Sorbitol Octanoate

Crop Production

Identification of Petitioned Substance

Chemical Name:
Sorbitol Octanoate

Other Names:
(D-Glucitol, octanoate)

Trade Names:
Avachem Sorbitol Octanoate Manufacturing Use Product
Avachem Sorbitol Octanoate [90%]
Avachem Sorbitol Octanoate [50%]

CAS Number:
108175-15-1

Other Codes:
OPP Chemical Code: 035400

Characterization of Petitioned Substance

Composition of the Substance:

Sorbitol octanoate is not a naturally occurring compound, but it is derived as a sugar ester synthesized via the condensation of a sorbitol (a naturally occurring sugar alcohol) with octanoic acid (a naturally occurring fatty acid). An ester is defined as an organic compound formed from an alcohol and an acid splitting out a molecule of water (Stenish, 1989). The active ingredient is an oily liquid that is miscible in water, forming a stable emulsion when shaken.

Properties of the Substance:

Product Chemistry (U.S. EPA, 2006)

Color	Amber
Physical State	Liquid
Odor	Faint sweet smell
Melting Point	Not applicable; not a solid
Boiling Point	Decomposes above 105 degrees Centigrade
Solubility	Forms an emulsion with water
Stability	Stable below 40 degrees Centigrade
Oxidizing or Reduction Action	Not Applicable
Flammability/Flame Extension	None; decomposes above 105 degrees Centigrade
Explodability	Non-explosive
Miscibility	Miscible in water

Specific Uses of the Substance:
Sorbitol octanoate is a bio-pesticide and is used to control certain soft-bodied pests which include: adeigids, aphids, caterpillars, glassy-winged sharpshooter, lace bug, leafhopper, mealy bug, plant bug, psyllid, soft scale, mites, tent caterpillars, thrips, and whitefly. Sorbitol octanoate is permitted by the U.S. Environmental Protection Agency (U.S. EPA Registration Nos. 70950-3 and 70950-5, OPP No. 035400) for

use as a bio-pesticide for foliar spray in fields, greenhouses, and nursery use including vegetables, herbs, spices, fruit crops, nut crops, field crops, hops, coffee, bananas, pineapple, ornamental landscape trees and shrubs, Christmas trees, roses, flowers, and bedding plants.

Sorbitol octanoate is used as a food emulsifier and post-harvest protective fruit coating. Sorbitol and octanoic acid are the two components of sorbitol octanoate, which are naturally occurring materials found in plant and animal products.

Approved Legal Uses of the Substance:

Sorbitol octanoate is chemically similar to certain sorbitan esters and other sugar fatty acid esters that have been approved by the Food and Drug Administration for direct food use as food emusifiers and post-harvest protective fruit coatings (21 CFR 172.836; 172.838; 172.840; and 172.842). Sorbitan esters are different from sorbitol octanoate in that sorbitol has one more water molecule than sorbitan. Sorbitol is a naturally occurring carbohydrate found in apples, plums, pears, cherries, dates, peaches, apricots, and other fruits (Lawson, 1997). Octanoic acid (caprylic acid) is a naturally occurring fatty acid found in plants, coconut oil, meat, and milk (Hall, 1995; Rogge et al., 1991; Tatsuka et al., 1993). Sorbitol is cleared for food use in unlimited quantities as an anti-dusting agent under 40 CFR 180.910.

Sorbitol octanoate is also approved for use as a contact-type biochemical insecticide/miticide (U.S. EPA Registration Nos. 70950-3; 70950-5; OPP No. 035400) to control soft-bodied pests.

Action of the Substance:

Sorbitol octanoate acts as a bio-pesticide by causing rapid suffocation and/or de-waxing the cuticle of the targeted pests, subsequently causing dessication via loss of body fluids. There are no neurological and/or physiological interactions with the targeted pests.

Status

U.S. Environmental Protection Agency:

In 2006, the U.S. EPA approved sorbitol octanoate for use as the active ingredient in the end-use product, Avachem Sorbitol Octanoate [90%] (Avachem Sucrose Octanoate Manufacturing Use Product for formulating into biochemical insecticide/miticide end-use product; EPA Registration No. 70950-3) and Avachem Sorbitol Octanoate [50%] for use as a biochemical insecticide/miticide end-use product; EPA Registration No. 70950-5 (U.S. EPA, 2006). The approved targeted pests are mites and soft-bodied insects on food and non-food crops, including certain ornamentals. The approved application method is spraying using ground equipment (U.S. EPA, 2006). The registration review by the U.S. Environmental Protection Agency concluded that no tolerance under the Federal Food, Drug, and Cosmetic Act is required for sorbitol octanoate residues in or on any food commodity. The U.S. Environmental Protection Agency arrived at this conclusion as a result of data that demonstrated no toxicity, except from ocular exposure (discussed in Evaluation Question #11 below; U.S. EPA, 2006). Both sorbitol and octanoic acid are included in the U.S. Environmental Protection Agency's List 4 inert ingredients, and thus of are of minimal concern.

