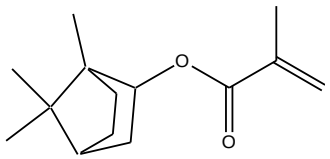
SIDS INITIAL ASSESSMENT PROFILE

CAS No.	7534-94-3
Chemical Name	Isobornyl Methacrylate (IBOMA)
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Physicochemical Properties

Isobornyl methacrylate **(IBOMA)** is liquid at room temperature. In a melting point study, the measured melting point was not detected, but a relaxation peak and an endothermic Specific heat capacity (Cp)-step was shown at -94 °C, characteristics for a glass transition (i.e., the test item solidifies amorphously in the glassy state). The measured boiling point value is 258°C; measured vapor pressure is 0.012 hPa at 25°C; measured water solubility is 5.44 mg/L at 20°C; measured octanol log K_{ow} values is 5.09. Estimated and measured values are highly concordant.

Human Health

No toxicokinetic, metabolism or distribution studies were identified for **IBOMA**. However, in general, methacrylates are known to be metabolized to methacrylic acid and the corresponding alcohols.

In rats, the oral LD_{50} value was 3,100 mg/kg bw (males) and 6,670 mg/kg bw (females) in an oral gavage study [pre-guideline]. The clinical signs included depression, hunched appearance, ataxia, excessive urination, and labored respiration. Animals that died during the study showed gastrointestinal inflammation and/or congestion of the lung lobes at the two highest dose levels (i.e., approximately 4,547 and 9,800 mg/kg bw for males and 9,800 and 21,070 mg/kg bw for females). **IBOMA** is not considered to be an acutely toxic substance via the oral route. No reliable acute toxicity studies were identified for the inhalation or dermal routes of exposure. Based on its low vapor pressure, **IBOMA** is unlikely to be hazardous via the inhalation route.

No guideline, or reliable, skin or eye irritation studies were identified for **IBOMA.** Following intracutaneous induction in a guinea pig maximization test [OECD TG 406], **IBOMA** did not evoke a skin reaction during challenge exposure when applied undiluted under occlusive conditions. As such, **IBOMA** was not sensitizing to skin under the conditions of the test.

Repeated-dose toxicity of **IBOMA** has been investigated in two subchronic dietary toxicity studies using rats and dogs, and in one oral gavage study [OECD TG 421] in rats. In the subchronic dietary rat study [Pre-guideline; similar to OECD TG 408], **IBOMA** was administered to 15 rats/sex/group, in the diet, *ad libitum*, at concentrations of 0, 1000, 3000, or 10,000 ppm (approximately 0, 50, 150, or 500 mg/kg bw/day) for 3 months. No deaths were reported at any concentration. Treatment-related effects included significantly decreased growth rate, food consumption and mean terminal body weights in males and females at 10,000 ppm compared to the controls. Increased liver weight relative to body weight (both sexes), and increased kidney and testis weight relative to body weight (males), was observed at 10,000

ppm. Histopathological findings in the liver at all concentrations ranged from biliary epithelial hyperplasia at 1000 ppm to severe bile duct hyperplasia at 10,000 ppm in both sexes. Histopathological changes in the kidneys of male and female rats were observed at all concentrations. At 10,000 ppm, hypertrophy of the deep proximal convoluted tubules was seen, while at 3000 and 1000 ppm, varying degrees of protein imbibition, slightly more severe than controls, was considered to be related to treatment. In addition, hypercellularity of the bone marrow was noted in animals at 10,000 ppm. A NOAEL could not be established because histopathologic changes were noted at all concentrations. The LOAEL for 3 months of dietary exposure to **IBOMA** was 1000 ppm (approximately 50 mg/kg bw/day) based on histopathologic changes in the kidneys and liver at all doses.

In the subchronic dietary dog study [Pre-guideline; similar to OECD TG 409], **IBOMA** was administered daily to 4 dogs/sex/group in the diet at concentrations of 0, 1000, 3000, or 10,000 ppm (approximately 0, 31, 95, or 352 mg/kg bw/day) for 13 weeks. No deaths were reported at any concentration. Toxicologically-significant effects were limited to the animals at 10,000 ppm and included slightly increased blood urea nitrogen (BUN), increased liver to body weight ratio, and minimal to slight degenerative changes in the epithelial cells of the kidney proximal convoluted tubules. The NOAEL for 13-weeks of dietary exposure to **IBOMA** in dogs was 3000 ppm (approximately 95 mg/kg bw/day). The LOAEL was based on clinical pathology (BUN), organ weights (liver), and histopathologic findings (kidney) at 10,000 ppm (approximately 352 mg/kg bw/day).

