

MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY
INTEROFFICE COMMUNICATION

TO: File for 1,3,5-Cycloheptatriene [CAS# 544-25-2]
FROM: Doreen Lehner
SUBJECT: Screening Level Determination for 1,3,5-Cycloheptatriene [CAS# 544-25-2]
DATE: March 4, 2014

The initial threshold screening level (ITSL) for 1,3,5-cycloheptatriene is 0.18 µg/m³ with an annual averaging time.

1,3,5-Cycloheptatriene [CAS# 544-25-2], also known as tropilidene, is a straw colored liquid that darkens to a distinct yellow upon exposure to air. It has a pungent and persistent odor and has a molecular weight of 92.14 g/mol.



Figure 1. Structure of 1,3,5-cycloheptatriene.

The following references or databases were searched to identify data to determine the screening level: U.S. Environmental Protection Agency (EPA) Integrated Risk Information System (IRIS), Registry for Toxic Effects of Chemical Substances (RTECS), American Conference of Governmental and Industrial Hygienists (ACGIH) Threshold Limit Values (TLVs), International Agency for Research on Cancer (IARC) Monographs, Chemical Abstract Service (CAS) - Online (searched 2/10/2014), National Library of Medicine, and the EPA Aggregated Computational Toxicology Resource (ACToR) Database.

Little toxicity data is available for 1,3,5-cycloheptatriene. There is an oral rat LD₅₀ of 57 mg/kg from Brown et al., (1967). Based on rule 232(1)(h) the ITSL can be determined from an oral LD₅₀ using the following equation:

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

Where:

W_A = the body weight of male and female Hooded Lister strain rats in kilograms. As the average weight of Hooded Lister rats is not reported in the key study, the default weight for a non-gender rat of unknown species is 0.395 kg is used (EPA, 1988).

I_A = the daily inhalation rate of male and female Hooded Lister strain rats in cubic meters/day which is determined by using the equation below from EPA (1988):

$$I_A = 0.80 \times W_A^{0.8206}$$
$$I_A = 0.80 \times 0.395 \text{ kg}^{0.8206} = 0.3733 \text{ m}^3/\text{day}$$

The values for I_A , W_A , and the LD_{50} are entered into the ITSL equation above:

$$ITSL = \frac{1}{500} \times \frac{1}{40} \times \frac{1}{100} \times \frac{57 \text{ mg/kg} \times 0.395 \text{ kg}}{0.167 \times 0.3733 \text{ m}^3/\text{day}} = 0.0001806 \text{ mg/m}^3 = 0.18 \text{ }\mu\text{g/m}^3$$

Based on Rule 232(2)(c) the averaging time for this ITSL is annual. Based on the above data, the ITSL for 1,3,5-cycloheptatriene is $0.18 \text{ }\mu\text{g/m}^3$ with an annual averaging time.

References:

Act 451 of 1994, Natural Resources and Environmental Protection Act and Air Pollution Control Rules, Michigan Department of Environmental Quality.

Brown VKH, Ferrigan LW, and Stevenson DE. 1967. The Acute Toxicity and Skin Irritant Properties of Tropilidene (Cyclohepta-1,3,5-triene). Ann. Occup. Hyg. Vol. 10. 123-126.

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

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