U.S. Food and Drug Administration:

Since 1983, the U.S. Food and Drug Administration allowed sucrose fatty acid esters including, sucrose octanoate esters, to be added to certain processed foods (21CFR 172.859). Sucrose fatty acid esters may be used as emusifiers or as stabilizers in baked goods and baking mixes, in chewing gum, in coffee and tea beverages with added dairy ingredients and/or dairy product analogs, in confections and frostings, in dairy product analogs, in frozen dairy deserts and mixes, and in whipped milk products. They also are used as texturizers in biscuit mixes, in chewing gum, in confections and frostings, and in surimi-based fabricated seafood products. They may also be used as components of protective coatings applied to fresh apples, avocados, bananas, banana plantains, limes, melons (honeydew and cantaloupe), papaya, peaches, pears, pineapples, and plums to retard ripening and spoiling. Sucrose fatty acid esters must be used in accordance with good manufacturing practices and in an amount not to exceed that reasonably required to accomplish the intended effect (21 CFR 172.5). Sorbitol octanoate is similar in chemical structure to sucrose fatty acid esters. On January 27, 2006, the U.S. EPA established an exemption from the tolerance requirements pursuant to the Federal Food, Drug, and Cosmetic Act, Section 408 for residues of sorbitol octanoate in or on all food commodities. The sorbitol octanoate constituents sorbitol (21 CFR 184.1835) and octanoic acid (21 CFR 184.1025) are classified as Generally Recognized as Safe (GRAS) by the U.S. Food and Drug Administration. More information about GRAS substances can be found at FDA, 2004 "Guidance for Industry: Frequently Asked Questions About GRAS."

International:

There are no CODEX Alimentarius Commission Maximum Residue Levels (MRLs) for residues of sucrose octanoate esters or sorbitol octanoate.

Evaluation Questions for Substances to be used in Organic Crop or Livestock Production

Evaluation Question #1: Is the petitioned substance formulated or manufactured by a chemical process? (From 7 U.S.C. § 6502 (21).)

Sorbitol octanoate is a synthesis of sorbitol and food-grade octanoic acid derived from tropical vegetable oils. Sorbitol is a polyol (sugar alcohol) that occurs naturally in a wide variety of fruits and berries. It is commercially produced by the hydrogenation of glucose. Short-chain fatty acids, including octanoic acid, are found in palm kernel oil and in coconut oil at concentrations of 3.0 to 4.5% and 5.8%, respectively. Sorbitol octanoate is manufactured by a process described in U.S. Patent No. 6,419,941, titled "Polyol Ester Insecticides and Methods of Synthesis ", dated July 16, 2002 (U.S. Patent and Trademark Office, 2002). The manufacturing process for sorbitol octanoate involves a single chemical reaction that is solvent-free and has no post-reaction purification steps, other than the optional removal of the esterification catalyst. One of the objectives is to have an environmentally acceptable process that produces no toxic by-products.

First, octanoic acid is placed in a reactor at a temperature sufficiently high to keep it in liquid form. Next, sorbitol is added in an amount that allows the production of a monoester, plus an additional 10% to drive the reaction to essentially completion. An esterification catalyst (sulphuric acid or phosphoric acid) is added. Phosphoric acid is preferred since neutralization at the completion of the reaction provides a phosphate salt that can either be left in the product (since phosphorus is an essential plant nutrient), or removal by filtration. The reactor is held at a temperature sufficiently high along with a pressure sufficiently low to allow water to be removed as the esterification reaction proceeds. The reaction is allowed to proceed until the remaining octanoic acid reaches a low equilibrium value. At the completion of the reaction, the solution is neutralized with an amount of base that is sufficient to neutralize all the mineral acid used as a catalyst, plus bring the solution to a desired pH for subsequent use. If calcium hydroxide is used as the base, calcium phosphate can be filtered out of the product.

Evaluation Question #2: Is the petitioned substance formulated or manufactured by a process that chemically changes the substance extracted from naturally occurring plant, animal, or mineral sources? (From 7 U.S.C. § 6502 (21).)

As described above, sorbitol octanoate is manufactured by a single step chemical process that requires raw materials (sorbitol and octanoic acid) to be extracted from naturally occurring sources. However, the petitioner does not specify whether natural sources of raw materials would be used to manufacture sorbitol octanoate for the petitioned use. The petitioner does not specify whether the various reagents used in the manufacturing process (sulphuric acid or phosphoric acid and calcium hydroxide) would be from natural or synthetic sources, but it is more likely that synthetic reagents would be used. During the process, these raw materials undergo a chemical reaction that substantially change their chemical composition, and produce the material under review (i.e., sorbitol octanoate). It would likely be cost prohibitive to extract and purify natural sources of raw materials for use in the manufacturing process. The highest yielding plant, *Nicotiana trigonophylla,* has less than three grams of naturally-occurring sugar ester per kilogram of plant material. (Barrington, 2004). Thus, it is likely that synthetic raw materials would be used in the manufacturing process.

