SIDS INITIAL ASSESSMENT PROFILE

CAS No.	764-41-0
Chemical Name	1,4-Dichlorobut-2-ene
Structural Formula	$Cl\text{-}CH_2\text{-}CH{=}CH\text{-}CH_2\text{-}Cl$

SUMMARY CONCLUSIONS OF THE SIAR

1,4-Dichlorobut-2-ene (CAS No. 764-41-0) consists of a mixture of *cis*-1,4-dichlorobut-2-ene (CAS No. 1476-11-5) and *trans*-1,4-dichlorobut-2-ene (CAS No. 110-57-6). 1,4-Dichlorobut-2-ene available in the US contains 95 - 98 % *trans*-1,4-dichlorobut-2-ene and 2 - 5 % of the *cis*-isomer. During manufacturing, mixtures of different composition may occur.

Human Health

For the toxicological endpoints addressed there have been taken into consideration besides the data for the title substance 1,4-dichlorobut-2-ene (*cis* and *trans*) also toxicity data for the pure isomers *cis*-1,4-dichlorobut-2-ene and *trans*-1,4-dichlorobut-2-ene.

There are no studies available concerning toxicokinetics, metabolism and distribution of 1,4-dichlorobut-2-ene. Results from toxicity studies with experimental animals show that 1,4-dichlorobut-2-ene is absorbed after inhalational, oral and dermal application.

1,4-Dichlorobut-2-ene is very toxic by inhalation with a 4 hours-LC_{50} of 450 mg/m^3 in rats; toxic symptoms are mainly of local nature like salivation, lacrimation and irritation of the respiratory tract. The dermal toxicity is moderate with an LD_{50} (rabbit) of ca. 735 mg/kg bw in a study with rather limited documentation. After oral application the substance is toxic with an LD_{50} (rat) ranging from > 120 and < 300 mg/kg bw accompanied by toxic effects like spasms and weakness. 1,4-Dichlorobut-2-ene is corrosive at the skin and eyes and extremely irritating to the respiratory tract. The RD_{50} in rats was calculated as 179 ppm (900 mg/m^3).

There are no valid data available concerning sensitization.

The main toxic effects after repeated exposure of rats to 1,4-dichlorobut-2-ene vapors are irritations of the respiratory tract characterised by flattening and metaplasia of the nasal and tracheal mucosal epithelium. At higher exposure concentrations ($\geq$ 1 ppm; $\geq$ 5.2 mg/m^3) mortality is increased. There is no chronic NOAEC derivable; the LOAEC is 0.1 ppm (0.52 mg/m^3; lowest concentration tested). A limited study gave information that repeated oral application of 100 mg/kg bw/day to rats led to discomfort, diarrhea, reduced body weight gain and high mortality. Histopathological effects included lung congestions as well as acute necroses in stomach, liver and spleen.

1,4-Dichlorobut-2-ene is mutagenic to bacteria and yeasts as well as to mammalian cells *in vitro*. *In vivo* a negative result was obtained in a micronucleus assay performed according to OECD TG 474 with inhalation exposure of rats although the highest concentration tested (52 mg/m^3) led to systemically toxic effects. In another non-guideline study with limited documentation 1,4-dichlorobut-2-ene showed a clastogenic activity after inhalational exposure of rats. Overall 1,4-dichlorobut-2-ene is mutagenic *in vitro* and there are some indications for a possible clastogenic activity *in vivo*.

1,4-Dichlorobut-2-ene has shown a tumorigenic activity in rats after chronic inhalation exposure leading to the dose-dependent increase of the incidence of benign and malignant nasal tumors. In studies with dermal application of 1,4-dichlorobut-2-ene to mice there is no indication for a tumorigenic potential at the skin. A retrospective cohort study gave no suspicion for any increased cancer risk of exposed employees. Due to the small cohort size no firm conclusion can be drawn concerning the cancer risk to humans exposed to 1,4-dichlorobut-2-ene.