In a reproduction/developmental toxicity screening study (OECD TG 421), three groups of 10 male and 10 female rats received **IBOMA** by daily oral gavage at 0 (corn oil), 25, 100, and 500 mg/kg bw/day. The males were dosed for 29 days and the females were dosed for up to 55 days. Hypersalivation was observed in a dose-related manner in males and females given 100 or 500 mg/kg bw/day. During the first week of the pre-mating period, males given 500 mg/kg bw/day gained less weight than controls. There were no other treatment-related effects on body weight, weight gain or food consumption during the study for males or females. There was a statistically significant increase in liver weight (males and females) and kidney weight (males only) at 500 mg/kg bw/day. No treatment-related findings were found in the reproductive organs examined. Microscopic findings in the liver included biliary proliferation/hypertrophy associated with fibrosis and macrophages infiltration (100 and 500 mg/kg bw/day, both sexes); disorganization of the hepatic cords (500 mg/kg bw/day, both sexes); and necrosis in the parenchyma (500 mg/kg bw/day, males). No treatment-related microscopic findings were observed at 25 mg/kg bw/day. In the kidneys, acidophilic globules were observed in the cortical tubular epithelium with a higher severity in males at 100 and 500 mg/kg bw/day, relative to controls. Based on the experimental conditions of the study, the NOAEL for systemic (parental) toxicity was 25 mg/kg bw/day.

In an Ames test [OECD TG 471], with multiple strains of *Salmonella typhimurium* and *Escherichia coli* WP2 uvrA, **IBOMA** was negative both with and without metabolic activation. In an *in vitro* chromosomal aberration test [OECD TG 473] using cultured human lymphocytes, **IBOMA** was negative with or without metabolic activation. Based on these results, **IBOMA** is not considered genotoxic under *in vitro* conditions.

No *in vivo* genetic toxicity studies were identified for **IBOMA**.

No data are available for the carcinogenicity of **IBOMA**.

In a reproduction/developmental toxicity screening test [OECD TG 421], three groups of 10 rats/sex/dose were administered **IBOMA** daily via oral gavage for 15 days prior to mating, during mating and gestation, and through lactation day (LD) 5. The dose levels were 0 (corn oil), 25, 100, or 500 mg/kg bw/day. The males were dosed for 29 days and the females were dosed for up to 55 days. The systemic toxicity effects for parental animals are described above. No treatment-related findings were noted in the reproductive organs examined. The male and female fertility indices were unaffected by treatment. All pregnant females had live pups, and the duration of gestation was similar in the control and **IBOMA** groups. There was no effect of treatment on the mean number of live born pups or on pup death after birth. There were no gross external pup abnormalities in the control or **IBOMA** groups. No significant differences were noted in the male and female pup body weight gain. No relevant findings were noted in pups sacrificed at PND 6. No treatment-related findings were found in the reproductive organs examined. Based on the experimental conditions of the study, the NOAEL for systemic toxicity was 25 mg/kg bw/day and the NOAEL for reproductive/developmental toxicity was 500 mg/kg bw/day (highest dose tested).

IBOMA possesses properties indicating a hazard for human health (repeated-dose toxicity), and the liver and kidney appear to be the main target organs. Adequate screening level data are available to characterize the human health hazard for the purposes of the OECD HPV Programme.

Environment

The predicted atmospheric half-life (AOP v.1.92) is 5.0 hours (12-hr day; 1.5 x 10^6 OH/cm^3). In general, methacrylates do not contain photolytically active groups (i.e., direct photolysis by absorption of light > 290 nm will not occur). Methacrylates are hydrolytically stable at acidic and neutral pH levels. For environments at a pH range between 5-7, hydrolysis is not expected to be a significant route of degradation for **IBOMA**; however, at higher pH levels (i.e., 9-11), methacrylates rapidly hydrolyze.

The level III fugacity model (EpiSuite 4.00) calculation for **IBOMA** with equal and continuous release (1000 kg/hr) to air, water, and soil suggests that **IBOMA** will distribute mainly to the soil (86.7%) with minor distribution to other compartments (11.9% to water, 0.8% to sediment, and 0.6% to air). With 100% release of 1,000 kg **IBOMA**/hr to water, 92.1% would remain in the water, 6.5% would distribute to sediment, 1.4% to air and <0.1% would enter the soil. Similarly, with 100% release of the same amount to soil, 99.7% is expected to remain in the soil with virtually no distribution to air, water or sediment.

