# SIDS INITIAL ASSESSMENT PROFILE

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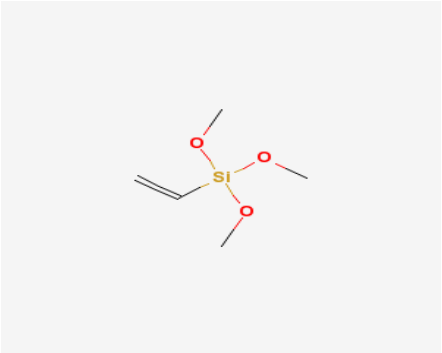
| **CAS No.** | 2768-02-7 |
| **Chemical Name** | Vinyl trimethoxysilane (VTMS) |
| **Structural Formula** |  |

## SUMMARY CONCLUSIONS OF THE SIAR

### Physical-Chemical Properties

### Reduced Testing Rationale

VTMS is hydrolytically unstable over a range of environmentally relevant pH and temperature conditions. At pH 7 and 50°C, the half-life is < 2.4 hours. This hydrolysis is expected to produce 3 moles of methanol and 1 mole of ethenyl silanetriol. Silanetriols (at concentrations greater than 500 mg/L) can condense to form highly cross-linked, high molecular weight polymers. In aqueous solutions, exposures to VTMS are likely to be transient and observed toxicity is likely due primarily to the hydrolysis products methanol, ethenylsilanetriol, and condensed silanetriol materials (high molecular weight polymers). Because VTMS is hydrolytically unstable, water solubility and partition coefficient were not measured; however, modeled values are provided for water solubility and partition coefficient.

The EPISuite program (v 4.0) developed by the U.S. Environmental Protection Agency and Syracuse Research Corporation has not been validated for chemicals that contain silanes in their molecular structure (although some measured data are included in the training data set); therefore, there is uncertainty associated with the calculated values and they should be used with caution whenever they are reported.

VTMS is a liquid with a melting point of -97 °C, a boiling point of 123 °C at 1013 hPa. The measured vapour pressure is15.93 hPa at 25°C. The estimated water solubility of VTMS is 5.043 x $10^5$ mg/L; the estimated log Kow is -0.032. The water solubility and log Kow values may not be applicable because the chemical is hydrolytically unstable.

### Human Health

Toxicokinetics, metabolism and distribution data are not available for VTMS.

The acute toxicity of VTMS has been studied by the inhalation, dermal and oral routes in rats. The combined 4 hour inhalation $LC_{50}$ in rats for VTMS was ca. 16.8 mg/L). The study was conducted in a manner consistent with OECD TG 403. Clinical signs included perinasal, periocular, perioral and

urogenital wetness, perioral and perinasal encrustation, unkempt fur, hypoactivity, blepharospasm, lacrimation, respiratory difficulties, ataxia, prostration, tremors, distended stomachs, and negative righting and pinch reflexes. Body weight gains for all exposure groups were depressed during post-exposure week 1. There were no findings at necropsy in surviving animals. The dermal $LD_{50}$ for VTMS for male rats was 4.00 mL/kg bw (ca. 3880 mg/kg bw) and for female rats was 3.36 mL/kg bw (3259 mg/kg bw). The study was conducted in a manner consistent with OECD TG 402. Discomfort, sluggishness, unsteady gait, and prostration were observed. Most deaths occurred at one to 5 days; surviving animals recovered by day 3. There were no findings at necropsy in surviving animals. Skin reactions included erythema, ecchymosis and desquamation. The oral $LD_{50}$ for VTMS for male rats was 7.34 mL/kg bw (ca. 7120 mg/kg bw) and for females was 7.46 mL/kg bw (7236 mg/kg bw). The study was conducted in a manner consistent with OECD TG 401. Sluggishness, red to brown discharge, lacrimation, piloerection, unkempt appearance, prostration, emaciation and unsteady gait were among the signs of toxicity observed. Deaths occurred at 2.5 hours to 4 days. Survivors recovered by day 5. Most survivors had no remarkable gross lesions; one female animal in the 8.0 mL/kg bw dose group was observed to have an enlarged kidney. The combined oral $LD_{50}$ of VTMS in rats was 8.20 mL/kg bw (ca. 7954 mg/kg bw). The study was conducted in a manner consistent with OECD TG 401. Signs of toxicity included lethargy, diuresis and diarrhea within 6 hours of administration followed by blood staining around mouth and nostrils at 24 hours. Deaths occurred up to 96 hours after administration. The oral $LD_{50}$ of VTMS in female rats > 300 mg/kg bw to 2000 mg/kg bw (OECD TG 423). Signs of toxicity included diarrhea, perianal soiling and reddish urine. Deaths occurred up to 3 days after administration of 2000 mg/kg bw. At necropsy, small thymi and spleens were noted in the animals that died at 2000 mg/kg bw. Histopathological examination showed atrophy of the cortex of the thymus and of the red and white pulp of the spleen.

