol
	Toxicity Value and Reference
Oral LD <sub>50</sub> , rat	>500 mg/kg bw (IUCLID 2001)
Dermal LD <sub>50</sub> , rat	>2000 mg/kg bw (IUCLID 2001)
Dermal LD <sub>50</sub> , rabbit	>1000 mg/kg bw (IUCLID 2001)
Inhalation LC <sub>50</sub> , rat	>20 mg/L (IUCLID 2001)
Eye Irritation, rabbit	Highly irritating (IUCLID 2001)
Skin Irritation, rabbit	Irritating; moderate to severe erythema and slight edema in the animals. Skin irritation was resolved within 21 days after exposure in all animals (IUCLID 2001)

### Subchronic Toxicity

2,4,7,9-Tetramethyl-5-decyn-4,7-diol: In a 28-day oral study of rats fed 0, 625, 1250, 2500, or 5000 ppm (equivalent to 0, 31.2, 62.5, 125, or 250 mg/kg/day, respectively); mortality, physical observations, body weight, and food consumption data, as well as gross necropsy observations did not reveal any adverse effects considered to be attributable to the administration of Surfynol 104 at any of the dose levels. The NOAEL is equal to 5000 ppm (highest dose tested).

In a 130 day oral study in dogs (0, 200, 250, or 300 mg/kg/day), all dogs survived for the duration of the study with few clinical signs. Occasional dogs in the mid- and high-dose groups (250 to 300 mg/kg/day) exhibited sporadic compound-related neurologic disturbances

(convulsions and tremors) during the study. All other observations, including feed consumption, body weight gains, organ weights (except liver), clinical chemistries, hematology, urinalysis, gross pathology, and histology were judged to reflect no compound-related/biologically significant changes. Mean liver weights and liver-to-body weight ratios in all Surfynol 104 treated groups were higher than in corresponding control groups; however, since no historical abnormalities were observed in these livers, the liver enlargement was judged to be due to hyperplasia of the hepatic endoplasmic reticulum, where xenobiotic/drug metabolizing enzymes are located. Based on the liver effects, a NOAEL could not be established. The LOAEL was determined to be 200 mg/kg/day.

#### Mutagenicity/Genotoxicity

2,4,7,9-Tetramethyl-5-decyn-4,7-diol: Nonmutagenic in Ames testing with *Salmonella typhimurium* strains both with and without activation. Negative in a cytogenetic assay using CHO (Chinese Hamster Ovary) cells *in vitro* both with and without activation.

#### Carcinogenicity

2,4,7,9-Tetramethyl-5-decyn-4,7-diol: No carcinogenicity studies currently available.

#### Developmental and Reproductive Toxicity

2,4,7,9-Tetramethyl-5-decyn-4,7-diol: In a one-generation reproduction study in Sprague-Dawley rats, as well as in a one-generation developmental/teratogenicity study in Sprague-Dawley rats (doses of 0, 500, 1000, or 2000 mg/kg/day), the only pertinent findings observed in the F0 parents were a slight decrease in the mean weaning weight of both male and female pups of the high-dose group; a slight decrease in lactation indices of the high-dose group; decreased body weight and feed consumption of the high-dose female group; and normal histology of the reproductive organs in the F0 parents. Fertility, viability, and gestation indices were not affected. In the reproduction phase of this experiment, there was a toxic effect at the 2000 mg/kg/day level, a borderline effect at the 1000 mg/kg/day level, and no effect at 500 mg/kg/day. The following pertinent findings were observed in the F1a rats: slight decrease in the mean rate of body weight gain in both sexes at the mid- and high-dose (there was also a significant decrease in this parameter in the low-dose male group during the first eight weeks); normal mean hematological findings, clinical chemistry findings, and urinalysis findings after 91 days on test; significant increase in the absolute and relative liver weights of both sexes at the mid- and high-dose; corresponding histopathology of the liver showing mild to moderate centrilobular cloudy swelling of hepatocytes of the mid- and high-dose rats. For both studies, the parental and offspring NOAELs were determined to be 500 mg/kg/day, with effects only observed at or above the limit dose (1000 mg/kg/day).

### **C. Metabolism and Pharmacokinetics**

No metabolism or pharmacokinetic data are available for these chemicals.

#### **D. Special Considerations for Infants and Children**

In a combined one-generation reproductive/developmental study in Sprague-Dawley rats, (doses of 0, 500, 1000, or 2000 mg/kg bw/day), both the parental and offspring NOAELs were determined to be 500 mg/kg bw/day. Based on this information there is no concern, at this time, for increased sensitivity to infants and children to 2,4,7,9-tetramethyl-5-decyn-4,7-diol and the structurally similar chemical 3,6-dimethyl-4-octyn-3,6-diol when used as inert ingredients in pesticide formulations. For the same reason, a safety factor analysis has not been used to assess risk and, therefore, the additional tenfold safety factor for the protection of infants and children is also unnecessary.

