

MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

INTEROFFICE COMMUNICATION

October 24, 2003

TO: C 6-8 branched alcohols file (CAS # 70914-20-4)

FROM: Gary Butterfield

SUBJECT: Screening level for C 6-8 branched alcohols

C6-8 branched alcohols are also listed in DuPont's MSDS as heptyl alcohols. This chemical is a high production volume (HPV) chemical, with the appropriate toxicological data and results of future tests being accumulated by EPA.

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 - May 2003), National Library of Medicine (NLM) - Toxline, and National Toxicology Program (NTP) Status Report.

The CAS and NLM on-line literature searches were conducted on October 21, 2003. There were no hits for toxicity information found for this chemical's CAS number.

A search of EPA's web site found several hits under this CAS number. There was a summary of an acute oral and acute inhalation study in the document by ExxonMobil Chemical (EPA 2002) that could be used to establish a screening level.

In the acute inhalation study a group of 5 male and 5 female Sprague-Dawley rats, Swiss albino mice, and Hartley guinea pigs were exposed to 152 ppm (nominal concentration) for 6 hours. This was the maximum vapor concentration attainable. A 14-day observation period followed the exposure. There were no deaths observed during this study. The LC50 is greater than 152 ppm.

In the acute oral study groups of 5 male Sprague-Dawley rats were administered a single gavage dose of 1, 1.47, 2.15, 3.16, 4.64, 6.81 or 10 g/kg. A 14-day observation period followed the dosing. All animals at the 6.81 and 10 g/kg dose levels died. Two rats at 4.64 g/kg died. One rat died in the 1, 2.15 and 3.15 g/kg dose levels. The LD50 was reported to be 3.9 g/kg.

It is generally advisable to use an inhalation study over an oral study when setting a screening level. However, the inhalation study has some faults - only one dose level was used, no actual LC50 was determined, and the concentration of exposure reported was based on a nominal concentration. The acute oral study had multiple dose levels spaced relatively closely, giving more confidence to the reported LD50 value, even though only one sex of rat was used.

Therefore, the acute oral study provides the best basis for setting the ITSL under R232(1)(h) as follows.

$$\text{ITSL} = \frac{3.9 \text{ g/kg}}{500 \times 40 \times 100 \times 0.167} \times \frac{1 \text{ kg}}{0.9 \text{ m}^3} = 13 \text{ ug/m}^3 \text{ annual average}$$

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

As a comparison to the above ITSL, a calculation based on the LC50 of 152 ppm and the equation from R232(1)(f) also results in an ITSL in the range of 13 to 16 ug/m³ (the range occurs from various possible molecular weights of the C6-8 branched alcohols). Thus, in this case, there is little difference between the oral LD50 based ITSL and the LC50 based ITSL. The above ITSL from the LD50 calculation is considered to be the best single point value for the ITSL.

References:

EPA OPPT. 2002. Olefin hydroformylation products category, robust summaries of environmental fate and effects. ExxonMobil Chemical.