

MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

INTEROFFICE COMMUNICATION

TO: File for 2,4,7,9-tetramethyl-5-decyn-4,7-diol (CAS # 126-86-3)
FROM: Doreen Lehner, Toxics Unit, Air Quality Division
DATE: August 18, 2016
SUBJECT: Screening Level for 2,4,7,9-tetramethyl-5-decyn-4,7-diol (CAS # 126-86-3)

An initial threshold screening level (ITSL) for 2,4,7,9-tetramethyl-5-decyn-4,7-diol will not be set. This compound is a solid at ambient temperature and pressure with a relatively low oral toxicity and therefore, emissions may be evaluated based on the National Ambient Air Quality Standards (NAAQS) for PM_{2.5} (footnote #26 of the Toxic Air Contaminant screening level list).

2,4,7,9-Tetramethyl-5-decyn-4,7-diol (CAS# 126-86-3) also known as diisobutyl-1,4-dimethyl-butynediol and Surfynol 104 is a waxy-like white solid with a molecular weight of 226.36 g/mol. 2,4,7,9-Tetramethyl-5-decyn-4,7-diol is a surfactant with a low surface tension with defoaming properties; low water solubility, high thermal stability and is stable in pH range 3 to 12. It is used: as a surfactant in pesticide formulations for growing crops; as an inert ingredient in herbicides, fungicides, and insecticides; as a surfactant, defoamer, rinse aid, viscosity reducer, lubricity additive, and wetting agent in detergents, paints, coatings, adhesives, metal working formulations, and shampoo (EPA, 2006).

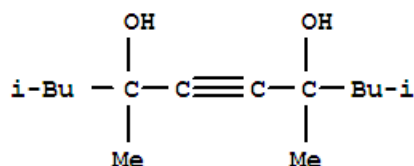


Figure 1. Structure of 2,4,7,9-tetramethyl-5-decyn-4,7-diol.

A literature review was conducted to determine the screening levels for 2,4,7,9-tetramethyl-5-decyn-4,7-diol. The following references and databases were searched: Chemical Criteria Database (CCD), United States Environmental Protection Agency (US EPA) Integrated Risk Information System (IRIS), National Institute for Occupational Safety and Health (NIOSH), American Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Values and Biological Exposure Indices (TLV/BEI) 2014 guide, National Toxicology Program (NTP) Study Database, International Agency for Research on Cancer (IARC), Acute Database, Chemical Abstract Service (CAS) Online (searched 8/12/16), National Library of Medicine (NLM)-online, EPA Aggregated Computational Toxicology Resource (ACToR) Database, U.S. EPA TSCATS database, and Hazardous Substances Data Bank (HSDB).

No inhalation toxicity data were found which could be used to establish an ITSL. However, 2,4,7,9-tetramethyl-5-decyn-4,7-diol does have oral toxicity data. In the first study, "...a 28-day oral study of rats fed 0, 625, 1250, 2500, or 5000 ppm (equivalent to 0,31.2, 62.5, 125, or 2580 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)" (EPA, 2006).

"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" (EPA, 2006).

"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)" (EPA, 2006).

A proposed ITSL could be developed using the 130-day oral dog study, which was the longest well-conducted study with the most sensitive endpoint (dose-dependent liver weight increases). The LOAEL of 200 mg/kg/day could be used in the determination of an RfD using the equation below:

$$\text{Potential RfD}(\text{mg}/\text{kg}/\text{day}) = \frac{\text{LOAEL}(\text{mg}/\text{kg}/\text{day})}{\text{UF}_A \times \text{UF}_H \times \text{UF}_S \times \text{UF}_L}$$

Where:

UF_A = interspecies variation. A factor used to account for uncertainty when extrapolating from valid results of long-term studies on experimental animals to humans.

UF_H = intraspecies variation. A factor used to account for variation in sensitivity among members of the human population.

UF_S = Uncertainty factor used to account for the extrapolation from less than chronic NOAELs to chronic NOAELs.

UF_L = Uncertainty factor used to account for the extrapolation from a LOAEL to a NOAEL.

The LOAEL from the 130-day oral dog study of 200 mg/kg/day can be used as an RfD using the above equation:

$$\text{Potential RfD}(\text{mg}/\text{kg}/\text{day}) = \frac{200(\text{mg}/\text{kg}/\text{day})}{10 \times 10 \times 10 \times 10} = 0.02 \text{ mg}/\text{kg}/\text{day}$$

Rule 232(1)(b) uses an oral RfD to determine an ITSL using the following equation:

$$\text{Potential ITSL} = \text{Oral RfD} \times \frac{70 \text{ kg}}{20 \text{ m}^3} = 0.02 \text{ mg}/\text{kg}/\text{day} \times \frac{70 \text{ kg}}{20 \text{ m}^3} = 0.07 \text{ mg}/\text{m}^3 = 70 \text{ }\mu\text{g}/\text{m}^3$$

The potential ITSL would be 70 $\mu\text{g}/\text{m}^3$. According to Rule 232(2)(b) a 24-hour averaging time period should be used, but as this ITSL is based on a 130 day oral dog study and $UF_S = 10$ is applied, it is appropriate to utilize a longer averaging time, which would be an annual averaging time. Therefore, the potential ITSL for 2,4,7,9-tetramethyl-5-decyn-4,7-diol would be 70 $\mu\text{g}/\text{m}^3$ based on an annual averaging time. As 2,4,7,9-tetramethyl-5-decyn-4,7-diol is considered to be a solid, the ITSL determined above exceeds the NAAQS for $\text{PM}_{2.5}$ therefore, an ITSL will not be determined and emissions of 2,4,7,9-tetramethyl-5-decyn-4,7-diol will be evaluated using the NAAQS standard for $\text{PM}_{2.5}$.

References:

Act 451 of 1994. Natural Resources and Environmental Protection Act and Air Pollution Control Rules. MDEQ.

EPA. 2006. Inert Ingredient – Reassessment Decision Documents: 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). United States Environmental Protection Agency Office of Prevention, Pesticides, and Toxic Substances. Available online at: <https://www.epa.gov/sites/production/files/2015-04/documents/diols.pdf>

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