# SIDS INITIAL ASSESSMENT PROFILE

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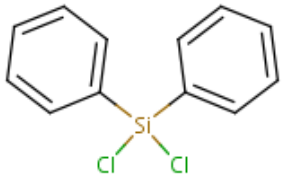
|---|---|
| **CAS No(s).** | 80-10-4 |
| **Chemical Name(s)** | Dichlorodiphenylsilane (**DClDPS**) |
| **Structural Formula(s)** | **DClDPS**:   |

## SUMMARY CONCLUSIONS OF THE SIAR

**Analogue Rationale**

Chlorosilanes, including **DClDPS**, react rapidly when exposed to moisture or polar reagents (those that are protic and as such contain a dissociable $H^+$), producing hydrogen chloride (HCl; CAS No. 7647-01-0) and diphenylsilanediol (CAS No 947-42-2)[1]. Each mole of **DClDPS** hydrolyses to form two moles of HCl and one mole of diphenylsilanediol. The hydrolysis half-life of **DClDPS** is < 1 minute at 1.5ºC for pH 4, 7, and 9.

*Human Health, Aquatic Toxicity and Environmental Fate Analogues*
(1) Hydrolysis products of **DClDPS** are used to characterize toxicity due to its very fast hydrolysis. Data for hydrolysis products HCl and diphenylsilanediol are used to represent repeated dose mammalian toxicity and acute aquatic toxicity. HCl is also used to represent acute toxicity, irritation, and genotoxicity.

(2) Structural analogues are used directly as read across substances, or through rapid hydrolysis to a structurally similar silanediol, to characterize the toxicity of **DClDPS**. A structurally analogous phenylchlorosilane, trichlorophenylsilane (TClPS, CAS No. 98-13-5), with the same expected rapid hydrolysis rate as **DClDPS,** is used to represent the biodegradation and chromosome aberration endpoints**.**

HCl was presented and agreed under the OECD Cooperative Chemicals Assessment Programme (http://www.oecd.org/env/hazard/data).

[1]When prepared under very controlled conditions, the hydrolysis product, diphenylsilanediol will crystallize from solution before it can react to form siloxanes. The crystal structure locks in the special configuration, thereby preventing the silanediols from condensing and allows separation of diphenylsilanediol for testing. In solution, diphenylsilanediol will condense to form oligomers. Under "normal" conditions, and depending on pH and concentration in water, silanediols such as diphenylsilanediol can condense to form highly cross-linked, high molecular weight polymers, further reducing the potential for exposure.

The read across strategy for **DClDPS** follows:

| Env. Fate | Mammalian toxicity | | | | Environmental effects |
|---|---|---|---|---|---|
| **Bio-degradation** | **Acute toxicity** | **Irritation** | **Repeated dose toxicity** | **Genetic toxicity (chromosome aberration)** | **Aquatic toxicity to Fish, Daphnid and Algae** |
| TClPS | HCl | HCl | Diphenylsilanediol, HCl | TClPS, HCl | Diphenylsilanediol, HCl |

**Physical-chemical Properties**

**DClDPS** is a colorless liquid at 20 °C and 1013 hPa with measured melting point of -22°C, measured boiling point of 305°C and estimated vapour pressure of 0.00078 hPa at 25 °C. The calculated octanol-water partition coefficient (log $K_{ow}$) is 5.06 (reliability = 4), and the estimated water solubility is 2.8 mg/L at 25 °C. The calculated water solubility and log $K_{ow}$ values may not be accurate because the substance is hydrolytically unstable.

**Human Health**

No data are available on the toxicokinetics, metabolism and distribution of **DClDPS**. However, **DClDPS** rapidly hydrolyses to HCl and diphenylsilanediol on contact with moisture. Damage to membranes caused by the corrosive nature of HCl might enhance the uptake of **DClDPS** or the silanol hydrolysis product. Hydrogen and chloride ions will enter the body's natural homeostatic processes. HCl will rapidly dissociate and its effects are thought to be a result of pH change (local deposition of $H^+$). Repeated dose exposure studies with diphenylsilanediol suggest the silanol is absorbed following oral exposure, distributed systemically and metabolized/eliminated through the liver and kidneys.

Acute inhalation studies were not located for **DClDPS**. The acute inhalation toxicity of **DClDPS** is expected to be well characterized by the effects of HCl exposure, rather than systemic effects of silanol hydrolysis products. The principal clinical signs are expected to be indicative of respiratory and ocular effects resulting from HCl exposure. Inhalation $LC_{50}$ values (one hour exposure) for HCl were determined to be 4.2 - 4.7 mg/L for rats and 1.7 mg/L for mice. The acute oral $LD_{50}$ values of HCl were determined to be 238 - 277 mg/kg bw for female rats. An acute toxicity study was not located for diphenylsilanediol.

