

MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

INTEROFFICE COMMUNICATION

September 29, 2003

TO: 4,4-dimethoxy-2-butanone file (CAS # 5436-21-5)

FROM: Gary Butterfield, Toxics Unit, Air Quality Evaluation Section
Air Quality Division

SUBJECT: Screening level for 4,4-dimethoxy-2-butanone

4,4-Dimethoxy-2-butanone is a liquid with a molecular weight of 132.16 g/mol. 4,4-Dimethoxy-2-butanone is also commonly known as acetylacetaldehyde dimethyl acetal, or 3-ketobutyraldehyde dimethyl acetal, among many other synonyms. The melting point is -82 degrees Celsius. The boiling point is 178 degrees Celsius.

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 May 5, 2003. There were very few hits found during the literature searches for this chemical.

Dow submitted to DEQ Air Quality Division the results of an acute oral study, Dow Chemical/Jeffery (1986), for this chemical. Groups of 3 male F344 rats were administered single gavage doses at dose levels of 100, 500 or 1,000 mg/kg. Survivorship was monitored during a 14 day observation period. All animals survived the whole 14 day study. From this study, the LD50 appears to be greater than 1,000 mg/kg.

A sanitized acute toxicity report (EPA OTS doc# 0534674) was available from EPA, which had been submitted for TOSCA purposes. Details that the submitting company thought would be confidential business information were removed (sanitized). The company's identity and lab that conducted the study were among the details removed. In this study, groups of 6 male albino rats, weighing 120 to 153 grams, were administered a single gavage dose. Three dose levels were used, 5,000, 7,500 and 10,000 mg/kg. The rats were observed for 7 days following administration of the dose. All rats survived the 5,000 mg/kg dose. There was 1/6 survivors at 7500, and no survivors at 10,000 mg/kg. The LD50 was reported to be 6,200 mg/kg.

This sanitized study is the only toxicity study available that reports an actual LD50 being determined. The results from the sanitized report are consistent with those from Dow/Jeffery

(1986). It was determined to be the best data available for establishing a screening level. The ITSL will be based on the rat LD50 of 6,200 mg/kg, and calculated from R232(1)(h) as follows.

$$\text{ITSL} = \frac{(6,200 \text{ mg/kg})}{500 \times 40 \times 100 \times 0.167} \times \frac{1 \text{ kg}}{0.9 \text{ m}^3} = 20 \text{ ug/m}^3 \text{ annual average}$$

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

References:

Acute Oral Toxicity of AAD in Rats (final report) with Cover Letter Dated 11-21-91 (Sanitized).
EPA NTIS/OTS0534674

Dow Chemical/Jeffrey. 1986. Acetylacetaldehyde dimethyl acetal, technical: acute toxicologic properties. HERL file # DR-0049-7074-001. Summary submitted by Dow to DEQ Air Quality Division.