

# MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

## INTEROFFICE COMMUNICATION

TO: File for octanoic acid (CAS # 124-07-2)

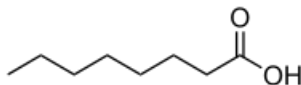
FROM: Doreen Lehner, Toxics Unit, Air Quality Division

DATE: September 12, 2016

SUBJECT: Screening Level for octanoic acid (CAS # 124-07-2)

The initial threshold screening level (ITSL) for octanoic acid (CAS # 124-07-2) is  $4.2 \mu\text{g}/\text{m}^3$  based on an annual averaging time. The original ITSL, established in 1999, was  $33 \mu\text{g}/\text{m}^3$  (annual averaging time) was based on an  $\text{LD}_{50}$  of 10,080 mg/kg (Jenner, 1964). In 2006, the EPA listed an  $\text{LD}_{50}$  of 1,283 mg/kg in the *Federal Register* (40 CFR 180) in a document on sorbitol octanoate. The EPA  $\text{LD}_{50}$  is a more appropriate value as EPA is using it in evaluating a sorbitol octanoate. Also the  $\text{LD}_{50}$  is significantly lower than the previous  $\text{LD}_{50}$  and therefore, the resulting value is more health protective than the higher  $\text{LD}_{50}$  of 10,080 mg/kg.

Octanoic acid (also known as caprylic acid and 1-heptanecarboxylic acid) is an eight-carbon, saturated fatty acid that is an oily liquid with an unpleasant, rancid-like taste and smell with a molecular weight of 144.21 g/mol. Octanoic acid is found naturally in the milk of various mammals, and as a minor constituent of coconut oil and palm kernel oil. Octanoic acid is used: in perfumes; in the manufacture of dyes; as an antimicrobial pesticide where food contact may occur as a surface sanitizer (example, on dairy equipment, food processing equipment, breweries, wineries, and beverage processing plants); as a disinfectant in health care facilities, schools/colleges, animal care/veterinary facilities, industrial facilities, office buildings, recreational facilities, retail and wholesale establishments, livestock premises, restaurants, and hotels/motels; and as an algaecide, bactericide, and fungicide in nurseries, greenhouses, and garden centers (Wikipedia, 2016).



**Figure 1.** Structure of octanoic acid.

A literature review was conducted to determine the screening levels for octanoic acid. The following references and databases were searched to derive the above screening levels: 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 8/23/16), National Library of Medicine (NLM)-online, EPA Aggregated Computational Toxicology Resource (ACToR) Database, U.S. EPA TSCATS database, and Hazardous Substances Data Bank (HSDB).

### ITSL Derivation:

RfC or RfD values were unavailable. There is no NIOSH recommended exposure limit data available or a threshold limit value from ACGIH. However, there are two LD<sub>50</sub>'s for octanoic acid. A rat oral LD<sub>50</sub> for octanoic acid of 10,080 mg/kg was determined from a study by Jenner, et al., (1964) where rats experienced general depressed activity and diarrhea shortly after oral dosing. Another rat oral LD<sub>50</sub> of 1,283 mg/kg from an acute oral toxicity study for octanoic acid in male rats (40 CFR, 2006). Based on Rule 232(1)(h) the ITSL is determined as follows:

$$ITSL = \frac{1}{500} \times \frac{1}{40} \times \frac{1}{100} \times \frac{LD_{50} (mg/kg) \times W_A}{0.167 \times I_A}$$

Where  $W_A$  is the body weight of an unspecified strain of male rat in kilograms (0.470 kg) (EPA, 1988) and  $I_A$  is the daily inhalation rate of a unspecified strain of male rat in cubic meters/day (EPA, 1988). These default values are utilized because the study report does not provide the values. The equation to determine the value for  $I_A$  is below:

$$I_A \left( m^3/day \right) = 0.80 \times W^{0.8206}$$

$$I_A \left( m^3/day \right) = 0.80 \times 0.470^{0.8206} = 0.430539983 \text{ } m^3/day$$

Inserting the above values for  $I_A$ ,  $W_A$ , and the LD<sub>50</sub> gives:

$$ITSL = \frac{1}{500} \times \frac{1}{40} \times \frac{1}{100} \times \frac{1,283 (mg/kg) \times 0.470kg}{0.167 \times 0.430539983 \text{ } m^3/day} = 0.004193383 \text{ } mg/m^3$$

$$= 4.193383 \text{ } \mu g/m^3 \approx 4.2 \text{ } \mu g/m^3$$

Based on Rule 232(2)(c) the averaging time for this ITSL is annual. Therefore, the initial threshold screening level (ITSL) for octanoic acid (CAS# 124-07-2) is 4.2 µg/m<sup>3</sup> based on an annual averaging time.

**References:**

40 CFR 180. Revised as of January 27, 2006. Federal Register Vol. 71, No. 18, pages 4512-4518. Sorbitol Octanoate; Exemption from the Requirement of a Tolerance.

EPA. 1988. Recommendation for and documentation of biological values for use in risk assessment. PB 88-179874.

Jenner PM, Hagan EC, Taylor JM, Cook EL, and Fitzhugh OG. 1964. Food flavorings and compounds of related structure. I. Acute oral toxicity. Food and Cosmetics Toxicology, Vol 2(3):327-343.

NREPA. 1994. Part 55, Air Pollution Control of the Natural Resources and Environmental Protection Act, 1994 PA 451, as amended.

Wikipedia. 2016. Caprylic acid. Available online at:  
[https://en.wikipedia.org/wiki/Caprylic\\_acid](https://en.wikipedia.org/wiki/Caprylic_acid)

DL:lh