Irritation data are not available for **DClDPS**. **DClDPS** rapidly hydrolyses to HCl and the associated silanol. HCl is corrosive and highly irritating to the skin, eyes and respiratory tract. As such, **DClDPS** is expected to be corrosive to the skin, cause serious damage to the eyes and be highly irritating to the respiratory tract. Sensitization data are not available for **DClDPS** or the expected hydrolysis products.

Repeated dose toxicity data are not available for **DClDPS**. Repeated oral exposure to the expected hydrolysis product, diphenylsilanediol and inhalation data for the hydrolysis product HCl are available. The NOAEL following repeated gavage exposure of rats to diphenylsilanediol for 21 days was 400 mg/kg bw (highest dose tested). In a 14-day study with beagle dogs, repeated dose administration of diphenylsilanediol at 500 mg/kg bw for 14 days produced effects that included neurological effects, marked reduction in body weight and effects on liver, kidney and adrenal gland. Exposure at 50 mg/kg bw produced some of these same effects, albeit at a lower incidence/severity. In repeated dose toxicity studies of HCl by the inhalation route, local irritant effects were observed in the groups of rats and mice exposed to 0.015 mg/L and above for 90 days. The inhalation NOAEC for systemic toxicity for HCl, excluding the local effects of irritation, has been determined to be 0.030 mg/L, with a LOAEC of 0.075 mg/L. The toxicity of **DClDPS** is expected to be well-characterized by the effects of HCl inhalation exposure, the prevalent route of the **DClDPS** exposure.

**DClDPS** did not induce gene mutations in bacterial cells *in vitro* [similar or equivalent to OECD TG 471]. TClPS was negative for induction of gene mutations in bacterial [similar to OECD TG 471] and mouse

lymphoma cells [OECD TG 476]. A chromosomal aberration study was not located for **DClDPS**. The hydrolysis products, diphenylsilanediol and HCl, did not induce gene mutations in bacterial cells. Positive results in the *in vitro* chromosome aberration test with HCl were considered to be the effect of low pH. Based on the available data, **DClDPS** is not expected to be genotoxic.

No data are available for the carcinogenicity of **DClDPS**.

Reproductive toxicity data are not available for **DClDPS** or the hydrolysis product diphenylsilanediol**;** no additional testing is needed because **DClDPS** is a site-limited intermediate and is produced and used in closed systems. Information for the hydrolysis product HCl is used to partially fill the reproductive toxicity endpoint for **DClDPS**. No reliable studies have been reported regarding toxicity to reproduction and development in animals after oral, dermal or inhalation exposure to hydrogen chloride/hydrochloric acid. Because proton and chloride ions are the normal constituents in the body fluid of animal species, low concentrations of hydrogen chloride gas/mist or solution do not seem to cause adverse effects to mammals. In fact, the cells of gastric glands secrete hydrochloric acid into the cavity of the stomach and orally administered sulfuric acid, which results in pH change as well, did not cause developmental toxicity to laboratory animals. These facts indicate that hydrogen chloride/hydrochloric acid is not expected to have developmental toxicity. In addition, no effects on the gonads were observed in a 90-day inhalation repeated-dose study up to concentrations of 0.075 mg/L.

**Diphenyldichlorosilane possesses properties indicating a hazard for human health [lethality from acute inhalation, corrosive and highly irritating to the skin, eyes and respiratory tract (based on the hydrolysis product, HCl) and repeated dose toxicity (based on the hydrolysis product, diphenylsilanediol)]. Data on reproductive toxicity are not available, however, based on use of this chemical in the sponsor country (closed system site-limited intermediate), additional testing for this endpoint is not needed. Adequate screening-level data are available to characterize the human health hazard for the purposes of the OECD Cooperative Chemicals Assessment Programme.**

**Environment**

Not all programs within EPI Suite have been validated for chemicals that contain the element Si, but recent upgrades to the Kow module, found in the current version of EPI Suite (v4.10), may improve estimates for silanes and siloxanes for this endpoint. However, there is still uncertainty associated with the calculated values and they should be used with caution whenever they are reported.

The chlorine group is the most active functional group for **DClDPS** and determines many aspects of its behaviour. Each mole of **DClDPS** undergoes rapid hydrolysis in the presence of moisture to form two moles of HCl and one mole of diphenylsilanediol. An OECD TG 111 (Hydrolysis as a Function of pH) test was conducted at 1.5ºC for **DClDPS**; half-lives of less than one minute were reported at pH 4, 7, and 9.

