

MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

INTEROFFICE COMMUNICATION

TO: File for 2-Methyltetrahydrofuran (CAS # 96-47-9)
FROM: Doreen Lehner, Toxics Unit, Air Quality Division
DATE: May 11, 2017
SUBJECT: Screening Level for 2-Methyltetrahydrofuran (CAS # 96-47-9)

The initial threshold screening level (ITSL) for 2-methyltetrahydrofuran (CAS # 96-47-9) is 420 $\mu\text{g}/\text{m}^3$ with an annual averaging time.

2-Methyltetrahydrofuran (also known as 2-methyloxolane, methyltetrahydrofuran, and tetrahydrofuran) is a clear, colorless to yellow liquid with an ether-like odor and has a molecular weight of 86.13 g/mol. 2-Methyltetrahydrofuran is used: as a specialty solvent for Grignard reagents; as a reactant in the production of 2-methylpyrrolidine and N-substituted 2-methylpyrrolidines; as a solvent in lithium batteries; and as a gasoline extender in fuel blends (NTP, 2000).

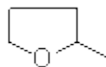


Figure 1. Structure of 2-methyltetrahydrofuran.

A literature review was conducted to determine an initial threshold screening level (ITSL) for 2-methyltetrahydrofuran. The following references and databases were searched to derive the above screening levels: 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) 2017 guide, National Toxicology Program (NTP) Study Database, International Agency for Research on Cancer (IARC), European Chemicals Agency (ECHA), Acute Database, Chemical Abstract Service (CAS) Online using SciFinder portal (searched 5/4/2017), National Library of Medicine (NLM)-online, EPA Aggregated Computational Toxicology Resource (ACToR) Database, US EPA TSCATS database, and Hazardous Substances Data Bank (HSDB).

There is very little toxicity information available on 2-methyltetrahydrofuran. There is an acute 50% mortality lethal concentration (LC₅₀) inhalation study on rats with 2-methyltetrahydrofuran at 6,000 ppm after a 4-hour exposure (Deichmann WB et al, 1969).

Derivation of the ITSL:

The ITSL will be based on the rat inhalation LC₅₀ of 6,000 ppm (4-hour) exposure based on Rule 232(1)(f) using the following equation:

$$ITSL = \frac{LC_{50}}{500 \times 100}$$

Before calculating the ITSL, the LC₅₀ must be converted from ppm to mg/m³ using the following equation:

$$mg/m^3 = \frac{ppm \times MW}{24.45}$$

The molecular weight of 2-methyltetrahydrofuran is 86.13 g/mol. Using the above equation:

$$mg/m^3 = \frac{6,000 \text{ ppm} \times 86.13 \text{ g/mol}}{24.45} = 21,136.19632 \text{ mg/m}^3$$

The rat LC₅₀ converted to mg/m³ can be used to determine the ITSL using the above equation:

$$ITSL = \frac{21,136.19632 \text{ mg/m}^3}{500 \times 100} = 0.422723926 \text{ mg/m}^3 = 422.723926 \text{ } \mu\text{g/m}^3$$

$$ITSL \approx 420 \text{ } \mu\text{g/m}^3$$

According to Rule 232(2)(c), the averaging time is annual. Therefore, the initial threshold screening level for 2-methyltetrahydrofuran (CAS# 96-47-9) is 420 μg/m³ with an annual averaging time.

References:

APCR. 2017. Air Pollution Control Rules, Promulgated pursuant to Part 55, Air Pollution Control, of the Natural Resources and Environmental Protection Act, Michigan Department of Environmental Quality. 1994, Act 451, as amended (NREPA).

Deichmann WB and Gerarde HW. 1969. Toxicology of Drugs and Chemicals. Fourth edition. New York: Academic Press. Pg. 395.

NTP. 2000. 2-Methyltetrahydrofuran 96-47-9. Basis of Nomination to the CSWG. Summary of data for chemical selection. Available online at:
https://ntp.niehs.nih.gov/ntp/htdocs/chem_background/exsumpdf/methyltetrahydrofuran_508.pdf

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