SIDS INITIAL ASSESSMENT PROFILE

CAS No.	79-50-5
Chemical Name	2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl (DL-lactone)
Structural Formula	CH ₃ OH CH ₃ OH

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

There is no information on the toxicokinetics of DL-lactone available.

The acute oral LD_{50} of DL-lactone in rats and mice is above 2000 mg/kg bw.

In a test with rabbits (OECD 404) DL-Lactone was not irritating to the skin. However, based on occupational exposure experience in humans, DL-lactone is expected to be irritating to the eyes and upon prolonged and intensive exposure also to the skin. No sensitisation potential is found in the guinea-pig maximisation test (OECD 406).

In a combined repeated dose reproduction/developmental toxicity screening study (OECD 422) female rats treated at an oral dose of 1000 mg/kg bw/day showed aggression and restlessness during part of the study period. Findings on body weight, food consumption, haematology, clinical chemistry, organ weights, macroscopy and histopathology were within normal ranges. The NOAEL for repeated dose toxicity was set at 200 mg/kg bw/day.

DL-lactone was negative in an Ames test (OECD 471) and an *in vivo* micronucleus test (OECD 474). There are no indications that DL-lactone possesses mutagenic properties.

In an OECD 422 repeated dose reproduction/developmental toxicity screening study with rats exposed to DL-lactone, no effects on reproductive performance, stage of spermatogenesis, pup mortality, weight, sex and viability were reported up to oral doses of 1000 mg/kg bw/day. Animals were dosed prior to and during mating, gestation and following gestation until lactation day 4. Based on the available data, DL-lactone does not show evidence of reproductive or developmental toxicity. The NOAEL for reproductive toxicity is ≥1000 mg/kg bw/day.

Environment

DL-lactone is a white crystalline powder with a melting point of 78°C, boiling point of 247°C and a vapour pressure of about 0.1 hPa at 25°C (calculated from experimental vapour pressure at 60°C). The substance is very soluble in water (> 500 g/l) and has a log Kow of -0.69 (OECD 107). Based on its pKa (>13) DL-lactone is most likely present in the unionised form under environmental conditions. The substance is readily biodegradable. Hydrolysis half-live for DL-lactone is expected to be one year at pH 4, 30 days at pH 7 and approximately 12 days at pH 9 (25°C).

Various model calculations (based on log Kow) indicate that DL-Lactone does not bioaccumulate in fish and/or

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worms.

DL-lactone has an LC₅₀ of >140 mg/L in fish, an EC₅₀ of >130 mg/L in daphnia and an EC₅₀ for biomass and growth rate of >78 mg/L (nominal 100 mg/L) in algae. Data on the toxicity towards micro-organisms of the d-isomer are indicative of an EC₅₀ for micro-organisms above 100 mg/L.

Exposure

For the year 2004 the global market for DL-lactone was estimated to be 1000-5000 tonnes. DL-lactone is used in the synthesis of cosmetics and pharmaceuticals. At the production site of the main producer in UK DL-lactone is further processed on-site in closed systems in the synthesis of Calcium D-Pantothenate. Only a small amount (<0.5%) is isolated and sold to a third party. According to the product registers in Nordic Countries (Norway, Sweden and Denmark) and in Switzerland DL-lactone is not used in industrial and consumer products.

Occupational exposure may occur during synthesis, mainly through completion of process sampling and potentially during drumming-off operations.

Based on a production mass balance at the manufacturing plant of the main producer in UK for the year 2004, a maximum of 0.4 % of the total produced DL-lactone is lost to the waste water and a maximum of 0.75 % to the distillation residues which are incinerated. Waste water is treated in an on-site wastewater treatment plant. Since DL-lactone is ready biodegrable releases to surface water with effluents will be low.

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

Human Health: The chemical is currently of low priority for further work. The chemical possesses properties indicating a hazard for human health (skin and eye irritation). These hazards do not warrant further work as they are related to reversible effects. They should nevertheless be noted by chemical safety professionals and users.

Environment: The chemical is currently of low priority for further work because of its low hazard profile.

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