

BASIC ACRYLIC MONOMER MANUFACTURERS, INC.

SUBSTANCE REVIEW: T-BUTYL ACRYLATE

(Last Updated: 5/7/12)

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Substance	Acronym	CAS Number
tert-Butyl acrylate	tBA	1663-39-4

Physicochemical Properties

Property	Results
Physical state at 20°C and 1013 hPa	Liquid Color: colorless Odor: fruit-like
Melting / freezing point	-69°C
Boiling point	119.2°C at 1013 hPa
Relative density	0.87 g/cm ³ at 20°C
Vapor pressure	20 hPa at 23.4°C
Surface tension	not surface active
Water solubility	approx. 2 g/l at 20°C
Partition coefficient n-octanol/water (log value)	2.32 at 25°C
Flash point	14°C (cc)
Flammability	Highly flammable upon ignition. The substance has no pyrophoric properties and does not liberate flammable gases on contact with water.
Explosive properties	non explosive
Self-ignition temperature	400°C
Oxidizing properties	no oxidizing properties
Granulometry	not applicable
Stability in organic solvents and identity of relevant degradation products	not applicable
Dissociation constant	not applicable

Environmental Fate

In contact with water, tBA will hydrolyze slowly. Photodegradation in air will proceed slowly, too. tBA was not readily biodegradable in an OECD 310 -Screening test. After 28 days a biodegradation degree of 50 - 60 % was determined. The 10-day-window criterion for ready biodegradability was not fulfilled. Based on these data, tBA is considered to be partly or moderately biodegradable.

Degradation products expected for tBA are acrylic acid and tert-butanol. Acrylic acid is readily biodegradable according to OECD criteria. The biodegradability of tert-butanol was investigated in a CO₂-Headspace test according to ISO 14593 (non-GLP). After 28 days a biodegradation degree of 70 - 80 % was reached. Tert-butanol was considered to be biodegradable. Taking all these data into consideration, tBA can be expected to be (inherently) biodegradable in the environment. Formation of persistent breakdown products is not expected.

Based on an experimental log Kow and calculated BCF, a potential for bioaccumulation is not to be expected. Adsorption of tBA 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

Tert-butyl acrylate is of moderate toxicity after a single ingestion and short-term skin contact. tBA is of pronounced toxicity after short-term vapor inhalation.

Oral: LD50 = ca. 1047 mg/kg bw (rat, BASF test)

- Dermal: LD50 ca. 2000 mg/kg bw (rabbit)
- Dermal: LD50 > 4000 mg/kg bw (rat)
- Inhalation: LC50 = 7.01 mg/L (rat, 4h)

Irritation/Sensitization

Tert-butyl acrylate is irritating to the respiratory system and the skin. tBA is not irritating to the eyes. After repeated skin contact with tBA sensitization is possible.

Repeated Dose Toxicity

The inhalation of 180 ppm tBA vapors (equivalent to 956 mg/m³) by male and female Wistar rats in a combined sub-chronic toxicity study with a reproduction / developmental toxicity screening test caused slight irritation of the eyes and upper respiratory tract, retarded body weight development, mild impairment of renal function in the males, a reduced general health status and two deaths during gestation in the females. NOAEC = 60 ppm (equivalent to 319 mg/m³) (Wistar rat, vapor inhalation, OECD TG 413, 422).

Genetic Toxicity

Tert-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

A combined sub-chronic toxicity study with a reproduction / developmental toxicity screening test with tBA did not reveal any potential of the substance to cause a developmental toxic / teratogenic effect at doses that were not toxic to the mother. Nor is it expected to impair reproduction. This is supported by data on the structural analogues n-butyl acrylate and methyl acrylate.

- NOAEC for fetotoxicity 319 mg/m³ (60 ppm)
- NOAEC teratogenicity \geq 956 mg/m³ (180 ppm)
- NOAEC for fertility of the parent animals 319 mg/m³ (60 ppm).

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

Tert-butyl acrylate is not hydrolyzed by a mammalian esterase to acrylic acid and the alcohol in vitro. No in vivo data are available.

Disclaimer

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