

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	1067-53-4
Chemical Name	Tris(2-methoxyethoxy)vinylsilane (VTMOEOS)
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR**Analog Justification**

VTMOEOS undergoes rapid hydrolysis, which occurs during testing, such that observed toxicity is likely due primarily to the hydrolysis products. The primary hydrolysis products are known to be 2-methoxyethanol (EGME) (CAS No. 109-86-4) and the corresponding vinyltrisilanol (CAS No. 143-48-6). 2-Methoxyethanol and a silanetriol have been used to supplement the existing partition coefficient, water solubility and acute aquatic toxicity (fish, aquatic invertebrate, and algae) data for VTMOEOS. Fugacity modeling of the vinylsilanetriol is also presented. Adequate data for the sponsored substance are presented for the remaining physical chemical properties, environmental fate and mammalian toxicity endpoints. Additional data on EGME are to be made available via the World Health Organization IPCS CICAD process.

Human Health

There are no human studies with VTMOEOS. No data were available on the toxicokinetics, metabolism and distribution of VTMOEOS.

The oral (gavage) LD₅₀ in rats of VTMOEOS was determined using OECD guideline 401 and is greater than 2000 mg/kg bw. Clinical signs included hypoactivity and tremors. Autopsy findings included gastrointestinal abnormalities, slight lung congestion, prominent acini with some mottling of the liver, pale kidneys and slight congestion of the adrenals. When dosed in a vehicle, signs of toxicity included piloerection and lethargy, followed by excessive salivation, sweating, diuresis, diarrhea and blood staining around mouth and nostrils. The dermal LD₅₀ of VTMOEOS in rats was determined using OECD guideline 402 and is greater than 2000 mg/kg bw. Desquamation was noted sporadically during the study. The dermal LD₅₀ of VTMOEOS in rabbits was 1560 mg/kg bw. Covered applications produced necrosis of the skin and when death followed, the lungs were hemorrhagic, livers congested, and kidneys pitted on the surface. VTMOEOS is mildly irritating to the skin (using OECD guideline 404 or similar) and eyes (using OECD guideline 405 or similar). No sensitisation data were available for VTMOEOS.

In a combined oral gavage OECD 422 study in rats there were no test article-related effects on mean body weights, body weight gains or food consumption in the toxicity phase females. Hematological effects were observed in both sexes in the 250 mg/kg/day toxicity phase group. These findings correlated with the microscopic finding of hypocellularity in the sternal bone marrow, in which aggregates of mature granulocytes were absent. Serum

chemistry parameters in the 250 mg/kg bw/day toxicity phase male and female groups were observed. Test article-related macroscopic changes, microscopic changes and/or reductions in organ weights were observed in the 75 mg/kg bw/day group males and the 250 mg/kg bw/day group males and females. The NOAEL for VTMOEOS for male systemic toxicity is 25 mg/kg bw/day. Based on effects on hematology and serum chemistry parameters and effects on lymphoid tissues for females at 250 mg/kg bw/day, which were similar to the effects noted for males, the NOAEL for female systemic toxicity is 75 mg/kg bw/day. Based on decreased fertility at 250 mg/kg/day, macroscopic and microscopic changes with corresponding decreases in weights for the male reproductive organs at 250 mg/kg bw/day and the reduced mean litter size in the 75 mg/kg bw/day group, the NOAEL for VTMOEOS for male and female reproductive toxicity was 25 mg/kg bw/day. The NOAEL for fetotoxicity/developmental toxicity is 75 mg/kg bw/day. A role for developmental toxicity in the reduced postnatal survival at this dose cannot be excluded. The NOAEL for teratogenicity is ≥ 75 mg/kg bw/day.

In vitro, VTMOEOS was negative in bacterial mutagenicity assays (OECD guideline 471 or similar) and did not induce chromosomal aberrations (OECD guideline 473) in CHO cells. No carcinogenicity studies were available for VTMOEOS.

Environment

VTMOEOS is hydrolytically unstable over a range of environmentally relevant pH and temperature conditions. The melting point of VTMOEOS is 30.15°C and the boiling point is 285 °C at 1013 hPa. The vapor pressure is 0.00104057 hPa at 25 °C. The estimated water solubility of VTMOEOS is 1000 g/L; the estimated log Kow is -1.14. The water solubility and log Kow values may not be applicable because the chemical is hydrolytically unstable. The water solubility and partition coefficient of 2-methoxyethanol range from 5 to 1000 g/L and -0.61 to -0.77, respectively. The estimated water solubility and partition coefficient of vinylsilanetriol are 1000 g/L and -2.01, respectively.

