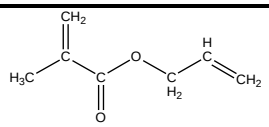
SIDS INITIAL ASSESSMENT PROFILE

CAS Nos	96-05-9
Chemical Names	Allyl Methacrylate
Structural Formulae	

SUMMARY CONCLUSIONS OF THE SIAR

Physical-Chemical Properties

Allyl methacrylate is a clear, colorless liquid with a melting point of -75 °C, boiling point of 141 °C, and measured vapor pressure of 7.7 hPa (5.77 mmHg) at 25 °C. The measured octanol-water partition coefficient (log K_{ow}) is 2.15 at 25°C, and water solubility is 2200 mg/L.

Human Health

No data were identified related to metabolism of allyl methacrylate. In general, methacrylates are readily absorbed and metabolized to methacrylic acid and the appropriate alcohol. Therefore, allyl methacrylate is expected to be metabolized to methacrylic acid and allyl alcohol.

In a 4-hour acute inhalation toxicity study in male and female rats exposed to allyl methacrylate vapour via whole body, the LC_{50} was 1.56 mg/L (310 ppm). Clinical signs included secretory responses (chromodacryorrhea, nasal discharge, excessive lacrimation, excessive salivation) and respiratory responses (labored breathing, gasping and moist rales) and signs of CNS depression (decreased motor activity and effects that included flattened posture, drooping eyelids, ataxia or tip-toe gait, decreased or no locomotor activity, stupor, no response to external stimulation, abnormal air righting reflex and decreased grip strength) that were considered to be general effects of allyl methacrylate exposure and not specific neurobehavioral effects; the surviving animals showed no such effects at 1 or 2 weeks after exposure. In a second study (nose only exposure), rats were exposed to allyl methacrylate vapour at 1.02 and 2.13 mg/L (198 and 414 ppm). Clinical signs during exposure included initial exaggerated breathing for approximately 2 hours followed by a decreased breathing rate. No treatment-related findings were noted at necropsy of surviving rats. The 4-hour inhalation LC_{50} from this study was estimated to be 1.47 mg/L (the geometric mean of the two concentrations tested). The oral LD_{50} of allyl methacrylate in male rats was 470 mg/kg bw. In the oral study, rats exhibited lacrimation (high-dose group) and piloerection. Necropsy findings in the survivors included dark yellow liver lesions and adhesions of the stomach and/or liver peritoneum. These oral data are adequate for SIDS because there is no indication in studies with acrylates/methacrylates in general that toxicity is greater in females than males, and the results from acute inhalation toxicity studies indicate that female rats are not more sensitive, and possibly slightly less sensitive, than male rats to allyl methacrylate. In two limited acute dermal toxicity studies in rabbits, LD_{50s} were 210 and 467 mg/kg bw.

Allyl methacrylate was not irritating to slightly irritating to rabbit skin and eyes. A case report indicated skin irritation in three of 11 humans exposed to 3% allyl methacrylate in olive oil. Acute inhalation studies with allyl methacrylate suggest the substance is a respiratory irritant. In a 4-hour acute inhalation toxicity study clinical signs included respiratory responses (labored breathing, gasping and moist rales). In a second study with nose only exposure, clinical signs during exposure included initial exaggerated breathing for approximately 2 hours followed by a decreased breathing rate. Allyl methacrylate was not a skin sensitiser in guinea pigs (OECD TG 406).

Repeated-dose toxicity of allyl methacrylate has been investigated in two studies. In a combined repeated-dose/reproduction/developmental toxicity screening test (OECD TG 422), the test substance was administered via gavage to 10 rats/sex/dose at 0 (corn oil), 3, 15 or 60 mg/kg bw/day. Males were treated once daily during the pre-mating and mating periods for a minimum of 4 weeks. Females were treated once daily during pre-mating, mating and gestation and through post natal day (PND) 5 (the day of birth was designated PND 1). Males were sacrificed after the mating period, and females were sacrificed with their litters on PND 6. Hypersalivation was observed in a dose-related manner in males and females given 15 or 60 mg/kg bw/day. Treatment-related effects at 60 mg/kg bw/day included one female with hypotonia and half-closed eyes on PND 5, one

