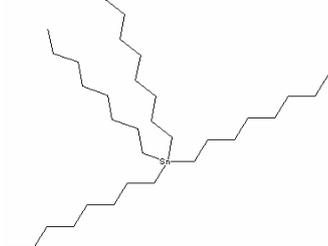


SIDS INITIAL ASSESSMENT PROFILE

CAS No.	3590-84-9
Chemical Name	Tetraoctyltin (TTOT)
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

The acute oral LD₅₀ of tetraoctyltin (TTOT) to rats was >2000 mg/kg bw. There are no data on acute dermal or inhalation toxicity, irritation, or sensitization.

The repeated-dose toxicity of TTOT (90.8% purity) to rats was evaluated in a combined repeated-dose and reproduction/developmental toxicity screening test (OECD TG 422). Based on the observed effects in the 7500 mg TTOT/kg diet group (decreased thymus weight, as well as thymic lymphoid depletion and macrophage accumulation), the NOAEL for sub-chronic toxicity was 1500 mg TTOT/kg diet (equivalent to 86–99 mg/kg bw/day for males and 80–141 mg/kg bw/day for females) and the LOAEL was 7500 mg TTOT/kg diet (445–480 mg/kg bw/day for males and 426–624 mg/kg bw/day for females).

TTOT was negative in a standard *in vitro* Ames assay using multiple strains of *Salmonella typhimurium* and with *Escherichia coli*, conducted with and without metabolic activation. TTOT was also negative in a standard *in vivo* mouse micronucleus test.

No adverse effects on fertility or reproductive performance and development were observed in the reproduction/developmental toxicity segment of the OECD 422 study, even at the highest (maternally toxic) dose tested of 7500 mg TTOT/kg diet. Based on the lack of observed effects, the NOAEL for reproductive and developmental toxicity of TTOT was 7500 mg TTOT/kg diet (445–480 mg/kg bw/day for males and 426–624 mg/kg bw/day for females).

Environment

Because of the insolubility of TTOT and strong adsorption of TTOT to labware, several physicochemical properties could not be readily measured and thus are based on modeled data. Estimated values derived from the current EPIWIN models developed by Syracuse Research Corporation should be used with caution, as the current versions have not been validated for estimating endpoints for chemicals that contain metals in their molecular structure. TTOT is a colorless to slightly yellow turbid liquid, with a measured freezing point of -102°C and a boiling point of 414–425°C at 1013.25 hPa (760 mm Hg). TTOT has a calculated vapour pressure of 9.4×10^{-6} hPa at 25°C, a relative density of 0.96-0.98 g/cm³ at 20°C, and a calculated log K_{ow} of 17.2. TTOT is only sparingly soluble in water with an estimated water solubility of 1.3×10^{-12} mg/L using a Log K_{ow} of 17.2. An additional estimation of the water solubility of TTOT was performed using an estimated log K_{ow} of 8.0, which is widely accepted as a realistic maximum value for this parameter; the resulting water solubility was 9.5×10^{-4} mg/L. Possible higher solubility suggested by the aquatic toxicity studies, where total tin was measured, may be due to differences in the percentage of impurities present (e.g., tin tetrachloride, trioctyltin chloride, and dioctyltin dichloride) that may either be more soluble or may hydrolyze to more soluble tin compounds. Measured vapour pressures present similar difficulties in that impurities may volatilize more readily than pure TTOT.

TTOT is stable in water due to a lack of hydrolyzable functional groups, and it is not readily biodegradable. Releases of TTOT to air are not expected to be significant due to its low vapour pressure. Vapour-phase TTOT would be expected to be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals, with a calculated rate constant of 79.5×10^{-12} cm³/molecule*sec and an estimated half life of 3.2 hours.

Based on a Level III fugacity model assuming emissions of 1000 kg/hr to soil, air, and water, TTOT is predicted to partition primarily to sediment and soil (68% and 28%, respectively, based on a log K_{ow} of 17.2; 84.5% and 10.5%, respectively, based on a log K_{ow} of 8.0). A calculated Henry's Law Constant of 562 atm.m³/mol predicts that TTOT will volatilize from water; half-lives from a model river and lake are estimated at 2.4 hours and 9.5 days, respectively. Calculated BCFs of 100 (based on a log K_{ow} of 17.2) and 2188 (log K_{ow} of 8.0) were determined using BCFWIN. These values are considered representative based on comparison with measured BCF values experimentally determined for a related material, tetrabutyltin, which had BCF values ranging from 38 - 310.

