SIDS INITIAL ASSESSMENT PROFILE

CAS No.	51000-52-3
Chemical Name	Neodecanoic acid ethenyl ester, vinyl neodecanoate
Structural Formula	CH_2=CH-O-CO-C(CH_3)(R^1)(R^2) where R^1 and R^2 contain seven alkyl carbons in total

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

There are no standard toxicokinetic studies on neodecanoic acid ethenyl ester. However, it is evident that the chemical is absorbed and distributed because there were specific organ effects in kidneys and liver following oral and inhalation dosing. Although it appears to be a very stable monomer that is not degraded, at least to a significant extent, by crude liver homogenates of rats *in vitro*. The acute toxicity tests indicate low toxicity by inhalation, dermal, and oral routes of exposure to rodents. In rats, the oral and dermal LD_{50} were > 8850 mg/kg bw and > 3540 mg/kg bw, respectively, and the 4-h LC_{50} was > 2.6 mg/L. With regards to irritation in animals, there is evidence of limited (minimal to non-irritating) potential to eyes and skin. However, the substance is not a sensitizer. Repeated dosing of neodecanoic acid ethenyl ester has shown a low degree of toxicity in rats by inhalation (0.25, 0.5 and 1.0 g/m3 for 6hr/day, 5d/wk, 13 weeks) or oral exposure (100, 250, 1000 mg/kg/d, for 28 d). The NOAEL for a 28-d oral exposure was 250 mg/kg bw/d based on specific kidney effects (so called male rat nephropathy) seen at 1000 mg/kg bw/d. The 13-week NOAEC for inhalation was 0.50 g/m3 or 61.7 ppm based on increased liver and kidney, and reduced body weights.

The mutagenic/genotoxic assays which were broadly consistent with modern guidelines show that neodecanoic acid ethenyl ester is not mutagenic or genotoxic *in vitro* (bacterial, yeast and mammalian cell gene mutation and rat liver chromosomal aberration) or *in vivo* (rat liver DNA integrity). No information is available for carcinogenicity. Results from a rat combined repeated dose toxicity study, including reproductive and developmental screening tests (OECD 422) show that neodecanoic acid ethenyl ester (1000, 250, and 100 mg/kg bw/d) is not toxic to reproductive functions such as fertility and there was no evidence of skeletal or visceral malformations or variations. There was a minor, not statistically significant decrease of about 5% in mean day 1 pup weights at the limit dose of 1000 mg/kg/d. The limited effects at the 1000 mg/kg/d limit dose indicate the chemical is not a specific developmental toxicant.

Environment

Neodecanoic acid ethenyl ester is a commercial mixture of isomers used mainly in the synthesis of polymers to make them more hydrolytically and UV-stable. It is a light viscous liquid, moderately volatile (Henry's Law Constant 1295.3 Pa.m^3/mol (1.3 x 10^{-2} atm.m^3/mol), measured boiling point 212°C and vapour pressure 0.386 hPa at 25 °C), of low water solubility (5.9 mg/L, measured), and with a moderate affinity towards organic matter (predicted Log Koc 2.75). While the measured octanol-water partition coefficient (Log Kow or Log P) is 4.9, the bioaccumulation potential from a fish study in which the substance was dosed via the feed indicates that the compound is rapidly eliminated (95% clearance in 14 days depuration, biomagnification factor 0.09). The assimilation efficiency of the hexachlorobenzene control was 47% (indicating high assimilation and in agreement with historical data), and 18% for neodecanoic acid ethenyl ester. The data were also used to derive a bioconcentration factor from an equation validated for compounds tested in aqueous-dosed bioaccumulation studies (BCF 1100 - 1390). However given that neodecanoic acid ethenyl ester is poorly soluble in water this range is likely to be a protective estimate. As stated earlier, the tertiary (neo-) carbon bonding and alkyl chain structure confers a high degree of stability to the molecule, thus it is expected to be strongly resistant to UV light and hydrolytic degradation. When modelling for its environmental distribution (Mackay Fugacity Level III) with

equal release to air, water and soil, it is predicted that the bulk transport should be to soil and sediment compartments (~78 and 14%, respectively), with very little to air and water (0.5 and 7.6%). This chemical was neither readily nor inherently biodegradable (OECD 301D, 14 – 17% degradation after 28 days; OECD 302C, 3 – 5% after 28 days). Microbial toxicity results show no adverse effects up to forced solubility limits (IC_{50} > 100 mg/L).

Neodecanoic acid ethenyl ester has been tested for its acute toxicity to fish, invertebrates and algae. No chronic studies have been conducted. Aquatic toxicity testing has been problematic due to its low water solubility and its likely adherence to glassware. The substance is acutely toxic to aquatic organisms: the lowest GLP results are fish LC_{50} 0.84 mg/L, invertebrates (marine copepod) EC_{50} 0.3 mg/L, and algae EbC_{50} 3.4 mg/L and ErC_{50} > 4.8 mg/L. As indicated above this chemical exhibited a low biomagnification factor, but according to OECD GHS criteria by its derived BCF would be considered to bioconcentrate since the derived BCF >500.

Exposure

Neodecanoic acid ethenyl ester is used exclusively in polymerization as a monomer to make the resulting products more hydrolytically and UV-stable. It is not meant to be used as an unreacted substance in any application. The primary uses include vinyl acetate latex polymers where the principal application is paints and coatings (65%), and adhesives i.e. re-dispersible powders (35%).

Four potential sources of environmental exposure have been identified: (1) Production; (2) Processing (monomer polymerization); (3) Formulation of the polymer into a coating; and, (4) Use by consumers and professional users. Production of neodecanoic acid ethenyl ester (or vinyl neodecanoate) takes place at one site in the Netherlands, and is performed in a continuous closed system as a "dry" process for 365 days/year. Releases from production are expected to be minimal. The total global production volume ranges from 46,000 to 230,000 tonnes/yr.

Exposure from processing is deemed as negligible as the chemical is non-dispersive and carried out in a closed system. Engineering controls are in place to minimize emissions, and transport from storage into a reactor tank is done in a completely closed environment. Any minimal waste water generated in the process would be fed to a waste water treatment plant (WWTP), and since neodecanoic acid ethenyl ester is normally directed to the oil phase in the oil / water separator before the WWTP it is treated as chemical waste, and hence incinerated.

Exposure from formulation of the polymer into a coating (i.e. paint) estimates a very small amount of unreacted residual neodecanoic acid ethenyl ester in the end product (0.006% max). It is assumed that dedicated equipment with very little cleaning is used for formulation, given the high quantities of product needed.

Exposures from uses (application) are more difficult to estimate. Based on the amount of unreacted residual monomer in an end-product such as paint (0.006%), an estimate of 350-600 kT paint containing residual neodecanoic acid ethenyl ester could be on the European market. The coating film is required to be stable for at least 3 years.

The circumstances of manufacture and use of neodecanoic acid ethenyl ester allow for a continuous control of human and environmental exposure, which are done in closed systems and under strict norms of safety. Occupational, consumer, and even environmental exposure are anticipated to be low, if not negligible. Despite the high toxicity seen in aquatic testing, exposure to the environment is anticipated to be low. In the event of an accidental spill there are mitigation plans in place to minimize exposure and potential hazards.

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

Human Health: The chemical is a low priority for further work due to its low hazard profile.

Environment: The chemical is a candidate for further work. The chemical possesses properties indicating a hazard for the environment (acute toxicity to fish and aquatic

invertebrates). Member countries are invited to perform an exposure assessment for the environment and if necessary a risk assessment.