## SIDS INITIAL ASSESSMENT PROFILE

CAS No.	60-24-2
Chemical Name	2-Mercaptoethanol
Structural Formula	HSOH C <sub>2</sub> H <sub>6</sub> O S

### SUMMARY CONCLUSIONS OF THE SIAR

#### Human Health

No data are available on toxicokinetics and metabolism of 2-mercaptoethanol in experimental studies. However, systemic toxic effects after exposure via different application routes suggested absorption and distribution after oral and dermal administration. The metabolite 2-mercaptoacetate was detected in the urine of a person who died from ingesting 2-mercaptoethanol.

The  $LD_{50}$  was 131 mg/kg bw in rats after acute oral exposure (OECD TG 401). The estimated  $LC_{50}$  after 4-hour inhalation exposure of rats was ca. 2000 mg/m<sup>3</sup>. In rabbits the  $LD_{50}$  after acute dermal exposure to 2-mercaptoethanol was 251 mg/kg bw. The clinical signs of systemic toxicity were mainly sedation, tremor and convulsions.

2-Mercaptoethanol was moderately irritating to rabbit skin in a 4-hour occlusive patch test. 2-Mercaptoethanol is corrosive to the rabbit eye, which was tested in studies according to the principles of the Draize test. Skin sensitizing effects were reported in a guinea pig maximization test (OECD TG 406).

In a study according to OECD TG 422 and 407 repeated oral application of 2-mercaptoethanol at 15, 50 and 75 mg/kg bw/day via gavage to rats for ca. 7 weeks resulted in clinical symptoms (excessive salivation, decreased body weight in males) and effects on the liver (organ weight increased and vacuolated liver cells in both genders) and the heart (degenerative cardiomyopathy in females at 50 and 75 mg/kg bw/day, in males at 75 mg/kg bw/day). The NOAEL was 15 mg/kg bw/day. 2-Mercaptoethanol neither induces gene mutation in *Salmonella typhimurium* nor chromosome aberration in human lymphocytes, both endpoints investigated in studies according to current guidelines (OECD TG 471 and 473, respectively). No mutagenic activity was detected in a mouse lymphoma assay (limited validity). Negative results were also obtained in a yeast recombination/mutation assay. Inconsistent results were reported in sister chromatid exchange (SCE) assays with CHO cells. No aneuploidy but an increased incidence of polyploid cells was observed in *in vitro* test systems indicating interaction with proteins or enzymes involved in mitosis. The *in vivo* micronucleus assay according to OECD TG 474 revealed no damage to the chromosomes or the mitotic apparatus of mouse bone marrow cells. Overall, available data showed no effects in gene and chromosome mutation assays, but revealed some evidence of polyploidy- inducing effects *in vitro*.

In a combined repeated dose toxicity study with the reproductive/developmental toxicity screening test (OECD TG 422, data on repeated dose toxicity see above) no effects were recorded on mating and fertility at 15 mg/kg bw/day. Doses of  $\geq$  50 mg/kg bw/day, which also induced general toxicity in males and females, prolonged the gestation

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period and/or affected delivery, with death of pregnant rats. The NOAEL for general toxicity, maternal toxicity, parturition and development of progeny is 15 mg/kg bw/day. The NOAEL for male reproductive performance and fertility is 75 mg/kg bw/day. The reproductive effects are not suitable for the differentiation between effects on female fertility and developmental effects. No data are available on carcinogenicity.

#### Environment

2-Mercaptoethanol is miscible with water. The substance has a vapour pressure of ca. 2 hPa at 25 °C, and a measured log Kow of -0.056 at 25 °C. The distribution modelling using Mackay, Level I, indicates water to be the almost exclusive (99.7 %) target compartment at 25°C. The calculated Henrys Law Constant of  $1.29 \times 10^{-2}$  Pa\*m<sup>3</sup>/mol indicates a low to moderate potential for volatilization from aqueous solution. The substance has a low potential for bio- and geoaccumulation. 2-Mercaptoethanol is not readily biodegradable according to OECD criteria. There is evidence for abiotic degradation in water. The half-life was influenced by the pH and temperature. At a constant temperature of 20 °C and pH 8.5 the half-life was 4 h, at a pH of 7.5 the half-life increased to 10 h, at a pH of 6.5 to > 100 h. The reaction of hydroxyl radicals with 2-mercaptoethanol in aqueous solution is insignificant. The substance is photodegraded by reaction with hydroxyl radicals (0.5 \* 10<sup>6</sup> molecule/cm<sup>3</sup>) in the atmosphere with an estimated half-life of 8.4 h. No information on direct photodegradation is available.

The following effect values are available from the short-term tests on aquatic species with fish, invertebrates and algae:

Leuciscus idus	$LC_{50}(96 h) = 37 mg/l$
Daphnia magna	$EC_{50} (48 h) = 0.4 mg/l$
Desmodesmus subspicatus	$E_r C_{50} (72 \text{ h}) = 19 \text{ mg/l.} (E_b C_{50} = 7.0 \text{ mg/l after } 72 \text{ h})$

For microorganisms (*Pseudomonas putida*) an EC<sub>50</sub> (17 h) = 125 mg/l was determined.