The overall OH rate constant is 0.00000000070836 cm³/molecule-sec with an estimated half-life of 0.23 days with a hydroxyl radical concentration of 5.0×10^5 molecule/cm³. Photodegradation as a mode of removal is unlikely as VTMOEOS is hydrolytically unstable. VTMOEOS is reactive and hydrolytically unstable, such that 2-methoxyethanol and vinylsilanetriols are rapidly generated upon contact with water or water vapor. Consequently, reaction with water vapor is likely the predominant degradation process for VTMOEOS in air and the overall reaction half-life in air should include both the oxidation half-life and the hydrolytic half-life. The overall reaction half-life in air is estimated to be less than 0.15 days because of rapid hydrolysis of the material with moisture in the atmosphere. The products resulting from VTMOEOS hydrolysis in the atmosphere are expected to further react with hydroxyl radicals. The overall OH rate constant for vinylsilanetriol is 0.0000000003665 cm³/molecule-sec with an estimated half-life of 0.4 days with a hydroxyl radical concentration of 5.0×10^5 molecule/cm³.

At pH 7 and 25° C, the half-life is 61.5 minutes the hydrolysis products are 2-methoxyethanol and corresponding vinylsilanetriols. Level III fugacity modeling for VTMOEOS, using loading rates for Air, Soil, and Water of 1000 kg/h for each medium, shows the following percent distribution: Air = 0.4%; Soil = 94%; Water = 5.6%; Sediment = 0%. However, VTMOEOS is unlikely to be found in the environment. Level III fugacity modeling for vinylsilanetriol, using loading rates for Air, Soil, and Water of 1000 kg/h for each media, shows the following percent distribution: Air = 0.0%; Soil = 39%; Water = 61%; Sediment = 0.1%. VTMOEOS is readily biodegradable. The biodegradation observed is likely reflective of the hydrolysis product, 2-methoxyethanol. The biodegradation rate for 2-methoxyethanol after 14 days is 100% and after 10 days is 65-77%. Bioaccumulation is not anticipated since this material is hydrolytically unstable.

VTMOEOS undergoes rapid hydrolysis in aquatic media, and thus the exposures to VTMOEOS are likely to be transient. The 96-hour LC50 of VTMOEOS for a freshwater fish (*Brachydanio rerio*) is >100 mg/L. There were no deaths at 100 mg/L, the highest concentration tested. The 96-hour EC50 of 2-methoxyethanol ranges from 15,500 to 16,000 mg/L for *Oncorhynchus mykiss*. 96-Hour LC50 values for 2-methoxyethanol have also been reported for *Lepomis macrochirus* (>10,000 mg/L) *Leuciscus idus* (>500 mg/L), *Menidia beryllina* (>10,000 mg/L), *Oryzias latipes* (> 89 mg/L) and *Salmo gairdneri* (14,997 mg/L). Studies have been performed with a silanol monomer, trimethylsilanol (CAS No. 1066-40-6). Although this silanol is not a hydrolysis product of VTMOEOS, it has been predicted to be one of the most toxic to aquatic organisms of all the silanols identified to date. A semi-static 96h study with trimethylsilanol and rainbow trout (*Oncorhynchus mykiss*) resulted in a NOEC of 128 mg/L and an LC₅₀ of 271 mg/L. The 48-hour EC50 of VTMOEOS is 314 mg/L for the water flea (*Daphnia magna*) under static conditions. The 48-hour EC50 of 2-methoxyethanol is greater than 85 mg/L for the water flea (*Daphnia magna*). The 48-hour EC50 of trimethylsilanol is 124 mg/L for the water flea (*Daphnia magna*) under semi-static conditions. In an algae study with *Scenedesmus subspicatus* and VTMOEOS, on the basis of biomass, the median

