


SIDS INITIAL ASSESSMENT PROFILE

CAS No.	1120-21-4
Chemical Name	<i>n</i> -Undecane
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR**Physical-chemical properties**

n-Undecane is a colourless liquid with a water solubility of 0.004 mg/L to 0.044 mg/L at 25 °C. Melting point and boiling point are -25.5 °C and 195.9 °C respectively. A calculated partition coefficient between octanol and water (Log K_{ow}) is 5.74. Vapour pressure of *n*-undecane is 50 Pa at 25 °C. An estimated soil adsorption coefficient (Log K_{oc}) is 3.42.

Human Health

n-Undecane vapour was readily absorbed by inhalation and was distributed to various tissues, especially fat tissues in rats. *n*-Undecane was also preferentially distributed to brain and a long-lasting redistribution from fat to brain can occur. The amount of *n*-undecane that can be absorbed through the skin was very small *in vitro*. After a single topical dose of *n*-undecane, maximum concentration in blood (C max) occurred shortly after the end of exposure (t max, ca. 30 min) in two healthy human volunteers.

The 8-h inhalation LC₅₀ value was above 2.82 mg/L (saturated vapor) for male rats. No toxic effects were observed in clinical signs, body weights, necropsy and histological observations.

The oral LD₅₀ value was above 2000 mg/kg for male and female rats in the acute study following OECD TG401. No toxic effects were observed.

The incidences of mild irritancy to skin by *n*-Undecane were reported only from lower reliability studies (pigs and rabbits). Prolonged or repeated skin contact may cause defatting and dermatitis. No experimental data are available for eye irritation.

No experimental data are available for skin sensitization in animals and humans.

The repeat dose and reproductive/developmental toxicity screening toxicity of *n*-undecane has been investigated in one study. In a repeat dose and reproductive/developmental toxicity screening study in rats following OECD TG422, *n*-undecane was administered daily via gavage to 12 animals/sex/dose at 0, 100, 300, and 1000 mg/kg bw/day, for 46 days for males and from 14 days before mating to day 3 of lactation for females. Salivation was observed, and the body weight gain was suppressed in males given 1000 mg/kg bw/day, and body weights were increased in females given 1000 mg/kg bw/day during the lactation period. A decrease in hemoglobin concentration, an increase in white blood cells count, a decrease in albumin, and increases in α_2 -globulin, glutamic-pyruvic transaminase, cholinesterase and total cholesterol were found in males given 1000 mg/kg bw/day. Liver and thymus weights were increased in males given 1000 mg/kg bw/day, and liver weights were elevated in females given 1000 mg/kg bw/day. No effects were detected at autopsy or after histopathological investigations. The NOAEL for repeat dose toxicity is considered to be 300 mg/kg bw/day for both sexes.

In a bacterial reverse mutation assay with *E.coli* WP2 *uvrA* and multiple strains of *Salmonella typhimurium* following OECD TG471 and 472, *n*-undecane was negative both with and without metabolic activation. An *in vitro* chromosomal aberration test using Chinese hamster lung (CHL/IU) cells was negative with and without metabolic activation following OECD TG473.

Undecane was shown to have tumour promoting activity in mice skin following dermal exposure three times per week with benzo[a]pyrene as an initiator for 440 days, although undecane alone did not induce tumours in mice skin. No other data are available on the carcinogenicity of *n*-undecane by other exposure routes.

The reproductive toxicity of *n*-undecane has been well investigated in a reproductive and developmental toxicity

screening test in rats following OECD TG422. In this study, *n*-undecane was administered daily via gavage to 12 animals/sex/dose at 0, 100, 300, and 1000 mg/kg bw/day, for 46 days for males and from 14 days before mating to day 3 of lactation for females. Reproductive toxicity in parental animals was not observed up to 1000 mg/kg bw/day. In offsprings of the 1000 mg/kg bw/day group, body weight gain was decreased. The NOAEL for reproductive toxicity is considered to be 1000 mg/kg bw/day, and the NOAEL for maternal and developmental toxicity is considered to be 300 mg/kg bw/day. However, the decreased body weight gain may be due to some general maternal toxicity.