A PNEC<sub>aqua</sub> =  $0.4 \,\mu$ g/l can be calculated based on the lowest toxicity value (EC<sub>50</sub> =  $0.4 \,\text{mg/l}$ ) for aquatic invertebrates (*Daphnia*) with the assessment factor of 1,000.

#### Exposure

In the EU there are three known producers of 2-mercaptoethanol. The production volume in the EU in the year 2003 was about 10,000 to 15,000 tonnes/year. Further producers of 2-mercaptoethanol are known in China (4), Mexico (1) Japan (1) and in the US (1) but no data on production volumes are available.

By far the largest use of 2-mercaptoethanol ( $\geq$  90 %) is the use under controlled conditions as an intermediate in the synthesis of organo-tin thermal stabilizers for plastics (polyvinyl chloride). After two steps of reactions 2-mercaptoethanol is entirely consumed.

App. 10 % of the total 2-mercaptoethanol production volume is either used as regulator in polymerization processes consumed by reacting with the polymer chain or as chain transfer agent and used as lab chemical (e.g. reduction agent in immune biochemistry). 2-Mercaptoethanol is also used as an intermediate for the synthesis of pickling agents for seed and as textile auxiliaries. Less than 1 % is transferred to the sodium salt and used as additive in low percentages at an early stage of the leather production process (de-hairing). This de-hairing process is performed at a pH > 9. After this first leather manufacturing step the waste is collected and separately totally oxidized to sulphate, sulphur and sulphite by catalytic aeration treatment. 2-Mercaptoethanol, sodium salt does not reach the aquatic environment via the industrial effluents – as it is either consumed as intended during the de-hairing process or abiotic degraded under the alkaline conditions. (Di)Sulphides are formed by reaction with the keratinic materials or by abiotic degradation. The sulphides are totally oxidized during the final step of the de-hairing process or during the pre-treatment step of the sewage formed.

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During production, transport and processing of 2-mercaptoethanol releases into the environment may occur accidentally. Significantly less than 25 kg are emitted in 2000 to the atmosphere from production and processing sites at BASF AG and no 2-mercaptoethanol loaded sewage was formed. Exposure of operators/workers can be as far as possible avoided due to a manufacturing process in closed system and due to efficient personal protective equipment. During cleaning and maintenance procedures formed sewage is collected and disposed by combustion. Further exposure information from other production sites and processing sites is not available.

It can be summarized that the European Product registers provide no evidence for the presence of 2-mercaptoethanol in consumer products. All entries of 2-mercaptoethanol containing products are found in the categories of industrial uses apart from one finding in the category "health, education and welfare". The known and recommended uses according to all 2-mercaptoethanol producers are listed above. At BASF the requirements of the chemical weapon convention are voluntary fulfilled for 2-mercaptoethanol. All customers are obliged to declare the uses of 2-mercaptoethanol and are assessed for their reputability. Reputability assessments also take place at all producers. The CWC regulation applies to all customers in Germany, Europe and outside of Europe and along the chain of downstream users. No industrial use entries of 2-mercaptoethanol products in the product registers are raising questions and doubts at the producers.

2-Mercaptoethanol was tabulated among 30 different thiols (mainly methanthiol and 3-mercaptopropionates) detected in reducing, intertidal sediments from Biscayne Bay (Florida, USA), the concentration ranges between 0.5 -  $20 \,\mu$ M. Thiols arise as a result of biotic and abiotic reactions.

At all possible scenarios exposure is limited by the very strong, disagreeable odor similar to hydrogen sulfide (odour threshold  $\leq 2 \text{ mg/m}^3$ ).

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

**Human Health:** The chemical is currently of low priority for further work. 2-Mercaptoethanol possesses properties indicating a hazard for the human health (irritating to the skin and corrosive to the eye, sensitisation, some evidence on polyploidy inducing effects *in vitro*, toxic after acute and repeated exposure, developmental and reproductive toxicity in the range of maternal general toxicity). Based on the data presented by the Sponsor country (relating to production by one producer and the use pattern in several OECD countries), the chemical is therefore strictly controlled in occupational settings, and any repeated or prolonged exposure of workers is practically excluded. Warning of possible exposure is given by the quality of odour and the odour threshold (0.4 - 2 mg/m<sup>3</sup>). Countries may desire to investigate any exposure scenarios that were not presented by the sponsor country.

**Environment:** The chemical possesses properties indicating a hazard for the environment. Based on data presented by the Sponsor country (relating to production by one producer and the use pattern in several OECD countries), exposure to the environment is anticipated to be low, and therefore this chemical is currently of low priority for further work. Countries may desire to investigate any exposure scenarios that were not presented by the sponsor country.

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