

isoamyl acetate

CAS number: 123-92-2

IUPAC: 3-methylbut-1-yl ethanoate;

SMILES (Simplified Molecular Input Line-Entry System): O=C(OCCC(C)C)CMolecular Formula: C₇H₁₄O₂

Mol. Wt.: 130.18

Colorless, flammable liquid with a banana-like odor (ACGIH, 1993).

Isoamyl acetate is commercially available as both a natural and synthetic product with a purity range of 95-99+%. (Allured Publishing Corp., 1993; Aldrich Chemical Co., Inc., 1994; Pfaltz & Bauer, 1994)

Use Pattern: Isoamyl acetate is used as a solvent for tannins, nitrocellulose, lacquers, celluloid, and camphor. It is also used as a flavoring agent in soft drinks, chewing gum, and candies. Isoamyl acetate is used during the manufacturing process of artificial silk, leather, pearls, photographic films, celluloid cements, waterproof varnish, bronzing liquids, metallic paints, dyeing, and finishing textiles (Howard, 1990).

Isoamyl acetate is used in the following products at the following typical concentrations (%): soap, 0.05; detergent, 0.005; creams, lotions, 0.003; perfume, 0.05 (Opdyke, 1975). Isoamyl acetate has reportedly been used in the following products at the following levels: non-alcoholic beverages, 28 ppm; ice cream, ices, etc, 56 ppm; candy, 190 ppm; baked goods, 120 ppm; gelatins and puddings, 100 ppm; and chewing gum, 2700 ppm (Furia & Bellanca, 1975).

Occurrence: Isoamyl acetate is a plant volatile. It is released during the fermentation process in making beer and whiskey. It is a sting pheromone of the honey bee (*Apis mellifera*), and can be used to attract large groups of honeybees to a small area. The compound is released by the honey bee when it stings and the resulting scent calls other bees to sting the victim. Isoamyl acetate is a pheromone for *Lobesia botrana* and *Manduca sexta*. Isoamyl acetate is used as an agent in respirator fit tests because of its intense, pleasant odor and its low toxicity. It may be released to the environment during this procedure (Howard, 1990). It has been identified in whiskey, beer, and cognac. The concentration of esters, including isoamyl acetate, in US lager beer is 25-50 ppm and is responsible for giving beer a fruity flavor (Howard, 1990). It has been found in the following food products: fried bacon, Beaufort cheese (Howard, 1990).

Production and Producers: Isoamyl acetate is derived by rectification of commercial amyl acetate (Lewis, 1993). It can also be prepared by esterification of commercial isoamyl alcohol with acetic acid (Opdyke, 1975). Two additional methods of preparation include esterification of pentyl alcohol with sodium acetate in the presence of sulfuric acid and by synthesis from pentane (Parmeggiani, 1983).

Isoamyl acetate is produced and supplied domestically in both bulk and research quantities by many manufacturers and distributors. There was little specific information on annual production volumes found in the available literature, but USITC reported a production volume of 112,000 pounds in 1984 (U.S. International Trade Commission, 1985). It was used in fragrances in the USA at about 10,000 lb/yr in the early 1970s (Opdyke, 1975).

Regulatory Status: An occupational exposure limit and guideline for isoamyl acetate has been established by the American Conference of Governmental Industrial Hygienists (ACGIH), the National Institute for Occupational Safety and Health (NIOSH) and the Occupational Safety and Health Administration (OSHA). The 8-hour time-weighted average (TWA) threshold limit value (TLV) for isoamyl acetate is 100 ppm (525 mg/m³) (ACGIH, 1993; NIOSH, 1992; OSHA, 1993).

Isoamyl acetate is listed in the EPA TSCA Inventory (Sax & Lewis, 1989).

Isoamyl acetate was Granted Generally Recognized as Safe (GRAS) status by FEMA in 1965 (Opdyke, 1975).

When isoamyl acetate, a hazardous material, is to be transported, Title 49 CFR, Transportation, Parts 1001 80, published by the US Dept of Transportation, contain the regulatory requirements and must be consulted (U.S. Department of Transportation, 1993).

Isoamyl acetate is a synthetic flavoring substance permitted for direct addition to food for human consumption, as long as (a) it is used in the minimum quantity required to produce its intended effect, and otherwise in accordance with all the principles of good manufacturing practice. (b) It consists of one or more of the following, used alone or in combination with flavoring substances and adjuvants generally recognizable as safe in food, prior sanctioned for such use, or regulated by an appropriate section in this part (U.S. Food and Drug Administration, 1994b).

The US Environmental Protection Agency has established regulations for the use of isoamyl acetate in or on raw agricultural commodities including exemption from the requirements of a tolerance (40 CFR 180.1001).