Valid data regarding the skin irritation potential of VTMS are not available; VTMS is not irritating to the rabbit eyes (OECD TG 405). Under the conditions of the guinea pig maximization test (OECD TG 406), VTMS or VTMS (hydrolysate) did not elicit a delayed contact hypersensitivity response in guinea pigs. Under the conditions of the Buehler test (OECD TG 406), VTMS was determined to be a skin sensitizer.

The repeated-dose toxicity of VTMS has been studied by the inhalation and oral routes in rats. Groups of 20 rats/sex/concentration were exposed six hours per day, five days per week, for 14 weeks to vapor of VTMS at target concentrations of 0, 0.06, 0.6 or 2.4 $mg/L^3$, respectively. Repeated inhalation exposure to 400 ppm VTMS resulted in effects primarily on the urinary bladder and kidney with the LOAEC of 0.6 mg/L and the NOAEC of 0.06 mg/L). In a combined repeated-dose/reproductive/developmental toxicity screening test [OECD TG 422], male and female rats were administered VTMS via gavage at 62.5, 250 and 1000 mg/kg bw/day for up to 42 days. Repeated oral exposure to VTMS resulted in effects primarily on the urinary bladder, intestine, kidney, and thymus in both sexes at all doses. The NOAEL was not established in this study. The LOAEL was 62.5 mg/kg bw/day (decreased urine osmolality and sodium, potassium and chloride concentrations (males) and slight decrease in body weight and body weight gain (females).

VTMS did not induce gene mutations in bacteria (Ames and bacterial reverse mutation assay) or mammalian cells (Sister chromatid exchange) *in vitro*. VTMS did not induce micronuclei in an *in vivo* test; however, it had a positive clastogenic effect *in vitro* in two chromosome aberration tests performed with metabolic activation only. VTMS is not considered to be genotoxic.

In the combined repeated-dose/reproductive/developmental toxicity screening test [OECD TG 422], there were no effects on reproductive performance of parental rats when VTMS was administered by oral gavage. The NOAEL was 1000 mg/kg bw/day for males, and 250 mg/kg bw/day for females (based on a reduced number of estrous cases). There were no effects on developmental parameters; the NOAEL for developmental effects was 1000 mg/kg bw. VTMS did not show any effects on the

reproductive organs in the 14-week repeated-dose toxicity study via inhalation. Exposure of pregnant rats to VTMS by inhalation during organogenesis resulted in a NOAEC of 0.15 mg/L for maternal toxicity. There was evidence of slightly delayed skeletal ossification in fetuses from the 1.8 mg/L group; the NOAEC for developmental effects was 0.60 mg/L . In the OECD TG 422 study, no effects were seen on the developmental parameters when VTMS was administered orally; the NOAEL for developmental toxicity was 1000 mg/kg bw/day.

**VTMS may present hazard for human health (potential for skin sensitization, oral repeated-dose toxicity and developmental toxicity (only at the high concentration via inhalation). Adequate screening-level data are available to characterize the human health hazard for the purposes of the OECD HPV Chemicals Programme.**