#### **V. Environmental Fate Characterization and Drinking Water Considerations**

Based on estimated values from the Agency's EPI Suite program, 2,4,7,9-tetramethyl-5-decyn-4,7-diol photodegrades rapidly in the atmosphere (half-life=3.021 hours), is soluble in water (1700 mg/L), nonvolatile, and exhibits negligible sorption to soil (Log Koc of 1.328). This chemical is classified as "not readily biodegradable." Biodegradation results based on Biowin suggest primary degradation may occur in weeks and ultimate degradation in weeks-months.

The estimated environmental fate characteristics for 3,6-dimethyl-4-octyn-3,6-diol are as follows: it rapidly photodegrades in the atmosphere (half-life=3.59 hours), is soluble in water (1810 mg/L), is nonvolatile, and exhibits negligible sorption to soil (Log Koc=1.00). This chemical is classified as "not readily biodegradable." Biodegradation results based on Biowin suggest primary degradation may occur in days-weeks, and ultimate degradation in weeks-months.

Based on their use restrictions and limitations when used as inert ingredients in pesticide products applied to growing crops, raw agricultural commodities after harvest, and animals, 2,4,7,9-tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol are likely to be present in drinking water sources, however, they are likely to occur at low levels based on use limitations and possible primary degradation before transport to a drinking water treatment facility. The fate and effects of potential primary degradates is not available, but are likely less than the parent compounds.

#### **VI. Exposure Assessment**

2,4,7,9-Tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol are approved for use as surfactants in pesticide formulations applied to growing crops, raw agricultural commodities after harvest, and animals. They are limited to 2.5% in pesticide formulations for application to growing crops and raw agricultural commodities after harvest, and to animals. Additionally, for growing crops, they are restricted to application to the soil prior to planting or to plants before the edible parts form.

For the general population, the primary route of exposure to these chemicals from their use as inert ingredients in pesticide products would most likely be through consumption of food

to which pesticide products containing them have been applied, and through drinking water (from runoff). Dermal exposure is also possible from residential use of pesticide products containing these inert ingredients, however, inhalation exposures are not expected because they are not volatile.

## **VII. Aggregate Exposures**

In examining aggregate exposure, the Federal Food, Drug, and Cosmetic Act (FFDCA) section 408 directs EPA to consider available information concerning exposures from the pesticide residue in food and all other non-occupational exposures, including drinking water from ground water or surface water and exposure through pesticide use in gardens, lawns, or buildings (residential and other indoor uses).

For 2,4,7,9-tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol, a qualitative assessment for all pathways of human exposure (food, drinking water, and residential) is appropriate given the use/application limitations and lack of human health concerns associated with exposure to these substances when used as inert ingredients in pesticide formulations.

## **VIII. Cumulative Exposure**

Section 408(b)(2)(D)(v) of FFDCA requires that, when considering whether to establish, modify, or revoke a tolerance, the Agency consider "available information" concerning the cumulative effects of a particular pesticide's residues and "other substances that have a common mechanism of toxicity."

Unlike other pesticides for which EPA has followed a cumulative risk approach based on a common mechanism of toxicity, EPA has not made a common mechanism of toxicity finding as to 2,4,7,9-tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol and any other substances, and these chemicals do not appear to produce toxic metabolites produced by other substances. For the purposes of this tolerance action, therefore, EPA has not assumed that 2,4,7,9-tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol have a common mechanism of toxicity with other substances. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see the policy statements released by EPA's Office of Pesticide Programs concerning common mechanism determinations and procedures for cumulating effects from substances found to have a common mechanism on EPA's website at <http://www.epa.gov/pesticides/cumulative/>.

## **IX. Human Health Risk Characterization**

There are limited applicable toxicity data available for 3,6-dimethyl-4-octyn-3,6-diol; however, the Agency has determined that 2,4,7,9-tetramethyl-5-decyn-4,7-diol is a suitable analog because of their structural similarities. When used as inert ingredients in pesticide products, these chemicals also have similar use patterns, restrictions/limitations, and potential exposures. Therefore, the available data for 2,4,7,9-tetramethyl-5-decyn-4,7-diol is used as the basis for the assessment of both chemicals. Based on the available data, 2,4,7,9-tetramethyl-5-decyn-4,7-diol is of low to moderate oral and inhalation toxicity, with acute effects of greatest

concern being eye and skin irritation. It is not mutagenic and no increased offspring sensitivity was observed in a one-generation reproduction study. Based on their structural similarity, the toxicity of 3,6-dimethyl-4-octyn-3,6-diol is expected to be similar to 2,4,7,9-tetramethyl-5-decyn-4,7-diol. The use/application limitations and likely biodegradation prior to transport to a drinking water treatment facility are expected to limit exposures of concern from residues of these chemicals (from food and drinking water) when used as inert ingredients in pesticide products.

