**MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY**

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**INTEROFFICE COMMUNICATION**

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TO: File for 2-Methylbutyraldehyde (CAS # 96-17-3)

FROM: Doreen Lehner, Toxics Unit, Air Quality Division

DATE: July 20, 2016

SUBJECT: Screening Level for 2-Methylbutyraldehyde (CAS # 96-17-3)

The initial threshold screening level (ITSL) for 2-methylbutyraldehyde (CAS # 96-17-3) is 700 µg/$m^3$ based on an annual averaging time.

2-Methylbutyraldehyde, also known as 2-methylbutanal, 2-ethylpropanal, and 2-formylbutane, is a volatile, colorless to pale yellow, clear liquid with an extremely pungent cocoa or coffee-like odor and a molecular weight of 86.1323 g/mol. It is a volatile organic compound found in household waste materials. Even though it is listed in with fragrant chemicals, there are no listed uses for 2-methylbutyraldehyde. The structure of 2-methylbutyraldehyde is shown below.

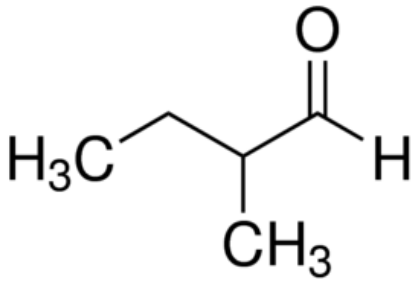


**Figure 1.** Structure of 2-methylbutanal.

A literature review was conducted to determine the screening level for 2-methylbutyraldehyde. 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 7/7/16), National Library of Medicine (NLM)-online, EPA Aggregated Computational Toxicology Resource (ACToR) Database, U.S. EPA TSCATS database, and Hazardous Substances Data Bank (HSDB).

There is very little toxicity information on 2-methylbutyraldehyde, therefore a rat inhalation $LC_{50}$ of 10,000 ppm (4 hour duration) is used to determine the ITSL (Carpenter et al., 1974). 2-methylbutyraldehyde concentrations in ppm were converted to µg/m$^3$ using equation 4-1b on page 4-20 in EPA (1994) with the assumptions that the testing was performed at 25°C and 760 mmHg, and that 1 g-mole of a perfect gas occupies 24.45 L

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

The molecular weight of 2-methylbutyraldehyde is 86.1323 g/mol. Using the equation above:

$$^{mg}/_{m^3} = \frac{10{,}000\ ppm \times 86.1323\ ^{g}/_{mol}}{24.45} = 35227.93456\ ^{mg}/_{m^3}$$

As per Rule 232(1)(f) an ITSL can be derived from a 4-hour inhalation $LC_{50}$ using the following equation:

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

Using the $LC_{50}$ value in mg/m$^3$ calculated above:

$$ITSL = \frac{35227.93456\ ^{mg}/_{m^3}}{500 \times 100} = 0.704558691\ ^{mg}/_{m^3} = 704.558691\ ^{\mu g}/_{m^3}$$

After rounding the ITSL is 700 µg/m$^3$. Rule 232(2)(c) states that the averaging time for an ITSL based on a 4-hour inhalation $LC_{50}$ is annual. Therefore, the ITSL for 2-methylbutyraldehyde (CAS# 96-17-3) is 700 µg/m$^3$ based on an annual averaging time.

**References**

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

Carpenter C, Weil CS, Smyth HF Jr. 1974. Range-Finding Toxicity Data: List VIII. Toxicology and Applied Pharmacology 28: 313-319.

EPA. 1994. Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry. Research Triangle Park, NC: U.S. Environmental Protection Agency, Environmental Criteria and Assessment Office EPA/600/8-90/066F.

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