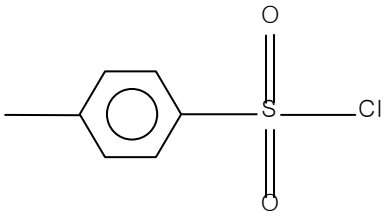
SIDS INITIAL ASSESSMENT PROFILE

CAS No.	98-59-9
Chemical Name	4-Methylbenzenesulfonyl chloride
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

There is no information on toxicokinetics, metabolism and distribution.

The acute oral toxicity study [OECD TG 423] of 4-methylbenzenesulfonyl chloride in rats showed that this chemical did not cause any significant changes in terms of LD_{50} at 2,000 mg/kg b.w for 1st and 2nd steps, and 5,000 mg/kg bw for limit test. Therefore, the oral LD_{50} value in female rats was greater than the highest tested dose (5,000 mg/kg bw). However, in a dose-finding study for an *in vivo* micronucleus test, at 200 mg/kg bw, all three female mice died.

Investigation was performed to observe effects of 4-methylbenzenesulfonyl chloride such as erythema and oedema on the abraded and intact backs of New Zealand White rabbits [OECD TG 404]. According to the results, the test substance induced irritation on the skins of rabbits. regarding eye irritation, a test was performed according to the FHSA protocol, in which the eyes were exposed for 24 hours then scored at 24, 48 and 72 hours after the exposure. Accordingly, 4-methylbenzenesulfonyl chloride induced corrosion and irritation on the eyes of New Zealand Albino Rabbits.

In the Combined Repeated Dose and Reproduction/Developmental Toxicity Screening Test in rats [OECD TG 422], 4-methylbenzenesulfonyl chloride was administrated by gavage at the dose levels of 0, 150, 350 and 750 mg/kg bw/day for 35 days and 36 ~ 51 days for male and female rats, respectively. Some clinical signs were observed at the dose level of 150 mg/kg bw/day in males such as intermittent (blood-like) salivation and staining around mouth; and in females such as intermittent (blood-like) salivation, staining around mouth, difficult delivery, poor nursing, irregular respiration. Based on these results, the LOAEL and NOAEL were determined to be 150 mg/kg/day and below the lowest tested dose (150 mg/kg/day) for both sexes, respectively.

In vitro bacterial gene reverse mutation tests [OECD TG 471 and 472] gave negative results in *Salmonella typhimurium* (strains TA98, TA1535 and TA1537) and *Escherichia coli* WP2 *uvr*A with and without metabolic activation. *Salmonella tryphimurium* (TA100 strain) showed positive mutagenic effects at concentrations of 1,250, 2,500 and 5,000 μg/plate without metabolic activation and the same strain (TA100) showed negative results with metabolic activation. Furthermore, an *in vivo* mutagenicity test, mammalian erythrocyte micronucleus assay (OECD TG 474) was negative. No firm conclusion can be reached from the available mutagenicity results.

In a reproduction/developmental toxicity screening test [OECD TG 422] with male and female rats, there were no significant treatment-related changes in terms of pregnancy, fertility, examination of pups etc. Therefore, LOAEL and NOAEL for reproduction and development are considered to be greater than 750 mg/kg bw/day.