There are no valid studies available concerning possible impairment of fertility by 1,4-dichlorobut-2-ene. From chronic inhalation studies with rats there are no indications for pathological changes of the male and female sex organs due to 1,4-dichlorobut-2-ene exposure. In a developmental toxicity study with rats 1,4-dichlorobut-2-ene showed no embryotoxic or teratogenic potential. The NOAEC for maternal toxicity is 2.6 mg/m^3 based on reduced body weight gain at 26 mg/m^3 and the NOAEC for developmental toxicity is 26 mg/m^3 (highest dose tested). Overall, 1,4-dichlorobut-2-ene is not anticipated to pose a hazard to fertility and has no specific effect on embryonic or fetal development.

Environment

1,4-Dichlorobut-2-ene is a yellowish liquid. The melting points are –48 (*cis*-isomer), 1 °C (*trans*-isomer), and between –48 °C and 1 °C for the mixture. The boiling points at 1013 hPa are 156 (mixture), 152.5 (*cis*-isomer), and 156.1 °C (*trans*-isomer). 1,4-Dichlorobut-2-ene (mixture) has a density of 1.189 g/cm^3 at 25 °C. The *cis*-isomer has a relative density of 1.188, and the *trans*-isomer of 1.183, both at 25 °C. The measured vapor pressure of the isomers mixture is 15.9 hPa, of the *cis*-isomer 4.4 hPa, and of the *trans*-isomer 3.9 hPa, all at 25 °C. The measured log K_{ow} of the *trans*-isomer is 2.18, calculated values for both isomers are 2.6. The solubility of the isomers mixture in water is 1.24 g/l at 20 °C, of the *cis*-isomer 0.58 g/l at 25 °C, and of the *trans*-isomer 0.85 g/l at 25 °C. The flash points are 59 °C (mixture), 49.9 °C (*cis*-isomer), and 53 °C *(trans*-isomer). The auto flammability (ignition temperature) is approx. 465 °C. 1,4-Dichlorobut-2-ene is flammable.

In the atmosphere 1,4-dichlorobut-2-ene is degraded by photochemically produced OH radicals. The half-life is calculated to be 12 hours for the *cis*-isomer and 10 hours for the *trans*-isomer. Due to the low absorption in the UV-B range, no direct photodegradation is expected. In a direct photodegradation experiment in demineralized water a half-life of 1 - 3 h was obtained. Under the same conditions, but in the presence of added hydrogen peroxide, the half-life decreased to $t_{½}$ < 30 minutes.
1,4-Dichlorobut-2-ene hydrolyzes in water forming organic hydrolysis products (e.g. 2,5-dihydrofuran) and hydrochloric acid. Hydrolysis half-lives of 1,4-dichlorobut-2-ene were measured as 3.2 days under neutral conditions, suggesting that hydrolysis may be an important fate process in moist soils and water.

According to a Mackay Level I calculation the favorite target compartment of 1,4-dichlorobut-2-ene (mixture and isomers) is air, with 98.1 % of the mixture in the gas phase. Henry's Law Constants, relating to the mixture, *cis*-, and *trans*-isomers of 1905 Pa m³/mol were calculated according to the Bond method, and of 54.2 Pa m^3/mol according to the Group-method. Henry's Law Constants of 57.4 - 160.3 Pa m³/mol were calculated from the ratio of the vapor pressure to the water solubility, respectively, indicating that the compounds have a high potential for volatilization from surface waters.
1,4-Dichlorobut-2-ene is not readily biodegradable. A closed bottle test in all essential parts identical with OECD TG 301 D was performed under GLP with a concentration of 1,4-dichlorobut-2-ene of 5.5 mg/l. After 28 days 20 % of the test substance had been biodegraded. In a closed bottle test, comparable to the OECD TG 301 D performed with a concentration of 1,4-dichlorobut-2-ene of 6.2 mg/l, no biodegradation was observed after 28 days.
The bioconcentration factor (BCF) of 9.5 for 1,4-dichlorobut-2-ene (mixture, *cis*-, and *trans*-isomers), calculated from the octanol-water partition coefficient, indicates that there is a low potential for bioaccumulation in aquatic organisms.
With PCKOCWIN v. 1.66 a K_{oc} of 149 for 1,4-dichlorobut-2-ene (mixture, *cis*-, and *trans*-isomers) is calculated. In addition, an adsorption coefficient (K_{oc}) of 215 was obtained experimentally for *cis*-1,4-dichlorobut-2-ene. These results indicate that 1,4-dichlorobut-2-ene is supposed to have a moderate accumulation potential in soil. However, due to hydrolysis and volatilization, accumulation in soil is not expected.

