# SIDS INITIAL ASSESSMENT PROFILE

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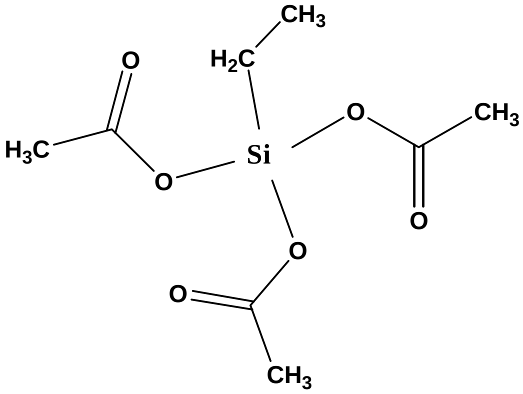
| **CAS No.** | 17689-77-9 |
| **Chemical Name** | Ethyltriacetoxysilane |
| **Structural Formula** |  |

## SUMMARY CONCLUSIONS OF THE SIAR

### Analogue Justification

Ethyltriacetoxysilane undergoes rapid hydrolysis in moist/aqueous environments (t1/2 is less than 13 seconds) to acetic acid and the corresponding trisilanol, thus observed toxicity is likely due primarily to acetic acid. Abiotic hydrolysis products of the test substance undergo continuous condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively). The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis. While the hydrolysis of ethyltriacetoxysilane is rapid, the polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available. The structural analogue methyltriacetoxysilane (CAS number 4253-34-3) has been used for in vitro bacterial gene mutation and chromosomal aberrations endpoints. The hydrolysis product, acetic acid (CAS number 64-19-7) and its salts [calcium acetate (CAS number 62-54-4), potassium acetate (CAS number 127-08-2) and sodium acetate (CAS number 127-09-3)]), have been used to assess the acute aquatic toxicity (fish, aquatic invertebrate and algae), repeated dose toxicity, fertility and developmental toxicity endpoints. Acetic acid and its salts are grouped together because of their close structural relationships and the salts are the neutralized form of the acid that can be more easily administered, their natural occurrence in plants and animals, and their fundamental role in cell metabolism, particularly in the tricarboxylic acid cycle (also known as the citric acid or Kreb's cycle), which is where humans get their energy. In addition the structural analogue vinyltriacetoxysilane (CAS number 4130-08-9) has been used to support the acute aquatic toxicity endpoints. Data from both ethyltriacetoxysilane and vinyltriacetoxysilane are representative of acetic acid, based on the rapid hydrolysis of these materials.

### Human Health

The acute toxicity of ethyltriacetoxysilane is described by an LD50 rat (oral) = 1462 mg/kg. Clinical signs included decreased activity; lethargy; lacrimation; salivation; irregular gait; hunched posture; decreased body weight, food consumption and fecal volume; red urine; red staining of the snout, eyes and extremities; and labored respiration. Although acute toxicity data for the inhalation or dermal routes of exposure are not available for ethyltriacetoxysilane, these exposures will likely result in local site of contact effects from acetic acid. Ethyltriacetoxysilane is severely irritating and corrosive to the skin, is expected to be severely irritating to the eyes of animals, and is likely to be a respiratory irritant based on production of acetic acid following hydrolysis.

In a 7-day oral range-finding study (gavage) rats were treated with undiluted ethyltriacetoxysilane (dose levels of 0, 17 (males), 23 (females), 100, 500 and 1000 mg/kg/d). Ethyltriacetoxysilane rapidly hydrolyzes (in seconds) to acetic acid and a trisilanol (3:1). The silanol generated is insignificant in both quantity and toxicity relative to the production of acetic acid and its associated toxicity. Animals from the 17 (males), 23 (females) and 100 mg/kg/day dose groups survived to day 7. Animals from the 500 and 1000 mg/kg/day dose groups were sacrificed after the third dose as a consequence of two deaths (one from each group), marked body weight loss, and severity of lesions (ulceration and erosion of stomach and esophagus) observed in necropsied animals. The stomach lesions observed resembled irritation from acetic acid production. This 7-day range-finder study indicated that a maximum dose level of less than 20 mg/kg/day would be required for a longer duration repeated dose study in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid. Based on the findings of the 7-day range-finder, a longer duration study will present technical difficulty questioning dosing accuracy and a very low nominal systemic dose. Additional testing (repeated dose, reproductive effects or developmental toxicity) with ethyltriacetoxysilane has not been conducted. Toxicity is represented by an irritative mechanism following single or repeated dosing, likely due to production of acetic acid during hydrolysis. NOAELs following repeated exposure to acetic acid and its salts range from 210 mg/kg bw/day (2-4 month acetic acid drinking water study; systemic toxicity) to 3600 mg/kg bw/day (acetic acid, sodium salt, 4 week dietary study; no effects reported). Signs of irritation/corrosion at the site of contact as well as systemic toxicity have been reported. Prolonged inhalation exposure to acetic acid results in muscle imbalance, increase in blood cholinesterase activity, decreases in albumins and decreased growth at concentrations greater than 0.01 mg/m3/day.