Environment

4-Methylbenzenesulfonyl chloride is a colorless to light yellow crystalline solid which is hygroscopic and highly reactive. It has a melting point of 71 °C, a boiling point of 145 - 146 °C at 15 mmHg, a density of 1.33 g/cm^3, a vapour pressure of 0.16 Pa at 25 °C and a Henry's law constant of 9.67 x 10^{-6} atm•m^3/mole at 25 °C. Due to the rapid hydrolysis of 4-methylbenzenesulfonyl chloride, water solubility and partition coefficient n-octanol/water cannot be measured. Hence a partition coefficient n-octanol/water (log P_{ow}) of 3.49 at 25 °C and a water solubility of 51.18 mg/L at 25 °C were estimated.
4-Methylbenzenesulfonyl chloride is hydrolysed to 4-methylsulfonic acid and half-lives ($t_{1/2}$) at 25 °C in water are 2.2 min at pH 4, 2.2 min at pH 7 and 2.6 min at pH 9. The substance is not readily biodegradable. The calculated half-life for photochemical-oxidative degradation in the atmosphere by OH radicals is 8.7 days. According to a level III fugacity modeling (EQC model) if 4-methylbenzenesulfonyl chloride is emitted to air, it will mainly partition to soil (97.6 %) and if it is released to water, it will mainly remain in water (79.2 %). If it is released to soil, it will mainly remain in soil (100 %). Based on rapid hydrolysis of the substance, bioconcentration of 4-methylbenzenesulfonyl chloride is not expected. 4-Methylbenzenesulfonic acid is a strong acid (pK = -1.34) and is completely dissociated at the environmental pH. According to a level III fugacity modeling (EQC model) if 4-methylbenzenesulfonic acid is emitted to air, it will mainly partition to soil (78.4 %) and if it is released to water, it will mainly remain in water (99.8 %). If it is released to soil, it will mainly remain in soil (80.6 %). The calculated BCF value of 4-methylbenzenesulfonic acid was 3.16. Both the substance and its hydrolysis product have a low potential for bioaccumulation.

The following toxicity data for aquatic organisms are available for 4-methylbenzenesulfonyl chloride:
Green algae (*Selenastrum capricornutum)*: EC_{g50} (72 h) > 100 mg/L (growth rate)
Invertebrates (*Daphnia magna):* EC_{50} (48 h) = 70 mg/L.
Fish (*Oryzias latipes*): LC_{50} (96 h) = 55 mg/L.

In preliminary tests with adjustment of pH with fish and daphnia, at 100 mg/L of 4-methylbenzenesulfonyl chloride, no effects were seen in fish and daphnia after 48 hours of exposure.

The following toxicity data for aquatic organisms are available for 4-methylbenzenesulfonic acid:
Green algae (*Chlorella vulgaris*): EC_{50}(24h) = 245 mg/L (unspecified)
Invertebrates (*Daphnia magna*) : EC_0(24h) > 2500 mg/L.
Fish (*Leuciscus idus melanotus*): LC_{50} (96h) > 500 mg/L
Microorganisms (anaerobic bact. from a domestic water treatment plant): SG(24h) > 5000 mg/L

No data are available on terrestrial organisms.

Exposure

In the Sponsor country, the production amount for 4-methylbenzenesulfonyl chloride was estimated to be about 542.7 tonnes in 2001. Around 689.8 tonnes were imported into Korea from China in 2001.
In the Sponsor country 4-methylbenzenesulfonyl chloride is produced as a by-product from the reaction of HSO_3Cl and toluene in the food additives industry and this chemical is used as a raw material for the production of foaming agents for the plastic and rubber industry, of riboflavin and antithrombotic drug in the pharmaceutical industry and of a condensing agent in the dye industry.
Environmental releases are unlikely to occur during industrial production and processing of 4-methylbenzenesulfonyl chloride as these processes take place in closed systems. If environmental releases occur during these operations, they will be in the form of the hydrolysis product 4-methylbenzenesulfonic acid.
There is a potential of exposure for workers via dust inhalation and dermal routes at the packaging process. Based on physico-chemical properties and the hygroscopic nature of this chemical, if workers are exposed, they are likely to be exposed to the acid. Although 4-methylbenzenesulfonyl chloride is used as a raw material in several industries, there is no direct use or consumer products containing the substance. Therefore, consumer exposure to the substance is not expected.

RECOMMENDATION

The chemical is currently of low priority for further work.

RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

The chemical possesses properties indicating a hazard for human health (e.g. irritation, uncertainty for genotoxicity). Based on data presented by the Sponsor country, exposure to humans 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.