Concerning the aquatic toxicity of 1,4-dichlorobut-2-ene there are acute test results available. The lowest reliable effect values for aquatic species with 1,4-dichlorobut-2-ene towards fish, *Daphnia*, and algae are (n = nominal concentration; m = measured concentration):

Poecilia reticulata (fish):	14 d-LC_{50}	=	0.086 mg/l (n)
Daphnia magna (invertebrates):	48 h-EC_{50}	=	0.156 mg/l (m)
Desmodesmus subspicatus (algae)	72 h-$EC_{50Growth\ rate}$	=	2.13 mg/l (m)

For microorganisms the lowest available toxicity value determined was 3 h-EC_{50} of 573 mg/l (n) (activated sludge).
Since acute test results for 1,4-dichlorobut-2-ene for three trophic levels are available, an assessment factor of 1000 was applied for the derivation of the $PNEC_{aqua}$ according to the EU Technical Guidance Document. The lowest effect concentration was found for the fish species *Poecilia reticulata*, 14 d-LC_{50} of 0.086 mg/l effect concentration,

therefore resulting in a $PNEC_{aqua}$ = 0.086 µg/l.

Exposure

1,4-Dichlorobut-2-ene is manufactured by chlorination of butadiene in closed systems. For 2002, the following 1,4-dichlorobut-2-ene manufacturing capacities were estimated:

USA	68 000 tonnes/a	(1 manufacturer)
EU	71 000 tonnes/a	(2 manufacturers)
Japan	67 000 tonnes/a	(3 manufacturers)
Armenia	3000 tonnes/a	(1 manufacturer)
China	no capacity data available	(2 manufacturers)
Global	> 209 000 tonnes/a	(9 manufacturers).

In Germany, the only manufacturer of 1,4-dichlorobut-2-ene has a manufacturing capacity of 10 000 - 50 000 tonnes/a and processes all products at the same site. 1,4-Dichlorobut-2-ene is used as an intermediate in chemical processes. Like 3,4-dichloro-1-butene, it is an intermediate in the manufacturing of chloroprene, furthermore a starting material in the production of 3-hexenedinitril (which can be hydrogenated to adiponitril, a hexamethylenediamine intermediate), butane-1,4-diole, tetrahydrofuran, and tetrachlorobutane. Essentially 100 % of the manufacturing volume is used for the production of 3,4-dichloro-1-butene and adiponitril.

In the Sponsor country 1,4-dichlorobut-2-ene is manufactured continuously and processed in closed systems. During manufacturing and processing, virtually no 1,4-dichlorobut-2-ene was emitted into the atmosphere (< 25 kg) and into the aquatic environment in 2004.
Due to the high volatility of the substance, occupational exposure to 1,4-dichlorobut-2-ene may occur through inhalation. In the Sponsor country, exposure is well controlled in occupational settings.

1,4-Dichlorobut-2-ene is not listed in the Nordic and Swiss Product Registers. There is no known route of consumer exposure via the environment. Since no consumer products are known to contain 1,4-dichlorobut-2-ene, consumer exposure to 1,4-dichlorobut-2-ene is not likely to occur.

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

Human Health: The substance is currently of low priority for further work. The chemical possesses properties indicating a hazard for human health (acute toxicity, repeated dose toxicity, skin and eye irritation, genotoxicity, carcinogenicity). Based on data presented by the Sponsor country (relating to production by 1 producer which accounts for approximately 5 % to 24 % of global production and relating to the use pattern in several OECD countries), adequate risk management measures are being applied in occupational settings and exposure of consumers is negligible. Countries may desire to check their own risk management measures to find out whether there is a need for additional measures.

Environment: The chemical possesses properties indicating a hazard for the environment (acute toxicity to fish, algae, and invertebrates). Based on data presented by the Sponsor country (relating to production by 1 producer which accounts for approximately 5 % to 24 % of global production and relating to the use pattern in several OECD countries), emissions into the environment are anticipated to be low. Therefore this chemical is currently of low priority for further work. Countries may desire to investigate any exposure scenarios that were not presented by the Sponsor country.