In the atmosphere, indirect photo-oxidation by reaction with hydroxyl radicals is predicted to occur with a half-life of 2.7 days. Any potential for photodegradation might be superseded by hydrolysis of the parent compound depending on the concentration of water vapour in the air. The biodegradation of supporting substance TClPS was determined in OECD TG 310; there was essentially no (1%) biodegradation of the test substance in 28 days. HCl is an inorganic compound and biodegradation tests are not applicable. Based on this information, **DClDPS** is not expected to be readily biodegradable. Due to rapid hydrolysis of **DClDPS**, any potential for biodegradation is likely to be of the hydrolysis products. Consequently, the only biodegradable materials in the test system will be silanols, and condensed silanol materials (high molecular weight polymers). At high concentrations (>500 mg/L), the silanols will condense to form highly cross linked, high molecular weight polymers that are water insoluble and effectively nonbiodegradable.

A level III fugacity model calculation with equal and continuous distributions to air, water and soil compartments suggests that **DClDPS** will distribute mainly to the air (47.6%) and soil (47.7%) compartments with minor distribution to the water and sediment compartments. Level III fugacity modeling using equal loading rates of 1000 kg/h each for air, soil and water predicts that the hydrolysis product, diphenylsilanediol, will distribute mainly to soil (76.9 %), with a smaller fraction to water (13.9 %) and negligible amounts to sediment and air. Based on the more realistic scenario of 100% release to air, the model predicts that diphenylsilanediol will be distributed mainly in air (94.5%), with minor distribution to water (3.3%) and

sediment (2.8%).

**DClDPS** is not expected to bioaccumulate in the aquatic environment based on rapid hydrolysis to diphenylsilanediol, which has an estimated BCF of 9.7 L/kg. The calculated bioconcentration factor for **DClDPS** is 1009 L/kg wet-wt.

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

| Test substance | Species | Result (mg/L) | Guideline; Test type |
|---|---|---|---|
| **Fish, acute toxicity** | | | |
| **Supporting hydrolysis products** | | | |
| Diphenylsilanediol | *Oncorhynchus mykiss* | 96-hr $LC_{50}$ = 39 (measured) | OECD TG 203; static |
| HCl | *Cyprinus carpio* | 96-hr $LC_{50}$ = 4.92 (pH = 4.3 ) | OECD TG 203; semi-static |
| **Aquatic invertebrate, acute toxicity** | | | |
| **Supporting hydrolysis products** | | | |
| Diphenylsilanediol | *Daphnia magna* | 48-hr $EC_{50}$ = 24 (measured) | OECD TG 202; static |
| HCl | *Daphnia magna* | 48-hr $EC_{50}$ = 0.492 (pH= 5.3) | OECD TG 202; not specified |
| **Aquatic plants, acute toxicity** | | | |
| **Supporting hydrolysis products** | | | |
| Diphenylsilanediol | *Pseudokirchneriella subcapitata* | 72-hr $E_rC_{50}$ = 9.0<br>72-hr $E_bC_{50}$ = 2.8<br>96-hr $E_rC_{50}$ = 11<br>96-hr $E_bC_{50}$ = 2.7<br>(measured) | OECD TG 201; static |
| HCl | *Pseudokirchneriella subcapitata* | 72-hr $E_rC_{50}$ = 0.492 (pH= 5.3) | OECD TG 201; static |

**Based on the properties of the hydrolysis products, HCl and diphenylsilanediol, DClDPS possesses properties indicating a hazard for the environment (acute toxicity to fish between 1 and 100 mg/L). Based on the hydrolysis product HCl, DClDPS posseses properties indicating a hazard for the environment (acute toxicity to aquatic invertebrates and to algae < 1 mg/L). Toxic effects are expected primarily from the hydrolysis products. DClDPS has a low potential for bioaccumulation and is not expected to be readily biodegradable. Adequate screening-level data are available to characterize the hazard for the environment for the purposes of the OECD Cooperative Chemicals Assessment Programme.**

**Exposure**

Production and import volumes (metric tonnes) for 2010 are summarized below.

| **United States** | | **Europe** | | **Japan** | |
|---|---|---|---|---|---|
| **Production** | **Import** | **Production** | **Import** | **Production** | **Import** |
| 454 - 2268 | 4.5 - 454 | 0 | 4.5 - 454 | 454 - 3629 | 0 |

Ranges are provided to protect confidential business information. **DClDPS** is used in formulations up to 100% as intermediates for silicone oligomers and polymers. No parent substance is expected to remain after end use.

**DClDPS** is produced and processed in closed systems; commercial customers use **DClDPS** in closed systems. Due to the dynamic and exothermic nature of the processes incorporating chlorosilanes, many engineering controls are always in place to prevent occupational exposure such as water scrubber devices and related equipment; closed sampling loop; and local and general ventilation. Employees involved in chlorosilane production and application use personal protective equipment (PPE) such as safety glasses or goggles, steel-

tipped shoes, flame-resistant clothing, hard hats, chemical resistant gloves, and respirator masks. Potential routes of exposure include inhalation and dermal exposure.

There are no consumer uses for **DClDPS**.

Environmental exposure is not expected.

Note: This document may only be reproduced integrally. The conclusions in this document are intended to be mutually supportive, and should be understood and interpreted together.