MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY
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INTEROFFICE COMMUNICATION
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TO: File for 1-Dodecene [CAS# 112-41-4]

FROM: Doreen Lehner

DATE: February 25, 2014

SUBJECT: Screening Level Determination for 1-Dodecene [CAS# 112-41-4]

The initial threshold screening level (ITSL) for 1-dodecene is 29 µg/m^3 based on an annual averaging time.

1-Dodecene [CAS# 112-41-4] (also known as α-dodecene, dodec-1-ene, and dodecylene) is an alkene consisting of a chain of twelve carbon atoms terminating in a double bond (Figure 1) and has a molecular weight of 168.319 g/mol. 1-Dodecene is classified as an alpha-olefin and is a colorless liquid with a mild, pleasant odor. 1-Dodecene is used: in the production of detergents; in gasolines, diesel fuels, and fuel oils; in the production of alkylated aromatics, amines and amine oxides, mercaptans, oxo alcohols, epoxides, and synthetic fatty acids; and as a cosmetic and flavor agent.

Figure 1. Structure of 1-dodecene.

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 2/19/2014), National Library of Medicine, and the EPA Aggregated Computational Toxicology Resource (ACToR) Database.

There is little information on 1-dodecene as most available information is on mixtures of 1-dodecene with other olefins. The OECD (2001) published a report examining available data and determined that the following alpha olefins: 1-hexene, 1-octene, 1-decene, 1-dodecene, and 1-tetradecene could be treated as a category in determining risk assessment. "The data indicate an increasing or decreasing trend or pattern from the shortest category member (C_6) to the longest category member (C_{14}) for various physiochemical properties and ecotoxicity (using a mixture of experimental data and estimation techniques), whereas there appears to be no difference across category members for biodegradation and health endpoints. Data presented relative the health effect endpoints of the C_6-C_{14} alpha olefins indicate no differences among the five category members for acute toxicity, repeat dose toxicity, genotoxicity and reproductive/developmental toxicity" (OECD, 2001).

The EPA (2005) has found an unpublished oral rat LD_{50} study. "Groups of 10 male Sprague-Dawley rats weighing 200-300 g were gavaged, after overnight fasting, with 1-dodecene, neat, at 10 g/kg body weight. The animals were observed for 14 days after dosing. Survivors were sacrificed and autopsied. There were no deaths and no visible signs of toxicity. All of the animals were gaining weight normally. The autopsy did not reveal any gross pathological changes" (EPA, 2005). Although an LD_{50} was not identified, it is possible to derive an ITSL conservatorship by using the LD_0 as a conservative surrogate for an LD_{50}.

Based on Rule 232(1)(h) the ITSL is determined using the equation below:

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

Where:
W_A = the body weight of the male Sprague-Dawley rat in kilograms.
I_A = the daily inhalation rate of the male Sprague-Dawley rat in cubic meters/day.

According to EPA (2005) the weight of the male Sprague-Dawley rats in the LD_{50} study is 200-300 g. The average weight is 250 g. I_A is calculated using the equation from EPA (1988) below:

$$I_A = 0.80 \times W_A^{0.8206}$$

Using the average weight of male Sprague-Dawley rats of 0.25 kg for W_A:

$$I_A = 0.80 \times 0.25 \, kg^{0.8206} = 0.2565 \, \frac{m^3}{day}$$

Using the ITSL equation above and inputing the calculated I_A, the average weight for Sprague-Dawley rats of 250 g, and the LD_{50}:

$$ITSL = \frac{1}{500} \times \frac{1}{40} \times \frac{1}{100} \times \frac{10,000 \, \frac{mg}{kg} \times 0.25 \, kg}{0.167 \times 0.2565 \, \frac{m^3}{day}} = 0.02918 \, \frac{mg}{m^3} = 29 \, \frac{\mu g}{m^3}$$

Based on rule 232(2)(c) the averaging time is annual. Based on the above data, the ITSL for 1-dodecene [CAS# 112-41-4] is 29 µg/m³ based on 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.

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

EPA. 2005. United States Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. Robust Summaries Dossier for Members of the Higher Olefins Category Containing C11 to C13 Olefins. Prepared by: American Chemistry Council Higher Olefins Panel. April 28, 2005.

OECD. 2001. Alfa Olefins CAS N°: 592-41-6, 111-66-0, 872-05-9, 112-41-4, 1120-36-1. SIDS Initial Assessment Report for 11th SIAM. Orlando, Florida, United States. UNEP publications. Available online at: http://www.inchem.org/documents/sids/sids/AOalfaolefins.pdf