Taking into consideration available toxicity and exposure information, the Agency has determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure (dietary and non-occupational sources of exposure) to 2,4,7,9-tetramethyl-5-decyn-4,7-diol and 3,6-dimethyl-4-octyn-3,6-diol when used as inert ingredients in pesticide formulations. Therefore, it is recommended that the exemptions from the requirement of a tolerance for these two chemicals under 40 CFR 180.910, 180.920, and 180.930 be considered reassessed as safe under section 408(q) of the Federal Food, Drug, and Cosmetic Act.

#### **X. Ecotoxicity and Ecological Risk Characterization**

##### 2,4,7,9-tetramethyl-5-decyn-4,7-diol (IUCLID 2001)

The 24 hour and 96hour LC<sub>50</sub> for carp was 42 mg/L with 0% mortality at 32 mg/L (LC<sub>0</sub>) and 100% mortality at 56mg/L (LC<sub>100</sub>). Effects on swimming behavior and pigmentation were induced at concentrations down to 18 mg/L, with no sublethal effects occurring at 10 mg/L.

For *Daphnia magna*, the 24 hour EC<sub>50</sub> was 99 mg/L and the 48 hour EC<sub>50</sub> was 91 mg/L. This chemical did not induce acute immobilization at 43 mg/L after 48 hours of exposure (NOEC).

2,4,7,9-Tetramethyl-5-decyn-4,7-diol affected growth of the freshwater species *Selenastrum capricornutum* significantly at 2.2 mg/L and higher. The NOEC for cell growth inhibition and growth rate reduction was 1.0 mg/L. However, a recovery of growth was observed during the last 48 hours of exposure with a NOEC of 4.6 mg/L for growth rate. Cell growth inhibition EC<sub>50</sub>=15 mg/L, cell growth rate reduction EC<sub>50</sub>(0-72 hours)=82 mg/L, (24-72 hours)=39 mg/L.

Based on the above results, 2,4,7,9-Tetramethyl-5-decyn-4,7-diol is classified as slightly toxic to fish and aquatic invertebrates and moderately toxic to aquatic plants.

##### 3,6-dimethyl-4-octyn-3,6-diol

There were no available measured data on the effects of 3,6-dimethyl-4-octyn-3,6-diol located in the Agency's public version of the Ecotox Database or elsewhere in the open literature. Quantitative structure activity relationships (QSAR) were generated for each compound and used to assess the toxicity of 3,6-dimethyl-4-octyn-3,6-diol.

Results of the QSAR for 2,4,7,9-tetramethyl-5-decyn-4,7-diol were approximately an order of magnitude more protective ( $LC_{50}$ 's ranged from 3.8 to 7.3 mg/L) when compared to the measured data for fish; estimates for other aquatic organisms were not generated because the current training dataset is insufficient to adequately predict effects concentrations for the propargyl-alcohol hindered compound class. Therefore, it is hypothesized that the results for 3,6-dimethyl-4-octyn-3,6-diol will likely overestimate the potential laboratory toxicity.

Based on the QSAR analysis, 3,6-dimethyl-4-octyn-3,6-diol is expected to be less toxic to aquatic organisms than 2,4,7,9-Tetramethyl-5-decyn-4,7-diol. QSAR  $LC_{50}$  results for fish were reported to range from 65 mg/L to 244 mg/L depending on the method of calculation.

On a chronic basis, QSAR results indicated that 2,4,7,9-tetramethyl-5-decyn-4,7-diol would be considerably more toxic to fish, with a NOAEC of approximately 1 mg/L, than 3,6-dimethyl-4-octyn-3,6-diol's estimated NOAEC of approximately 6 mg/L to 32 mg/L depending on method of analysis.

## REFERENCES:

HSDB, Hazardous Substances Data Bank, <http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+@rel+126-86-3>.

HPDB, Household Products Database, <http://hpd.nlm.nih.gov/cgi-bin/household/search?queryx=78-66-0&tbl=TblChemicals&prodcats=all>.

IUCLID - International Uniform Chemical Information Database, Data Set for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol, 12/18/2001.

US EPA. EPI Suite, <http://www.epa.gov/opptintr/exposure/docs/episuite.htm>.

US EPA. High Production Volume Challenge Program: 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. 2002. Available at [http://www.epa.gov/chemrtk/hpv\\_1990.htm](http://www.epa.gov/chemrtk/hpv_1990.htm).