Groups of 20 mice/sex were given 0.025% sodium acetate in the drinking water (about 60 mg/kg bw/day) for 1 week before breeding, during a 9-day breeding period and (females only) throughout pregnancy, lactation and until the offspring were weaned at 3 weeks of age. The male offspring were given the same solution until they were 5-7 weeks old and were then examined in a 24-hour activity test. No effects on fertility were observed. Examination of the litters revealed no overt deformities, and pup weights were normal at day 1 and day 21. The activity of offspring of the treated group was lower than that of controls during the first 12 hours but was similar during the second 12 hours. It is unknown if the decreased activity observed in the sodium acetate treated group to was a result of exposure in utero and/or post-weaning, since the pups were exposed during both time periods. Acetic acid had no effects on implantation or on maternal or fetal survival in rats, mice or rabbits dosed via gavage on days 6-19 to doses up to 1600 mg/kg/day. The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls. Sodium acetate had no effect on parents or offspring when mice were administered 1000 mg/kg bw, by gavage on days 8-12 of gestation.

*In vitro*, ethyltriacetoxysilane and methyltriacetoxysilane were negative in bacterial mutagenicity assays Methyltriacetoxysilane did not induce chromosomal aberrations in CHO cells.

**Environment**

The melting point of ethyltriacetoxysilane is 8.4°C and the boiling point is 227 °C at 1013 hPa. The vapor pressure is 0.05 hPa at 20 deg C. The estimated water solubility of ethyltriacetoxysilane is 42 g/L; the estimated log Kow is 0.74. The water solubility and log Kow values may not be reliable because the chemical is hydrolytically unstable. The overall reaction half-life in air is estimated to be less than 3 minutes because of rapid hydrolysis of the material with moisture in the atmosphere. Photodegradation as a mode of removal is therefore unlikely because ethyltriacetoxysilane is hydrolytically unstable in this medium. In addition, photodegradation of the parent silane is not expected to be a significant degradation process in the aquatic environment due to the rapid rate of hydrolysis. Although, the vapor pressure indicates that ethyltriacetoxysilane resides in the atmosphere and may undergo photodegradation due to ozone and/or hydroxyl radicals, due to extremely rapid hydrolysis, the substance is not expected to reside in the air compartment and the vapor pressure of the substance may not be relevant.

Ethyltriacetoxysilane is hydrolytically unstable ($t_{1/2} < 13$ seconds) over a range of environmentally relevant pH and temperature conditions. At pH 7, the half-life is = <13 seconds. Rapid hydrolysis of this material produces acetic acid and trisilanols.

Level III Fugacity modeling, using loading rates for Air, Soil, and Water of 1000 kg/h for each medium, shows the following percent distribution: Air = 47.3%; Soil = 47.4%; Water = 5.3%; Sediment = 0.0. However, ethyltriacetoxysilane is unlikely to be found in the environment, as this material is hydrolytically unstable. Ethyltriacetoxysilane is readily biodegradable; however this material rapidly hydrolyzes and generates 3 moles of acetic acid for every mole of parent material. Thus, the biodegradation observed is likely reflective of the hydrolysis product, acetic acid. The biodegradation rate for acetic acid after 14 days under aerobic conditions is 74%. Bioaccumulation is not anticipated since this material is hydrolytically unstable.

