# BASIC ACRYLIC MONOMER MANUFACTURERS, INC.

## SUBSTANCE REVIEW: I-BUTYL ACRYLATE

**(Last Updated: 5/7/12)**

**Disclaimer**

| Substance | Acronym | CAS Number |
|---|---|---|
| **i-Butyl acrylate** | iBA | 106-63-8 |

### Physicochemical Properties

| Property | Results |
|---|---|
| Physical state at 20°C and 1013 hPa | Liquid<br><br>Color: colorless<br><br>Odor: like ester |
| Melting / freezing point | -61 °C |
| Boiling point | 132 °C at 1013 hPa |
| Relative density | 0.8896 g/m$^3$ @ 20 °C |
| Vapor pressure | 10 hPa at 25 °C |
| Surface tension | not surface active |
| Water solubility | 1.8 g/l at 25 °C |
| Partition coefficient n-octanol/water (log value) | 2.38 at 25 °C |
| Flash point | 30 °C (cc) |
| Flammability | Flammable upon ignition.<br>The substance has no pyrophoric properties and does not liberate flammable gases on contact with water. |
| Explosive properties | non explosive |
| Self-ignition temperature | 350 ° C at 1013 hPa |
| Oxidizing properties | no oxidizing properties |
| Granulometry | not applicable |
| Stability in organic solvents and identity of relevant degradation products | not applicable |
| Dissociation constant | not applicable |
| Viscosity | 0.822 mPa.s at 21.1 °C |

## Environmental Fate

In contact with water, Isobutyl acrylate will hydrolyze slowly. Photodegradation in air will proceed slowly, too. In water, sewage treatment plants and soil rapid degradation is expected, since i-BA was readily biodegradable in an OECD 310-Screening test. Based on an experimental log Pow and calculated BCF, a potential for bioaccumulation is not to be expected. Adsorption of isobutyl acrylate to the solid soil phase is not expected.

Fugacity model calculation (Mackay Level I) revealed the atmosphere as the main target compartment for distribution which is also indicated by the substance's physicochemical properties.

## Ecotoxicity

When evaluated as a group, the acrylate esters have similar ecotoxicity data. LC50 values in freshwater fish ranged from 1.81 and 5.2 mg/L, EC50 values in freshwater invertebrates (Daphnia magna) were between 1.3 and 8.74 mg/L, and EC50 values in freshwater algae were between 1.71 and 14.6 mg/L, respectively. Thus, effect values were all in the same range of concentrations with Daphnia magna as the most sensitive freshwater species by a narrow margin. A 21-day chronic life-cycle study with Daphnia magna is available with ethyl acrylate with a respective NOEC of 0.19 mg/L, and another with n-butyl acrylate with a NOEC of 0.136 mg/L. In addition, several NOEC values from studies in algal species are available ranging from 0.45 to 3.85 mg/L.

## HUMAN HEALTH EFFECTS

Acute Toxicity
Iso-butyl acrylate is of low toxicity after a single ingestion. iBA is of moderate toxicity after a short-term inhalation and after short-term skin contact.

- Oral: LD50 = 4895 mg/kg bw (rat)
- Dermal: LD50 ca. 793 – 4000 mg/kg bw (rabbit)
- Inhalation: LC50 = 10.5 mg/L (rat, 4h)

Irritation/Sensitization
Iso-butyl acrylate is irritating respiratory system and skin. iBA is suspected to be a skin sensitizer, based on the structural similarity to n-butyl acrylate.

Repeated Dose Toxicity
No repeated dose toxicity studies are available with iBA; therefore data of the structural analogue n-butyl acrylate are taken to assess toxicity after repeated exposure.

In a chronic (2 years) repeated dose study by the inhalation route a LOAEC of 86 mg/m³ was determined in rats for local effects (nasal mucosa irritation) with n-butyl acrylate. The respective NOAEC for systemic effects was 773 mg/m³. After subchronic exposure by vapor inhalation over 3 months the NOAEC for systemic and toxic effects was 570 mg/m³ and the LOAEC was 1110 mg/m³ based on body weight decrease, clinico-chemical changes, and changed organ weights. The NOAEC for local effects (histological changes in the nasal mucosa and olfactory epithelium) was 111 mg/m³ and the LOAEC is 570 mg/m³.

Following a 90-day oral administration of n-butyl acrylate in the drinking water, the NOAEL was 84 (male) and 111 (female) mg/kg bw/d for F344 rats, respectively. This dose level administered in drinking water approaches the maximum solubility limit of butyl acrylate in water and thus was the highest concentration that could be reasonably given.

Genetic Toxicity

Iso-butyl acrylate was not mutagenic in the Ames test and not clastogenic in vivo in the mouse micronucleus test.

This is also supported by the data of the structural analogue n-butyl acrylate: in vitro, n- butyl acrylate was negative in the Ames Assay with and without metabolic activation. An in vitro micronucleus assay and an in vitro UDS assay in Syrian hamster embryo fibroblasts were both negative without metabolic activation. In vivo, n-butyl acrylate showed no genotoxic (cytogenetic) effects after vapor inhalation exposure in rats and hamsters.

Developmental/Reproductive Toxicity

No experimental data are available for iBA concerning developmental or reproductive toxicity, but the structural analogue n-butyl acrylate was tested.

The results of subchronic and chronic animal studies gave no indication of a fertility impairing effect caused by butyl acrylate. In addition, there are data from the structural analogue methyl acrylate. In a two-generation study in which groups of rats were whole-body exposed to methyl acrylate vapors, no effects on reproductive function (i.e. fertility) were observed. The NOAEC for reproductive function was 75 ppm (= ca. 268 mg/m³).

At concentrations where no maternal toxicity was observed, butyl acrylate did not cause developmental toxicity or teratogenicity. A developmental toxicity study in rabbits conducted with the structural analogue methyl acrylate did not give any indication for a developmental toxic or teratogenic effect.
No teratogenicity occurred after inhalation of butyl acrylate in animal studies.

In high maternal toxic vapor concentrations only, butyl acrylate caused fetotoxic effects. After oral gavage at very high doses to mice which caused severe maternal toxicity, butyl acrylate caused malformations. Those effects are considered secondary to the maternal toxicity.

Carcinogenicity

The structural analogue n-butyl acrylate showed no evidence of carcinogenicity in a 2-year vapor inhalation study in Sprague-Dawley rats up to the highest tested dose (135 ppm = 773 mg/m³) and in a lifetime skin painting study in C3H/HeJ mice at approx. 8 mg/kg bw.

Toxicokinetics

Based on the results from an in-vitro study with isobutyl acrylate and in-vivo data from the structural analogue n-butyl acrylate, it can be presumed that isobutyl acrylate will be rapidly absorbed and metabolized after oral exposure in rats. The major portion of iBA will be hydrolyzed by carboxyesterase to acrylic acid and iso-butanol. The subsequent metabolism follows that for acrylic acid, and involves metabolism to carbon dioxide via the propionate degradation pathway (acrylic acid --> 3-hydroxypropionic acid --> malonyl semialdehyde --> acetyl S CoA --> --> tricarboxylic acid cycle --> --> CO2). Metabolism of iso-butanol proceeds via the alcohol and aldehyde dehydrogenase pathway.

## Disclaimer

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