SIDS INITIAL ASSESSMENT PROFILE

CAS No.	1653-19-6
Chemical Name	2,3-Dichlorobuta-1,3-diene
Structural Formula	$CH_2=CCl-CCl=CH_2$

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

There are no studies available concerning toxicokinetics, metabolism, and distribution of 2,3-dichlorobuta-1,3-diene. Results from toxicity studies with experimental animals show that 2,3-dichlorobuta-1,3-diene is absorbed after inhalation as well as after oral and dermal application.

2,3-Dichlorobuta-1,3-diene is moderately toxic after acute inhalation exposure with an LC_{50} of 408 ppm (2080 mg/m^3)/4 h in rats. After 2 hours exposure the LC_{50} has been calculated as 931 ppm (4750 mg/m^3) for rats and 145 ppm (740 mg/m^3) for mice in a study with limited documentation. There are no dermal LD_{50} data available but limited studies in rats, mice, and rabbits provide evidence for systemic toxicity after dermal application. The oral LD_{50} has been determined as 222 mg/kg bw for rats and 110 mg/kg bw for mice in a study with limited documentation; target organs are the stomach due to the irritant nature of the substance as well as spleen, liver, and kidney.

A 50 % solution of 2,3-dichlorobuta-1,3-diene is not corrosive to the skin of rabbits (4°hours, occlusion). However, data from two unreliable studies suggest that 2,3-dichlorobuta-1,3-diene is irritating to the skin of rabbits. There are no valid studies on eye irritation available. However, according to data given in a monograph, 2,3-dichlorobuta-1,3-diene is irritating to the eyes of rabbits. 2,3-Dichlorobuta-1,3-diene is irritating to the respiratory tract.
There are no data available concerning sensitization.

There are no valid dermal or oral repeat dose studies and no standard repeat dose inhalation studies in experimental animals available. However, in the context of a one generation study with 11 weeks of whole body exposure of rats to 2,3-dichlorobuta-1,3-diene vapor it was possible to identify a NOAEC for general toxicity of 5 ppm (25.5 mg/m^3), at the LOAEC of 50 ppm (255 mg/m^3) decreases in body weight, and food efficiency as well as minimal to mild degeneration and regeneration of the nasal olfactory epithelium associated with mild to moderate atrophy of Bowman's glands are observed. Males show generally more severe nasal lesions than pregnant females, which had a 14-day recovery period. The same LOAEC of 50 ppm (255 mg/m^3) is found in a subacute range-finding inhalation study, associated with the one generation reproduction toxicity study, with rats; due to deficiencies in study design it is not possible to define a clear NOAEC from this study. Due to the fact that the substance is a chemical intermediate being manufactured and processed in closed systems exposure to the chemical is negligible. Therefore more in depth examinations of repeated dose toxicity of this substance are not warranted.
In humans occupational exposure to 2,3-dichlorobuta-1,3-diene in concentrations of $\leq$ 2 ppm ($\leq$ 10.2 mg/m^3) is probably not linked to possible health hazards like cardiovascular diseases and respiratory problems.

2,3-Dichlorobuta-1,3-diene is mutagenic in bacteria with and without addition of a metabolic activation system. In a micronucleus assay performed according to OECD TG 474 2,3-dichlorobuta-1,3-diene shows no clastogenic activity *in vivo* after whole body exposure of rats to vapor concentrations of up to 200 ppm (1020 mg/m^3). Overall, 2,3-dichlorobuta-1,3-diene shows a mutagenic activity *in vitro*.

There are no animal carcinogenicity studies with 2,3-dichlorobuta-1,3-diene available. A retrospective cohort mortality study with men occupationally exposed to 2,3-dichlorobuta-1,3-diene during chloroprene production showed no higher risk for them of dying from lung cancer or other causes than the general population. However, these results were based upon a relatively small number of workers and there may not have been sufficient

statistical power to detect an excess mortality risk, if it had existed.

In a one-generation reproduction toxicity study (OECD TG 415) in rats 2,3-dichlorobuta-1,3-diene shows no impairment of fertility and no adverse effects on the fetus after exposure of the parental generation up to parentally toxic concentrations. The NOAEC for reproductive toxicity and early embryonic development is 50 ppm (255 mg/m^3; highest concentration tested) and the NOAEC for toxic effects in P1 rats is 5 ppm (25.5 mg/m^3) after 11 weeks inhalation exposure to 2,3-dichlorobuta-1,3-diene. In a teratogenicity study (OECD TG 414) 2,3-dichlorobuta-1,3-diene leads to embryotoxic effects (decreased fetal weight) in the presence of clear maternal toxicity (decreases in maternal body weight, body weight gain and food consumption as well as clinical signs of toxicity during exposure) at the highest concentration tested (50 ppm = 255 mg/m^3). Therefore the maternal and fetal NOAECs were both considered to be 10 ppm (51 mg/m^3). Overall, 2,3-dichlorobuta-1,3-diene shows no specific effects on fertility or embryonic or fetal development.