***n*-Undecane may present a hazard for human health (repeated dose toxicity). Adequate screening-level data are available to characterize the human health hazard for the purposes of the OECD HPV Chemicals Programme.**

Environment

In the atmosphere, *n*-undecane is expected to be degraded by hydroxyl radicals. A calculated half-life time of 0.854 days and a rate constant of $12.5 \times 10^{-12} \text{ cm}^3/\text{molecule}\cdot\text{sec}$ were obtained by AOPWIN for the indirect photo-oxidation by reaction with hydroxyl radicals in air. *n*-Undecane is not expected to directly photolyze due to a lack of absorption in the environment UV spectrum.

n-Undecane is not hydrolysed due to the lack of hydrolysable functional groups. *n*-Undecane is considered to be readily biodegradable. *n*-Undecane was degraded 100 % by BOD under aerobic conditions after 4 weeks cultivation period according to OECD Guideline 301C. No measured data of bio-accumulation of *n*-undecane is available. A bioconcentration factor of 120.9 was calculated with BCFWIN using a log K_{ow} of 5.74. A bioconcentration factor of 1420 was also calculated with the Arnot-Gobas method, which indicates that *n*-undecane has a moderate bioaccumulation potential.

Fugacity level III calculations show that *n*-undecane is mainly distributed to the water compartment (69.9 %) and air compartment (24.4 %) if equally and continuously released to the air, soil and water. A Henry's law constant of $7.04 \text{ atm}\cdot\text{m}^3/\text{mole}$ at 25 °C suggests that volatilization from water surfaces may be an important fate process.

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

Fish [<i>Oryzias latipes</i>]:	96 h LC ₅₀ >0.013 mg/L (measured)
Invertebrate [<i>Daphnia magna</i>]:	48 h EC ₅₀ = 0.011 mg/L (measured)
Algae [<i>Pseudokirchneriella subcapitata</i>]:	72 h ErC ₅₀ >0.0059 (measured; growth rate)
	72 h EbC ₅₀ >0.0059 (measured; biomass)

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

Invertebrate [<i>Daphnia magna</i>]:	21 d NOEC = 0.0057 mg/L (measured)
	21 d LOEC = 0.0083 mg/L (measured)
Algae [<i>Pseudokirchneriella subcapitata</i>]:	72 h NOEC >0.0059 mg/L (measured; growth rate)
	72 h NOEC >0.0059 mg/L (measured; biomass)

***n*-Undecane possesses properties indicating a hazard for the environment (acute aquatic toxicity values less than 1 mg/L for invertebrate, and chronic aquatic toxicity value less than 0.01 mg/L for invertebrate). However, the substance is readily biodegradable and has moderate bioaccumulation potential. Adequate screening-level data are available to characterize the hazard to the environment for the purposes of the OECD HPV Chemicals Programme.**

Exposure

The annual production volume of *n*-undecane in the sponsor country is expected to be 1,000-10,000 tonnes. The worldwide production volume of *n*-undecane is not available. In the Sponsor country *n*-Undecane is separated and purified by distillation from *n*-paraffins which is isolated from desulfurized kerosene by selective adsorption with molecular sieve.

n-Undecane is used as feedstock for detergents and other industrial materials, reaction solvents and solvents for industrial cleaning in the sponsor country. *n*-Undecane is also used in consumer products like car wax, oil for lamp in the sponsor country. Uses for petroleum research, organic synthesis and distillation chaser are also known. It is reported that *n*-undecane is contained in gasoline. According to IUR information by US-EPA, *n*-undecane is used in consumer products like lubricants, greases and fuel additives. Therefore, consumer

exposure is expected through the use of these products.

n-Undecane is produced in continuous closed system where little potential exists for environmental exposure in the sponsor country. Vent gas from the system is burnt. Waste water, which may be released from the system through maintenance, is treated in the waste water treatment plant with activated sludge before it is released in the environment.

Occupational exposure to *n*-undecane through inhalation and dermal contact are possible. Swedish Permissible exposure limit for *n*-undecane is 350 mg/m³.