MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

INTEROFFICE COMMUNICATION

September 14, 2004

To: 3-(1,1-dimethylethoxy)-heptane file (CAS # 71945-54-5)

From: Gary Butterfield

Subject: Screening level for 3-(1,1-dimethylethoxy)-heptane

3-(1,1-Dimethylethoxy)-heptane is also known as tert-butyl-3-heptyl ether. It is a colorless liquid.

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), National Institute for Occupational Safety and Health (NIOSH) Registry for Toxic Effects of Chemical Substances (RTECS), American Conference of Governmental and Industrial Hygienists (ACGIH) Threshold Limit Values (TLVs), Michigan Department of Environmental Quality (DEQ) library, International Agency for Research on Cancer (IARC) Monographs, Chemical Abstract Service (CAS) Online (1968 - Feb 2004), National Library of Medicine (NLM) - Toxline, and National Toxicology Program (NTP) Status Report.

The CAS and NLM on-line literature searches were conducted on Jan 21, 2004. There was no toxicity information located on 3-(1,1-dimethylethoxy)-heptane during the literature searches. Due to a lack of available data the ITSL for 3-(1,1-dimethylethoxy)-heptane was initially set at the default trace value of 0.1 ug/m3 with annual averaging, under R232(1)(i) in April 2004.

However, Dow Chemical conducted an acute oral toxicity test during July of 2004 in order to generate some actual toxicity data, Brooks and Golden (2004). A group of three F344 female rats, weighing 142 to 153g, were administered a dose of 3-(1,1-dimethylethoxy)-heptane at 2000 mg/kg. None of the rats died during the 14 day observation period. An ITSL can be generated by use of the 2000 mg/kg as a surrogate LD50 in the calculation of an ITSL from the equation in R232(1)(h), as follows.

$$\text{ITSL} = \frac{2000 \text{ mg/kg}}{(500 \times 40 \times 100 \times 0.167)} \times \frac{1 \text{ kg}}{0.9 \text{ m3}} = 6 \text{ ug/m3} \quad \text{annual average}$$

The default rat inhalation rate of 0.9 m3/kg/day was used in the above calculation.

This ITSL, based on the surrogate LD50 of 2000 mg/kg, is considered to be health protective as it is lower than an ITSL value that was calculated on an actual LD50. Because the actual LD50 is probably much greater than 2000 mg/kg - there were no deaths observed in this study.

References:

Brooks and Golden. 2004. 3-(1,1-dimethylethoxy-)heptane: acute oral toxicity study in Fischer 344 rats. Unpublished study conducted by the Dow Chemical Company, Midland, Michigan.