female with increased total bilirubin concentration and another with increased biliary acid concentration that correlated with pathological findings in the liver (yellowish areas in 2/5 animals and foci of degenerated/necrotic hepatocytes, together with slight periportal fibrosis, slight biliary proliferation, and greenish-pigment-laden macrophages in 3/5 females). Other treatment-related findings included increased absolute thymus weights in the 15 and 60 mg/kg bw/day males group ($p< 0.05$). Based on liver effects, the LOAEL was 60 mg/kg bw/day and the NOAEL was 15 mg/kg bw/day.

In a 28-day dermal toxicity study, the test substance was administered under occlusive condition to rabbits (6 animals/sex/dose) at 0, 25, 50 or 100 mg/kg bw for 6 hrs/day, 5 days/week, for 4 weeks. A recovery high dose group was monitored for three additional weeks after dosing. Four female rabbits, two from the 50 mg/kg bw/day group and two from the 100 mg/kg bw/day group, died during the dosing phase of the study. Body weights and food consumption of the high-dose males were decreased throughout the dosing phase. No treatment-related clinical signs or changes in hematology, blood chemistry, or urine measurements were observed. Slight hemorrhage in the fascia of the skin at the treatment site in the high dose group animals was the only observation at termination. Microscopic effects were hyperplastic thickening of the epidermis with hyperkeratosis of the treatment-site skin, primarily in the high dose group. Following the recovery period, the animals from the high dose group appeared normal. A NOEL of 25 mg/kg bw/day was identified from this study.

In a bacterial reverse mutation assay with multiple strains of *Salmonella typhimurium*, allyl methacrylate was negative both with and without metabolic activation. In an *in vitro* chromosomal aberration test using human lymphocytes allyl methacrylate was negative. Based on these results, allyl methacrylate is not considered genotoxic *in vitro*. No *in vivo* mutagenicity studies were identified for allyl methacrylate.

No data are available for the carcinogenicity of allyl methacrylate.

In the repeated-dose/reproductive/ developmental toxicity screening test in rats (OECD TG 422) described above, no effects were observed following oral exposure of males and females to allyl methacrylate on reproductive performance, fertility or development in pups. The NOAEL for reproductive performance and developmental toxicity was 60 mg/kg bw/day (the highest dose tested).

The developmental toxicity of allyl methacrylate has also been investigated in rats via inhalation in an OECD TG 414 developmental toxicity study. Pregnant rats (19-25/group) were exposed to allyl methacrylate vapour via whole body inhalation for 6 hrs/day during gestation days 6 to 20 at 0, 12, 25, 50, and 100 ppm (corresponding to 0, 0.063, 0.131, 0.262, 0.524 mg/L). Maternal weight gain was reduced at $\geq$ 12 ppm. The mean number of implantation sites and number of live fetuses was comparable across all groups. Although slight increases in the incidence of non-live implants and of resorptions at 50 and 100 ppm were observed, these were not statistically significant. There was a concentration-related decrease in fetal body weight that achieved a statistical significance at 100 ppm. No compound-induced teratogenic effects were observed. The NOAEL for maternal toxicity was not achieved. The NOAEL for developmental toxicity was 50 ppm (0.262 mg/L/day) based on decreased fetal body weight. Based on these data, allyl methacrylate may result in developmental toxicity via inhalation (decreased fetal body weights).

Allyl methacrylate possesses properties indicating a hazard for human health (skin, respiratory and slight eye irritation, acute toxicity, repeated-dose toxicity, and developmental toxicity via the inhalation route). Adequate screening-level data are available to characterize the human health hazard for the purposes of the OECD HPV Programme.