<u>Evaluation Question #3:</u> Is the petitioned substance created by naturally occurring biological processes? (From 7 U.S.C. § 6502 (21).)

Sorbitol octanoate is designed to mimic the pest control properties of naturally-occurring sugar ester isolates of *Nicotiana gossei Domin* and other *Nicotiana* species that have been demonstrated to have insecticidal activity. The highest yielding plant, *Nicotiana trigonophylla,* has less than three grams per kilogram of plant material. (Barrington, 2004). The low concentration plus the cost of extraction means that the naturally occurring sugar esters are not an economically viable or environmentally sound source of sugar ester active ingredients for pest control purposes. In addition to the tobacco plant, sugar esters have been found in wild tomato, wild potato, and in the petunia plant (Chortyk et al., 1996).

<u>Evaluation Question #4:</u> Is there environmental contamination during the petitioned substance's manufacture, use, misuse, or disposal? (From 7 U.S.C. § 6518 (m) (3).)

As stated in Evaluation Question #1, sorbitol octanoate is manufactured by reacting sorbitol with octanoic acid using an esterification catalyst (sulphuric or phosphoric acid). At the completion of the reaction, an amount of base is added to neutralize all the mineral acid used as a catalyst and to bring the solution to a desired pH for subsequent use. Therefore, no corrosive residues from the manufacturing process should have to be disposed.

Sorbitol octanoate rapidly hydrolyzes to sorbitol and octanoic acid, both of which are naturally occurring compounds which are common human dietary components of no toxicological concern. Both sorbitol and octanoic acid are included in the U.S. Environmental Protection Agency's List 4 inert ingredients, and thus of are of minimal concern. Sorbitol octanoate bio-degrades with an apparent post-application half-life of approximately 7 to 10 days (U.S. EPA, 2006).

<u>Evaluation Question #5:</u> Is the petitioned substance harmful to the environment? (From 7 U.S.C. § 6517 (c) (1) (A) (i) and 7 U.S.C. § 6517 (c) (2) (A) (i).)

Sorbitol octanoate rapidly hydrolyzes to sorbitol and octanoic acid, both of which are naturally occurring compounds which are common human dietary components of no toxicological concern. Both sorbitol and octanoic acid are included in the U.S. Environmental Protection Agency's List 4 inert ingredients, and thus of are of minimal concern. Sorbitol octanoate bio-degrades with an apparent post-application half-life of approximately 7 to 10 days (U.S. EPA, 2006).

<u>Evaluation Question #6:</u> Is there potential for the petitioned substance to cause chemical interaction with other substances used in organic crop or livestock production? (From 7 U.S.C. § 6518 (m) (1).)

There is no information available to indicate that sorbitol octanoate will interact with other substances used in organic crop or livestock production.

<u>Evaluation Question #7:</u> Are there adverse biological or chemical interactions in the agro-ecosystem by using the petitioned substance? (From 7 U.S.C. § 6518 (m) (5).)

There is no information available to indicate that sorbitol octanoate has adverse biological or chemical interactions in the agro-ecosystem. Sucrose octanoate esters, which are chemically similar to sorbitol octanoate, are practically non-toxic to honey bees (LD50 > 80 micrograms per bee; U.S. EPA, 2006).

<u>Evaluation Question #8</u>*:* Are there detrimental physiological effects on soil, organisms, crops, or livestock by using the petitioned substance? (From 7 U.S.C. § 6518 (m) (5).)

There is no information available to indicate that using sorbitol octanoate has detrimental physiological effects on soil, organisms, crops, or livestock. Field trials with sorbitol octanoate have not shown any phytotoxicity. Sorbitol octanoate has no neurological and/or physiological interactions with the targeted pests, but rather kills the targeted pest through suffocation and/or dessication (U.S. EPA, 2006).

<u>Evaluation Question #9:</u> Is there a toxic or other adverse action of the petitioned substance or its breakdown products? (From 7 U.S.C. § 6518 (m) (2).)