Environment

2,3-Dichlorobuta-1,3-diene is a colorless to yellowish, water sensitive liquid with a melting point of –40 °C and a boiling point of 98 °C at 1013 hPa. 2,3-Dichlorobuta-1,3-diene has a relative density of 1.1829 at 20 °C and a vapor pressure of ca. 132.7 hPa at 25 °C. The calculated log K_{OW} is 3.02. The flash point is 13 °C, the auto flammability (ignition temperature) is ca. 420 °C.

2,3-Dichlorobuta-1,3-diene hydrolyzes in water at 50 °C with a half-life of 1.2 hours, forming short chain alcohols and ketones and hydrochloric acid. In the atmosphere 2,3-dichlorobuta-1,3-diene is degraded by photochemically produced OH radicals. The half-life is calculated to be about 3 days.
According to the Mackay fugacity model Level I, the favorite target compartment of the 2,3-dichlorobuta-1,3-diene is air with 99.93 %. The calculated value reflects the properties of the undissociated molecule without taking into account the sensitivity of 2,3-dichlorobuta-1,3-diene towards hydrolysis. A high volatility from water is indicated by the calculated Henry's law constant of 5.16 x 10^3 Pa m^3/mol at 25 °C.
2,3-Dichlorobuta-1,3-diene is not readily biodegradable as conducted in a respirometry test corresponding to OECD TG 301F with an elimination rate of 1 %.
The bioconcentration factor (BCF) of 42, calculated from the octanol-water partition coefficient, for 2,3-dichlorobuta-1,3-diene, and the low octanol-water partition coefficients for both presumed organic hydrolysis products (calculated log K_{OW} of 0.67 and -1.34 for 2,3-dihydroxybuta-1,3-diene and 2,3-butanedione, respectively), indicate a low potential for bioaccumulation of these compounds. A K_{OC} value of 107 was calculated with PCKOCWIN v. 1.66 suggesting a low sorption potential of 2,3-dichlorobuta-1,3-diene onto the organic phase of soil or sediments.

The lowest reliable toxicity values for aquatic species are (n = nominal concentration; m = measured concentration; c = calculated concentration):

Danio rerio (fish):	96 h-LC_{50}	=	10 mg/l (n)
Fish (ECOSAR)	96 h-LC_{50}	=	0.6 mg/l (c)
Daphnia magna (invertebrates):	48 h-EC_{50}	=	1.5 mg/l (m)
		=	22 mg/l (n)
Desmodesmus subspicatus (algae):	72 h-$EC_{50\text{growth rate/biomass}}$	=	> 2.1 mg/l (m)
		=	> 100 mg/l (n).

For bacteria (activated sludge) the lowest available toxicity value determined was a 3 h-EC_{50} of 1700 mg/l (nominal). For the hydrolysis product 2,3-butanedione, a 40 h-EC_{50} of 146 mg/l was determined in the protozoa *Tetrahymena pyriformis* (documentation insufficient for assessment).
Since acute test results for 2,3-dichlorobuta-1,3-diene 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 of 1.5 mg/l was found for invertebrates (*Daphnia magna).* However, no analytical monitoring was performed during the fish test with this volatile and rapidly hydrolyzing test substance. To further complement the information for this endpoint, a QSAR calculation was performed which yielded an LC_{50} of 0.6 mg/l. By applying an assessment factor of 1000 on both the lowest measured and calculated concentrations, the $PNEC_{aqua}$ is predicted to be 0.6 µg/l to 1.5 µg/l.

Exposure

2,3-Dichlorobuta-1,3-diene is manufactured by elimination of hydrogen chloride of both 1,2,3,4-tetrachlorobutane and 2,3,4-trichlorobut-1-ene. There are no data on the global production volume of 2,3-dichlorobuta-1,3-diene,

however, the manufacturing volume is estimated to be 10 000 - 20 000 tons/a. In Germany, the only manufacturer of 2,3-dichlorobuta-1,3-diene has a manufacturing capacity of 1000 - 5000 tons/aand processes all products at the same site.

2,3-Dichlorobuta-1,3-diene is produced and processed in a closed system and is used only as a co-monomer in the manufacturing of polychloroprene rubbers at the production site. In the Sponsor country, these rubbers account for approximately 20 % of the total polychloroprene rubber production volume. No other use pattern is known in the Sponsor country. Depending on the desired quality, the 2,3-dichlorobuta-1,3-diene content of the polymerization mixture may reach up to 10 % of the monomers.

In the Sponsor country during manufacturing and processing in closed systems, virtually no 2,3-dichlorobuta-1,3-diene 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. In the Sponsor country, all 2,3-dichlorobuta-1,3-diene is processed on-site by the manufacturer into solid polychloroprene rubber types. 2,3-Dichlorobuta-1,3-diene is not detectable in these rubbers with a detection limit of 1 mg/kg.

2,3-Dichlorobuta-1,3-diene 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 2,3-dichlorobuta-1,3-diene, consumer exposure to 2,3-dichlorobuta-1,3-diene is not likely to occur.

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

Human Health: The chemical possesses properties indicating a hazard for human health (acute and subacute toxicity, irritation, *in vitro* mutagenicity). Based on data presented by the Sponsor country (relating to production by 1 producer which accounts for approximately 5 % to 50 % of global production and relating to the use pattern in several OECD countries), exposure is well controlled in occupational settings, and exposure of consumers is negligible. 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 and 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 50 % 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.