**Environment**

The hydrolysis half-life for VTMS is <2.4 hours at 50 °C and pH7. Estimated t1/2 at 25C using the Taft Equation and the measured hydrolysis rates are 8.2 seconds at pH 4, 16 minutes at pH 7 and 11 seconds at pH 9. In the atmosphere, indirect photo-oxidation by reaction with hydroxyl radicals is predicted to occur with a half-life of 0.372 days. An OECD TG 301F resulted in 51 % biodegradation after 28 days. VTMS is not readily biodegradable under aerobic conditions. Based on the rapid hydrolysis of this material, any potential for biodegradation is likely to be of the hydrolysis products. Consequently, the only biodegradable materials in the test system will be methanol, silanetriol, and condensed silanetriol materials (high molecular weight polymers). The hydrolysis product, methanol, is readily biodegradable; however, ethenylsilanetriol and the condensed silanetriol materials are not expected to be readily biodegradable. Level III Fugacity modeling, using loading rates of 1000 kg/h each for air, soil, and water, shows the following percent distribution of VTMS when it is released simultaneously to all three compartments: Air = 2.58%; Soil = 46.3%; Water = 51%; Sediment = 0.937%. However, VTMS is unlikely to be found in the environment, as this material is hydrolytically unstable. A Henry's law constant of 8.72 x $10^{-5}$ atm-$m^3$/mole at 25°C (8.84 Pa-$m^3$/mole) suggests that the volatilization of VTMS from the water phase is not expected to be high. VTMS reacts to form methanol and ethenylsilanetriol through hydrolysis. The BCF for VTMS and ethenylsilanetriol cannot be predicted accurately, but are expected to be low. Methanol has a low estimated bioaccumulation potential (BCF= 3.2). Furthermore, due to these properties, current estimation models are not capable of calculating physicochemical or environmental fate values with a known degree of accuracy. No information on the environmental fate of ethenylsilanetriol was found. However, based on studies on related monomeric silanols, it is expected that the adsorption of ethenylsilanetriol onto surfaces and condensation to disiloxanes in dilute aqueous solution may be important properties of this chemical. Ethenylsilanetriol is expected to partition primarily to water, soil and sediment due to its high water solubility and potential to bind to mineral surfaces. In water and air, ethenylsilanetriol may degrade photolytically. Slow biodegradation in water and soil might also occur.

Due to the rapid hydrolysis of VTMS, aquatic organisms are likely exposed to the parent material and its hydrolysis products, methanol, ethenyl silanetriol, and silanol oligomers.

The following acute toxicity test results have been determined for aquatic species:

Fish [zebra fish :*Brachydanio rerio*]: 96h-$LC_{50}$ >100 mg/L (nominal)

Invertebrate [*Daphnia magna*]: 48h-$EC_{50}$ = 168.7 mg/L (nominal)

Algae [*Scenedesmus subspicatus*]: 72h-$ErC_{50}$ > 100 mg/L (growth rate method) (nominal)

Algae [*Scenedesmus subspicatus*]: 72h-$EbC_{50}$ > 100 mg/L (area under growth curve method) (nominal);

72h-NOEC = 10 mg/L

**VTMS may not present hazard for the environment based on its low hazard profile. Adequate screening-level data are available to characterize the environmental hazard for the purposes of the OECD HPV Chemicals Programme.**

**Exposure**

In the Sponsor Country, production volume in 2005 was 953 tonnes. In that year, an additional 230 tonnes of VTMS were imported into the Sponsor Country. In 2009, a total use of 16.9 tons/year was registered in the Danish Product Register. In 2006, the total use in the Nordic countries (Denmark, Sweden, Finland and Norway) was 1253 tons, according to the SPIN database. The main use category was "manufacture of rubber and plastic products". In Japan, the 2005 production volume was approximately 1000 tonnes and no VTMS was imported.

VTMS is a coupling agent used for plastics and wire and cable pipes. VTMS can be used as moisture scavenger in sealants; but there is no information that they are used as moisture scavengers in latex. VTMS can be used as a co-monomer in the preparation of latex dispersions with the purpose to promote adhesion of the latex dispersion on inorganic surfaces. The amount of VTMS used in industrial products is usually only 1-2 percent. The substance is reacted during use and little or no chemical is expected in final products. There are no consumer uses of VTMS.

In order to prevent the rapid hydrolysis and subsequent loss of this material in production, it is handled in closed systems [hard-piped]. Necessary engineering controls during production are recommended and include proper ventilation, containment, safety equipment and actual hardware designed to minimize exposure through splashing, or exposure to the air. VTMS is transported from the production site as the parent silane.

During industrial processing, the substance reacts completely and is no longer available for worker exposure. The substance hydrolyzes releasing methanol and silanetriols that can condense to form highly cross-linked, high molecular weight polymers. At the industrial customer level, the material may be used in open systems. Likely engineering controls during use include local ventilation (hoods) when the substance is being transferred or used in its application. Exposure due to non-accidental releases are expected to be low, and may include dermal and inhalation exposure during transfer and use.

Exposure to the environment is expected to be low.