FOREWORD INTRODUCTION

1,4-DICYANOBUTANE

CAS N°: 111-69-3

SIDS INITIAL ASSESSMENT PROFILE

CAS Nr.	111-69-3
Chemical Name	1,4-Dicyanobutane
Structural formula	$N\equiv C\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}C\equiv N$

RECOMMENDATION OF THE SPONSOR COUNTRY

presently of low priority for further work

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE RECOMMENDATIONS

The worldwide production volume of 1,4-Dicyanobutane is ca. 500 000 - 1 000 000 t/a. It is a chemical intermediate, mainly for the production of hexamethylenediamine. 1,4-Dicyanobutane is stable in neutral solution and is classified as "inherently biodegradable" with a "low bioaccumulation potential". The most sensitive environmental species to 1,4-Dicyanobutane is the fish *Leuciscus idus* (48h-LC50 = 384 mg/l).

The lowest acute oral, dermal and inhalation LD(C)50 are 20 mg/kg (rabbit), >2000 mg/kg (rat & rabbit) and 1.71 mg/l/4h respectively. The NOEL in a 13w inhalation study in rats was determined as 0.030 mg/l.
1,4-Dicyanobutane is considered as a slight irritant to the eye. It did not show any genotoxic effets in bacterial and non-bacterial tests in vitro as well as in a chromosomal aberration test in vivo.
Fertility of rats was not affected after inhalational exposure of up to 0.1 mg/l (22 days for females; 74 days for males). Oral administration of up to 80 mg/kg/d did not induce teratogenic responses.

The aquatic local PEC due to its use as a chemical intermediate is estimated to be 108 µg/l, based on a "worst-case" scenario. In conclusion, 1,4-Dicyanobutane presently represents no risk to the environment.
1,4-Dicyanobutane is only produced and transformed in closed systems. Exposure measurements in several plants confirm negligible exposure. It therefore presently presents no concern for humans.

IF FURTHER WORK IS RECOMMENDED, SUMMARISE ITS NATURE

none

SIDS SUMMARY

1,4-Dicyanobutane

CAS-NO.: 111-69-3			PROTOCOL	RESULTS
PHYSICAL CHEMICAL				
2.1	Melting-Point		NA	1°C
2.2	Boiling-Point		NA	295°C (at 101.3 kPa)
2.3	Density		NA	ca. 965 kg/m^3
2.4	Vapour Pressure		NA	0.33 Pa at 25°C
2.5	Partition Coefficient (Log Pow)		exp.	-0.32
2.6 A	Water solubility		NA	83 g/l at 20°C
B	pH		/	at °C
	pKa		/	/
2.12	Oxidation : Reduction potential		/	mV
ENVIRONMENTAL FATE / BIODEGRADATION				
3.1.1	Photodegradation		calc. (Atkinson)	In air $T_{1/2}$ = 11.6 days
3.1.2	Stability in water		EEC/67/548 (GLP)	$T_{1/2}$ > 1 year
3.2	Monitoring data			In air = / mg/m^3 In surface water = < 0.01 µg/l In soil / sediment = < 0.3 µg/g In biota = / µg/g
3.5	Biodegradation		OECD 301 C	35-43% (NO_2) 53-66% (NH_3)
ECOTOXICOLOGY				
4.1	acute/prolonged toxicity to fish	Pimephales promelas	APHA	LC_{50} (96 hr) = 1930 mg/l
		Leuciscus idus	DIN 38412 part 15	LC_{50} (48 hr) = 384 mg/l
4.2	acute/prolonged toxicity to aquatic invertebrates (daphnia)	Daphnia magna	DIN 38412 part 11	EC_{50} (24 hr) = 445 mg/l
4.3	toxicity to aquatic plants e. g. algae	Selenastrum capricornutum	EEC/67/548 (GLP)	EC_{50} (72 hr) = > 100 mg/l NOEC (72 hr) = 100 mg/l
4.4	toxicity to microorganisms	Pseudomonas putida	NA	EC_{10} (30 min) = 408 mg/l
4.5.1	chronic toxicity to fish			
4.6.1	toxicity to soil dwelling organisms			
4.6.2	toxicity to terrestrial plants			