Ethyltriacetoxysilane undergoes rapid hydrolysis in aquatic media, and thus the exposures to ethyltriacetoxysilane are likely to be transient. Limited data are available for ethyltriacetoxysilane, therefore, data from a structural analog, vinyltriacetoxysilane, as well as the primary hydrolysis product, acetic acid are used to address the acute aquatic toxicity endpoints. The 96-hour LC50 of ethyltriacetoxysilane for *Brachydanio rerio* is 251 mg/L (the test media was not neutralized). Studies have been conducted on a structural analog, vinyltriacetoxysilane, as well as the primary hydrolysis product, acetic acid. The 96-hour LC50 of vinyltriacetoxysilane for *Oncorhyncus mykiss* is 51 mg/L and for *Lepomis macrochirus* is 68 mg/L (in both cases the test media was not neutralized).. The 72 hour LC50s for acetic acid are 75, 79-88 (pH $\leq$5.9) and 251 mg/L (several species of fish). The 48 hour EC50 for ethyltriacetoxysilane is 62 mg/L for *Daphnia magna*. The 48 hour EC50 of vinyltriacetoxysilane is 100 mg/L for *Daphnia magna* (the test media was not neutralized. Under static conditions, the 48 hour EC50 for acetic acid is 65 mg/L for aquatic invertebrates (the test media was not neutralized). When the test solutions are neutralized, the static EC50 for acetic acid is 6000 mg/L. In renewal systems with aquatic invertebrates, 48 hour EC50s for acetic acid are 100 mg/L and 180 mg/L Ethyltriacetoxysilane toxicity to *Scenedesmus subspicatus* provided a 72 hour EC50 of 73 and 76 mg/L for biomass and growth rate, respectively (the test media was not neutralized). When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of the parent material is comparable to the reported toxicity of acetic acid ($EC_{50}$ = 50-450 mg/L, depending on test species). Studies have been performed with a silanol monomer, trimethylsilanol (CAS No. 1066-40-6). Although this silanol is not expected to be produced following hydrolysis of methyltriacetoxysilane. A semistatic 96h study with trimethylsilanol and rainbow trout (*Oncorhynchus mykiss*) resulted in a No Observed Effect Concentration (NOEC) of 128 mg/L and an $LC_{50}$ of 271 mg/L.

**Exposure**

The commercial use of this material is almost exclusively as a cross linker for silicone sealants and adhesives. The final formulated sealant and adhesive is sold in consumer, industrial and construction markets. In production, this material is mostly handled in closed systems. Necessary engineering controls during production include proper ventilation, containment, safety equipment and actual hardware designed to minimize exposure, through splashing, or exposure to the air. Transfer of this material is in closed pipe, drums, or tanks rather than in open systems to minimize loss of this material (through hydrolysis). Ethyltriacetoxysilane is transported from the production site as the parent silane to sealant formulators. The parent silane partially reacts during sealant formulation and then completely reacts during curing of the sealant into the polymer matrix and is no longer available for consumer or worker exposure. Ethyltriacetoxysilane does not volatilize during cure of sealants. Instead this material hydrolyzes and condenses, releasing acetic acid. Therefore, there is no human exposure to ethyltriacetoxysilane from use in silicones sealants. Generally, ethyltriacetoxysilane is used as a cross linker at 3% to 5%. As ethyltriacetoxysilane is compounded into a consumer or industrial sealant or adhesive, it reacts with the silicone. After curing the parent silane becomes crosslinked into the silicone rubber matrix and no longer exists, this greatly reduces the potential for consumer or worker exposure. Any toxicological effects of the silane are greatly reduced as a result of this crosslinking process. The production volume of ethyltriacetoxysilane in the sponsor country was 891 tonnes in 2001.

The reactive nature of this material destroys the parent material in any moisture-containing environment, thus limiting environmental exposure to the parent silane. In a spill situation, the parent material is hydrolyzed; the rapid hydrolysis means that the parent silane is unlikely to be found in the environment. If ethyltriacetoxysilane monomer is slowly released into the environment such that resulting concentrations of the parent compound are low, it is less likely that polymerization will occur and more likely that free triol or short-chain oligomers will result. The spectrum of by-products will depend upon the initial concentration of the parent compound.

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

**Human Health:** The chemical possesses properties indicating a hazard for human health (severe irritation and corrosivity caused by acetic acid). Due to the extremely rapid hydrolysis to acetic acid and the corresponding trisilanol and based on exposure data presented by the Sponsor country, the parent material will not be available for exposure, and therefore this chemical is currently of low priority for further work. The identified hazards should nevertheless be noted by chemical safety professionals and users.

**Environment:** The chemical has properties indicating a hazard for the environment (acute aquatic EC/LC50 values between 1 and 100 mg/l). However the chemical is currently of low priority for further work for the environment because of its rapid hydrolysis and its limited potential for bioaccumulation.