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effective concentration was 72 h EbC50 = 304 mg/L and 72 h EbC10 = 79 mg/L. On the basis of growth rate, a median effective concentration was achieved at (0-72 hr) ErC50 = 611 mg/L; (0-72 hr) ErC10 = 136 mg/L. The NOEC was 75 mg/L. The 48 hr EbC50 is greater than 93 mg/L for 2-methoxyethanol and *Pseudokirchneriella subcapitata*. The most sensitive endpoints for *Pseudokirchneriella subcapitata* exposed to trimethylsilanol were cell density and area under the growth curve (biomass). The 72-hour EC50 value was 555 mg/L with 95% confidence limits of 141 and 612 mg/L. The 72-hour NOEC, based on cell density, area under the growth curve (biomass) and growth rate was 70 mg/L. The 96-hour EbC50 value was 625 mg/L with 95% confidence limits of 555 and 702 mg/L. The 96-hour NOEC, based on area under the growth curve (biomass), was 70 mg/L. Three plant species, *Triticum aestivum* (wheat), *Brassica alba* (mustard), and *Lepidium sativum* (cress) were tested at concentrations of 0, 1, 10 and 100 mg VTMOEOS/kg soil. Five seeds of each species were planted in four replicates. Seedling wet weights were evaluated on day 17. The EC50 for emergence of seedlings and wet weight for wheat, cress and mustard were 29, 94 and >100 mg/kg, respectively; the NOECs for all three species were >100 mg/kg.

Exposure

VTMOEOS undergoes rapid hydrolysis, which occurs during testing, such that observed toxicity is likely due primarily to the hydrolysis product 2-methoxyethanol, with some potential exposure to trisilanols, and silanol oligomers. The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration (the silanetriol has a tendency to condense at concentrations greater than 500 ppm) and pH, and since both change over time it is not feasible to isolate specific silanols for analysis (the structures continue to evolve until they either reach equilibrium or precipitate out of solution).

In the Sponsor Country, production volume of VTMOEOS in 2001 was 285 tonnes with imports of 270 tonnes. In production, this material is 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 (hydrolysis).

VTMOEOS is bi-functional molecule, containing organo functional groups, which can form strong covalent crosslink with polymers and hydrolysable groups capable of forming strong covalent bonds with the hydroxyl groups on silica surfaces. This functionality allows reaction both with organic and inorganic fillers. It can be used as an adhesive and an accelerant. The major uses of VTMOEOS are in wire and cable, as a pre-treatment for clay filler. VTMOEOS is transported from the production site as the parent silane. The parent silane partially reacts during use by the customer and then completely reacts during curing into the polymer matrix and is no longer available for consumer or worker exposure. VTMOEOS does not volatilize during the cure of crosslinked EPDM or polyolefins. Instead this material hydrolyzes and condenses, producing 3 moles of 2-methoxyethanol and one mole of vinylsilanetriol for each mole of parent silane. Therefore, there is no human exposure to VTMOEOS from use in cross-linked ethylene propylene diene monomer (EPDM) and polyolefin based thermoplastics. Potential routes of exposure for workers include dermal contact and inhalation, although dermal exposures are minimal as chemical protective gloves and/or clothing would be required during handling. There is no known production process that involves aerosolized material or sprayed material. The product is stored on site in tanks, bins, drums and pails. At the customer level, the material is used in closed systems. Open systems as such are not known to be used in the production of treated filler. Industrial customers purchase VTMOEOS in closed vessels (such as Intermediate Bulk Containers) from the manufacturer. The VTMOEOS is pumped from these containers into a treating chamber, where hydrolysis of VTMOEOS occurs. Note that the chamber is not sealed (vapour tight) vessel, but is a closed container with an exhaust system tied into an incinerator. Necessary engineering controls during use are likely to include local ventilation. Exposure due to non-accidental releases are expected to be minimal, and may include dermal and inhalation potential. The treated clay is sold to medium voltage wire and cable manufacturers, for buried utility applications. The wire and cable is formed in an extruder. Industrial customers exposure to 2-methoxyethanol is expected to be negligible as the initial loading rate onto the clay is 0.5 % or less. Contact with the final product (laying buried cable) is small.

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

Human Health: The chemical possesses properties indicating a hazard for human health (reproductive and haematological effects). Due to the rapid hydrolysis to 2-methoxyethanol and the corresponding trisilanol and based on exposure data presented by the Sponsor country, the parent material and its hydrolysis products, including 2-methoxyethanol, will not be available for exposure, and therefore this chemical is currently of low priority for further work. These properties should nevertheless be noted by chemical safety professionals and users.

Environment: The chemical is currently of low priority for further work because of its low hazard profile.