Environment

Hydrolysis of allyl methacrylate, as with other methacrylates, is not expected to occur at pH values below 9; therefore, hydrolysis does not occur under normal environmental conditions. In the atmosphere, indirect photo-oxidation of allyl methacrylate is predicted to occur with an estimated half life of 2.8 hours with an OH-rate constant of 4.59×10^{-11} cm^3/molecule-sec. obtained using EPISuite. Allyl methacrylate does not contain photolytically active groups and, therefore, direct photolysis by absorption of light > 290 nm will not occur. A test conducted according to OECD TG 301D with allyl methacrylate resulted in 67.3% degradation over 28 days and met the 10-day window criterion. Allyl methacrylate is readily biodegradable under aerobic conditions.

The level III fugacity model calculation with equal and continuous distributions to air, water and soil compartments suggests that allyl methacrylate will partition primarily into soil (57.3%) and water (40.8%), with smaller amounts in air (1.75%) and sediment (0.1%). A Henry's law constant of 1.90 x 10^{-4} atm-m3/mole (19.3 Pa-m3/mole) (bond method) suggests that volatilization of allyl methacrylate from the water phase is expected to be moderate.

The bioaccumulation potential is estimated to be low based on a BCF value of 12.2 calculated with BCFWIN based on the low

log K_{ow} of 2.15.

The following acute toxicity test results have been determined for allyl methacrylate in aquatic species:

Fish [*Pimephales promelas*]	96-h LC_{50} = 0.61 mg/L (measured)
Invertebrates [*Daphnia magna*]	48-h EC_{50} = 2.4 mg/L (measured)
Algae [*Pseudokirchneriella subcapitata*]	72-h ErC_{50} = 59.6 mg/L (growth rate) (measured)
	96-h ErC_{50} = 77.2 mg/L (growth rate) (measured)
	72-h EbC_{50} = 19.3 mg/L (biomass) (measured)
	96-h EbC_{50} = 28.8 mg/L (biomass) (measured)

Allyl methacrylate possesses properties indicating a hazard for the environment (acute toxicity to fish, invertebrates and algae from <1 to 100 mg/L). However, allyl methacrylate is readily biodegradable and has a limited potential for bioaccumulation. Adequate screening-level data are available to characterize the environmental hazards for the purposes of the OECD HPV Programme.

Exposure

The world-wide estimated total annual production volume of allyl methacrylate is 1,000 to 10,000 metric tons.

Allyl methacrylate is manufactured using closed systems and can be produced by two different methods: (1) reaction of allyl alcohol and methacrylic acid and (2) trans-esterification of allyl alcohol and methyl methacrylate. It is further purified through distillation. Allyl methacrylate is a reactive monomer intermediate that is used in the production of polymers. The monomer is both manufactured and processed in closed systems. These closed systems are process units where most, if not all, of the equipment is vented to a scrubbing system or flare. Allyl methacrylate is primarily used as a cross-linking agent to improve the hardness and heat resistance of resins. In addition, it can be used as a rubber improver and coating modifier. Allyl methacrylate can also be used to manufacture intermediate compounds, which are then used to produce polymers. Methacrylate polymers have an uninterrupted carbon backbone and are very stable. With the additional cross-linking provided by reactions of the allyl side chain, the polymers can only be destroyed by a very high supply of energy (e.g. pyrolysis). Therefore, the polymer will not revert back to its original monomeric form during degradation under usual industrial and environmental conditions.

The monomer is both manufactured and processed in closed systems, which limits occupational exposure. Since there is potential inhalation exposure to allyl methacrylate and it has an offensive odor, special measures are taken to minimize or prevent worker exposure. There are no current occupational exposure limit values for allyl methacrylate. All customers are major resin or chemical producers with fully developed industrial hygiene procedures and equipment to minimize potential exposure. After initial manufacture of the resin, the material may be washed to remove residual monomers. In the production of water borne primary dispersions, the residual monomers are reacted away by a boost (addition of peroxide) or a distillation step, which is expected to limit consumer exposure. A typical residual monomer level of allyl methacrylate in finished resins is 1 - 2 ppm.

Since allyl methacrylate is a chemical intermediate that is both manufactured and processed in closed systems and wastes are incinerated or treated biologically, exposure from releases to the environment is expected to be limited.