In a recent biodegradation study [OECD 301 D], **IBOMA** reached the 60% pass level within the 10-day window and 70% after 28 days. **IBOMA** is considered to be readily biodegradable. The calculated Henry's law constant (HENRYWIN v. 3.0) for **IBOMA** is 36.6 Pa-m3/mole (3.61 x 10^{-4} atm-m^3/mole), which suggests that volatilization from the water phase is expected to be moderate. Based on the measured log K_{ow} of 5.09 and the relatively low measured water solubility (5.44 mg/L at 20°C and 6.35 mg/L at 30°C), there is a potential for bioaccumulation (estimated BCF = 1060, regression-based method; BCFBAF v. 3.00). An estimated Log K_{oc} value of 3.4 indicates that IBOMA has a moderate sorption to soil and sediment.

The following aquatic acute toxicity results have been determined for **IBOMA**:

An acute toxicity to fish [OECD TG 203] study yielded a 96-hour LC_{50} for zebrafish, *Danio rerio*, of 1.79 mg/L (measured);

An acute toxicity to *Daphnia magna* [OECD TG 202] study indicated that the 48-hour **IBOMA** EC_{50} was 1.1 mg/L (nominal). A more recent *D. magna* study [OECD TG 202] reported a measured 48-hour EC_{50} of > 2.57 mg/L. A saturated solution of 2.57 mg/L was the maximum dissolved concentration of **IBOMA** that could be achieved under the test conditions in the test medium;

An aquatic plant toxicity to *Pseudokirchneriella subcapitata* [OECD TG 201] study produced 72- and 96-hour E_rC_{50} (algal growth) values of 2.28 and 2.66 mg/L, respectively, and E_bC_{50} (biomass) values of 0.835 and 0.913 mg/L, respectively; the NOEC at 72- and 96-hours was 0.251 and 0.254 mg/L, respectively, based on both the growth rate and biomass.

IBOMA possesses properties indicating a hazard for the environment (acute toxicity to fish, daphnia, and algae from less than 1 to 10 mg/L). IBOMA has some potential for bioaccumulation. IBOMA is readily biodegradable. Adequate screening-level data are available to characterize the environmental hazard for the purposes of the OECD HPV Programme.

Exposure

The world-wide estimated total annual production volume of **IBOMA** is 1000 to 10,000 metric tons. The percentage breakdown by country/region is considered confidential. **IBOMA** is manufactured using only closed systems. On a commercial scale, **IBOMA** is produced by the reaction of camphene and methacrylic acid. **IBOMA** may also be made through the reaction of isobornyl alcohol and methacrylic acid; however, this is a secondary method and is not used on a commercial scale. **IBOMA** is purified through distillation.

With respect to the impurities in the commercial-scale material, it is normal to have both camphene and isobornyl alcohol impurities. Although isobornyl alcohol is not used as a reactant on a commercial scale, the alcohol impurity results from the hydrolysis of camphene with water.

IBOMA is manufactured and processed in closed systems which limit environmental exposure. Waste streams containing

IBOMA are typically treated as hazardous waste through incineration or, for aqueous waste streams, at on-site biological treatment facilities. For other uses (e.g., providing properties of abrasion and/or water and chemical resistance), **IBOMA** may enter the environment in small quantities.

IBOMA is used as a reactive monomer intermediate in the manufacture of resins. Nearly all (>95%) of the monomer is polymerized by large industrial paint and coatings companies. The polymers made with **IBOMA** are used in paints and coatings for industrial applications in metal, glass, and plastics; the polymers are not used in consumer paints or coatings. Very small amounts of polymers are used in other industrial or commercial applications: adhesives, polymer concrete, and optical products. After initial manufacture of the resin, the material is washed to remove residual monomers. Typical residual monomer levels of **IBOMA** in finished resins are 10-20 ppm. Therefore, consumer exposure to **IBOMA** is expected to be negligible.

The majority of **IBOMA** is shipped in bulk containers (e.g., IBCs, tank trucks, rail cars) rather than in drums. As a result, the material is transferred/pumped directly from bulk containers to process equipment using closed piping with vapor recovery systems. Exposure and release are generally limited to fugitive emissions.

The general public and consumers are not expected to ever be exposed to **IBOMA** in monomer form. The only people that may be exposed to **IBOMA** would be a very limited number of workers either producing the monomer or workers in coatings and adhesive resins facilities that use the **IBOMA** to make acrylate resins.