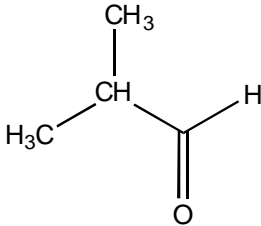


SIDS INITIAL ASSESSMENT PROFILE

CAS No.	78-84-2
Chemical Name	Isobutanal
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR**Analog justification**

Based on structure-activity considerations, data on the isobutanal analogs butyraldehyde (CAS No. 123-72-8), propionaldehyde (CAS No. 123-38-6) and isovaleraldehyde (CAS No. 590-86-3) were incorporated into the SIAR and SIDS Dossier to provide a more complete evaluation of the toxicity of isobutanal.

Human Health

Studies have been conducted that identify tissues and organs most sensitive to the effects of isobutanal. Direct contact produced an irritant response, and repeated inhalation exposure to 500 ppm and higher can lead to lesions of the tissues of the nasal mucosa. A developmental toxicity study indicated that isobutanal does not pose a hazard to developing fetuses at exposure concentrations up to 4000 ppm. Effects on male reproductive organs occurred at 4000 ppm and were accompanied by significant toxicity and mortality. Sperm motility after repeated exposure to rats was significantly decreased at 500 and 1000 ppm but was comparable to the controls at 2000 and 4000 ppm, with an overall conclusion that the effect of isobutanal on sperm motility was negative. There is *in vitro* and *in vivo* evidence that isobutanal causes mutagenic and genotoxic effects in mammalian cells. NTP carcinogenicity studies in rats and mice did not reveal any carcinogenic activity for isobutanal.

Environment

Isobutanal is a liquid at ambient temperatures with a melting point of -66 °C. It is soluble in water (25 g/L at 20 °C, 89 g/L at 25 °C), has a high vapor pressure (18.4 kPa at 20 °C; 172 mm Hg or 22.9 kPa at 25 °C) and a low octanol water partition coefficient (Log Kow = 0.77 at 25 °C). Isobutanal oxidizes slowly upon exposure to air, forming isobutyric acid; peroxides or peracids may also form. It is considered a highly flammable liquid which can easily be ignited by heat, sparks or flame. Its flashpoint is less than -18 °C. The flammability limits are 1.6% (lower) to 10.6% (upper).

Based on Level III distribution modeling, the majority of isobutanal released into the environment would partition into the water (64.8%), soil (27.4%) and air (7.72%). Measured and calculated concentrations in surface waters are below predicted no-effect concentrations. Modeling predicts that isobutanal is biodegradable and is not expected to accumulate in the environment.

For isobutanal, a static test with fathead minnows (*Pimephales promelas*) was reported to give a 96-hour LC₅₀ of

23 mg/L. With *Daphnia magna* Strauss, the reported 48 h EC₅₀ was 277 mg/L. The isobutanol toxicity to algae was tested with *Scenedesmus subspicatus* to give a 72-hour LC₅₀ of 84 mg/L.

Exposure

The worldwide production of isobutanol in 1993 *ca.* 700 807 metric tonnes (1545 million pounds); of this, 258,500 metric tonnes (*ca.* 570 million pounds), are produced in the US. This chemical finds sole use as a chemical intermediate. It is produced and used exclusively in closed systems and transport is by bulk carrier.

Toxics Release Inventory data reported for 1999 show that in the U.S., 118.6 metric tonnes (261,000 pounds) were released to the environment. The vast majority of this material, 118.0 metric tonnes (260,000 pounds), was released to the air, whereas 0.55 metric tonnes (1,200 pounds) were released into water. In addition to direct releases, 297.7 metric tonnes (656,000 pounds) were transferred to publicly owned treatment facilities and another 328.9 metric tonnes (725,000 pounds) to other off-site locations giving a total off-site waste transfer of approximately 626.6 metric tonnes (1,382,000 pounds).

In view of its primary use as a chemical intermediate, its low persistence in the environment, its low potential for adverse environmental impacts, and the unlikely occurrence of human exposure except in occupation situations, isobutanol is considered to be of low priority for further work.

RECOMMENDATION AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Isobutanol is currently of low priority for further work for human health and the environment.