There is no information to indicate that sorbitol octanoate or its breakdown products, sorbitol and octanoic acid have toxic or adverse actions. Based on the toxicology information/data submitted and other information available to the U.S. Environmental Protection Agency, there is a reasonable certainty that no harm will result from aggregate exposure to residues of sorbitol octanoate to the U.S. population, including infants and children, under reasonably foreseeable circumstances, when the biochemical pesticide is used in accordance with product label directions and good agricultural practices. Sorbitol octanoate may be applied up to and including the day of harvest of the crop. This includes all anticipated dietary exposures and all other non-occupational exposures for which there is reliable information. Sorbitol octanoate is in Toxicity Category IV for acute oral toxicity in rats and mice, acute dermal toxicity, acute inhalation toxicity, and primary dermal irritation in rabbits. The U.S. Environmental Protection Agency arrived at this conclusion based on the information/data submitted (and publicly available) demonstrating negligible toxicity of the chemically-similar sucrose octanoate esters, sorbitan esters, and sorbitol octanoate's constituents (sorbitol and octanoic acid; 40 CFR 180.1262).

<u>Evaluation Question #10:</u> Is there undesirable persistence or concentration of the petitioned substance or its breakdown products in the environment? (From 7 U.S.C. § 6518 (m) (2).)

The U.S. EPA (2005) determined that there is no adverse effect on endangered species or other non-target organisms following the use of sorbitol octanoate, as the active ingredient in a bio-pesticide. There is no evidence of toxicity to any non-target organisms or effects on critical habitat. Exposure to non-target organisms is mitigated by the rapid degradation of sorbitol octanoate in the environment. Sorbitol octanoate rapidly hydrolyzes to sorbitol and octanoic acid, both of which are naturally occurring compounds which are common human dietary components of no toxicological concern. Both sorbitol and octanoic acid are included in the U.S. Environmental Protection Agency's List 4 inert ingredients, and thus of are of minimal concern. Sorbitol octanoate bio-degrades with an apparent post-application half-life of approximately 7 to 10 days (U.S. EPA, 2006).

<u>Evaluation Question #11:</u> Is there any harmful effect on human health by using the petitioned substance? (From 7 U.S.C. § 6517 (c) (1) (A) (i), 7 U.S.C. § 6517 (c) (2) (A) (i) and), 7 U.S.C. § 6518 (m) (4).)

Sorbitol octanoate causes severe irritation to the eye (Toxicity Category II), however, the irritation is temporary and resolved in 14 days (U.S. EPA, 2006). Protective eyewear is required during handling and application.

<u>Evaluation Question #12:</u> Is there a wholly natural product that could be substituted for the petitioned substance? (From 7 U.S.C. § 6517 (c) (1) (A) (ii).)

There is no wholly natural product that could be substituted for sorbitol octanoate. Natural oils such as cottonseed, soy, or peanut oil could possibly be used as a bio-pesticide and act on the targeted pest through suffocation and dehydration. However, applying these natural oils in a nursery or field setting may be a problem, due to the fact that they are oils. Sorbitol octanoate is an emulsion and can be applied to crops and plants with mechanical spray equipment. Sucrose octanoate esters are chemically similar to sorbitol octanoate and they are registered as a bio-pesticide with the U.S. Environmental Protection Agency. Sucrose octanoate esters are allowed for use in organic crop production (7 CFR 205.601).

<u>Evaluation Question #13:</u> Are there other already allowed substances that could be substituted for the petitioned substance? (From 7 U.S.C. § 6517 (m) (6).)

Sucrose octanoate esters are chemically similar to sorbitol octanoate and they are registered as a bio-pesticide with the U.S. Environmental Protection Agency. Sucrose octanoate esters are allowed for use in organic crop production (7 CFR 205.601). Only sucrose octanoate esters act in a similar manner as sorbitol octanoate. Other possible substances include ammonium carbonate (for use as bait in insect traps and there can be no direct contact with organic food or crops), boric acid (no direct contact with organic food or crops), and sticky traps or barriers. These substances could possibly be used in conjunction with pheromones to attract pests to insect or sticky traps. Elemental sulphur, lime sulphur, insecticidal soaps, and horticultural oils are other permissible substances that may be effective in insect control. However, like sucrose octanoate esters, they would have to be applied to plants or shrubs in either dry or liquid form.

Evaluation Question #14: Are there alternative practices that would make the use of the petitioned substance unnecessary? (From 7 U.S.C. § 6517 (m) (6).)

As found in 7 CFR 205.205, organic crop producers must implement a crop rotation including, but not limited to sod, cover crops, green manure crops, and catch crops that provides for pest management in annual and perennial crops. In addition, cultural practices that remove habitat for pest organisms and the selection of plant species and varieties that are resistant to prevalent pests are important alternative practices. Pest infestations may also be controlled by the introduction of predators and parasites of the pest, development of habitat for natural enemies of the pests, and the use of non-synthetic controls such as lures, traps, and repellants. Possible substances include ammonium carbonate (for use as bait in insect traps and there can be no direct contact with organic food or crops), boric acid (no direct contact with organic food or crops), and sticky traps or barriers. These substances could possibly be used in conjunction with pheromones to attract pests to insect or sticky traps.

References

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