Aquatic toxicity studies were conducted in accordance with OECD Test Guidelines and exposure concentrations were measured on the basis of total tin, then converted to and reported as the named substance. All of the measured tin (including contributions from more water-soluble tin compounds, impurities, or hydrolysis products) was attributed to the named substance, TTOT. A 100% Water Accommodated Fraction (WAF), prepared at a loading rate of 100 mg TTOT/L, induced no visible effects in zebra fish (*Brachydanio rerio*) (96-h LC_{50} > 0.52 mg TTOT/L). A filtered, saturated solution immobilized *Daphnia magna* in all concentrations tested (24-h EC_{50} < 0.13 mg TTOT/L). A 100% WAF, prepared at a loading rate of 100 mg TTOT/L, induced no treatment-related deaths or adverse effects on growth or reproduction of *D. magna* (21-day EC_{50} [reproduction] > 0.068 mg TTOT/L; overall LOEC > 0.068 mg TTOT/L; and overall NOEC \geq 0.068 mg TTOT/L). A filtered, saturated solution of TTOT showed no to only very slight (7%) growth inhibition to the green alga *Scenedesmus subspicatus* (72-h EC_{50} > 0.21 mg TTOT/L). A possible explanation for the disparity between the chronic and acute toxicity may be attributed to the tendency for this material to adsorb to surfaces and cause immobilization due to a physical rather than toxicological mechanism. The reason for this may be the difference in WAF preparations of the two studies. In addition, the possibility of water soluble impurities present at the lowest concentration tested causing the observed toxicity can also not be ruled out.

Exposure

In 2000, worldwide production of TTOT was estimated at 2,500 to 7,500 tonnes. TTOT is produced in North America, Europe, and Asia-Pacific, and is only used as an industrial intermediate in the synthesis of other octyltin compounds. In individual dioctyltin and monoctyltin compounds, or in mixtures used as stabilizers, TTOT may be present at levels < 0.1 percent. TTOT may be present at levels up to 5% in trioctyltin chloride which is used as an intermediate in the production of other trioctyltin compounds. TTOT may be transported to the other organotin producers; however, all produced TTOT is consumed during its conversion to other compounds. There are no commercial applications for TTOT. Releases to the environment could occur via losses during the production of this intermediate, or during its conversion to other octyltin chemicals.

In the production of TTOT, the operations are usually sealed to prevent releases to the atmosphere. No information is available on the release of organotin compounds from the Toxics Release Inventory in the U.S. because manufacturers are not required to report releases under Section 313 of the Emergency Planning and Community Right-to-Know Act. The recommended method of disposal is incineration in an approved hazardous waste incinerator, which converts the organotin to inorganic tin.

The most prominent routes of potential exposure to TTOT in an occupational setting are inhalation and dermal contact. Exposure in the workplace is controlled through equipment design (engineering controls) and regular air monitoring. Engineering controls, such as local mechanical exhaust ventilation at sources of air contamination can be utilized to provide ventilation to control exposure levels below airborne exposure limits. Also, the use of personal protective equipment (PPE), such as chemical-resistant goggles, rubber gloves, and approved respirators is routinely advised. Worker exposure is confined to manual operations such as material addition, transfer, or sampling. For operations that specifically involve manual handling of organotin compounds (not TTOT specifically), recently measured exposure potentials were 50% to just greater than the threshold limit value (TLV) of 0.1 mg/m³.

Additionally, in the U.S. the small percentage of TTOT that is transported from the manufacturing site would be packaged in intermediate bulk containers (totes) which are returned through the tote manufacturer or the chemical supplier to designated facilities for treatment of residues and recycling of the container. The use of bulk shipments minimizes exposure to workers.

RECOMMENDATIONS AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health: The chemical is currently of low priority for further work. This chemical possesses properties indicating a hazard to human health (repeated-dose toxicity). Based on data presented by the Sponsor country

(relating to production in one country which accounts for unknown fraction of global production) and relating to the use pattern in one country, exposure to humans is anticipated to be low, and therefore this chemical is currently of low priority for further work. Countries may desire to investigate any exposure scenarios that were not presented by the Sponsor countries.

Environment: The chemical is a candidate for further work. The chemical possesses properties indicating a hazard for the environment (acute toxicity to aquatic invertebrates). Member countries are invited to perform an exposure assessment for the environment, and if necessary a risk assessment.