SIDS SUMMARY

1,4-Dicyanobutane

CAS-NO.: 76-03-9		SPECIES	PROTOCOL	RESULTS
TOXICOLOGY				
5.1.1	acute oral toxicity	rat rabbit	NA NA	LD_{50} = 138 – 300 mg/kg LD_{50} = 19 – 22 mg/kg
5.1.2	acute inhalation toxicity	rat	NA	$LC_{50\ (4h)}$ = 1.71 - 2.0 mg/l
5.1.3	acute dermal toxicity	rabbit	NA	LD_{50} = > 2000 mg/kg
5.4	repeated dose toxicity	rat	inhal.; 6h/d; 5d exp; 2d w/out exp; 5d exp	NOEL = 0.03 mg/l
		rat	inhal.; 6h/d; 5d/w; 4w	NOEL = 0.033 mg/l(males) NOEL = 0.064 mg/l(females)
		rat	inhal.; 6h/d; 5d/w; 13w	NOEL = 0.031 mg/l
5.5	genetic toxicity in vitro			
	bacterial test (gen mutation)		Ames/OECD 471	- (with and without metabolic activation)
	non bacterial in vitro test	mice lymphoma	OECD 476	- (with and without metabolic activation)
		rat hepatocytes	OECD 482	- (with and without metabolic activation)
5.6	genetic toxicity in vivo (chrom. aberr.)	rat	OECD 475	negative
5.8	toxicity to reproduction	rat	inhal.; 13, 31.8 & 104 mg/m3; 22d (GLP)	no effect on female fertility
		rat	inhal.; 12.9, 30.6 & 99 mg/m3; 74d (GLP)	no effect on male fertility
5.9	developmental toxicity / teratogenicity	rat	oral; 30, 50 & 80 mg/kg/d, days 6 through 19 of gestation (GLP)	NOEL = 80 mg/kg (F1) NOEL = 30 mg/kg (P)
5.11	experience with human exposure			Human skin irritation observed due to accidental exposure

SIDS INITIAL ASSESSMENT REPORT

1. GENERAL SUBSTANCE INFORMATION

Identity

Chemical name: 1,4-Dicyanobutane

CAS-Nr.: 111-69-3

EINECS Nr.: 203-896-2

Synonyms Adiponitrile

Empirical Formula: $C_6H_8N_2$

Structural Formula: $N\equiv C\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}C\equiv N$

Purity: > 90 - 99.9 %

Physico-chemical properties

Adiponitrile is a stable, colourless liquid (melting point 1 ℃; boiling point 295 ℃), highly soluble in water (83 g/l) and with a low vapour pressure (0.3 Pa at 20℃).

2. GENERAL INFORMATION ON EXPOSURE

There are only 4 major producers/importers within the EU. The production volume in the EU is ca. 100 000 to 500 000 t/a. The manufacturing capacity in the USA (3 production sites) was 641 000 t/a in 1995 (US-EPA, 1996). The worldwide production is estimated to be less than 1 000 000 t/a.
The only identified use of adiponitrile is as an intermediate, mainly for the production of hexamethylenediamine, which is used for the manufacture of Polyamide 6-6 (for the risk assessment of hexamethylenediamine, CAS Nr 124-09-4 see OECD-SIAR prepared by Canada). Furthermore, adiponitrile is used as an intermediate for the synthesis of adipoguanamine, corrosion inhibitors and rubber accelerators (US-EPA, 1996). A US survey of occupational exposure revealed that 1 - 970 workers are potentially exposed in the USA at 1 - 9 facilities (US-EPA, 1996).

Production

Adiponitrile is obtained by the reaction of butadiene on cyanhydric acid:

butadiene + cyanhydric acid → pentene nitrile

pentene nitrile + cyanhydric acid → adiponitrile + methyl glutoro nitrile

Because of the high toxicity of the raw materials used, a full containment system (closed system) is in place at the French production sites. There are no aqueous emissions. All the reaction by-products are incinerated. The production of adiponitrile is continuous and the sysnthesis is stopped every 2 years for control. All the exposure controls of ambient air at the production site were below the detection level.

A continuous monitoring of the raw material emissions i.e. cyanhydric acid also demonstrated a non-exposure to the products used.

Transformation

Adiponitrile is an intermediate for the synthesis of hexamethylenediamine (diamino-1,6-hexane). Adiponitrile in the presence of an hydrogen catalyst is reduced to hexamethylene diamine:

$$N{\equiv}C\text{-}(CH_2)_4\text{-}C{\equiv}N \xrightarrow{H_2} H_2N\text{-}(CH_2)_6\text{-}NH_2 + H_2O$$

From the French transformation unit, the following data is available:

- adiponitrile is entirely transformed during the reaction;
- no emissions of adiponitrile occur during the process;
- as the water from the dehydration step contains some hexamethylenediamine derivatives, this residue is incinerated as well;
- the water used to clean the filters and the reactor are rejected to the waste water treatment plant;
- the process is continuous and the synthesis is stopped every 18 months to 2 years for control.

At another European production/transformation site the estimated releases to surface water after treatment are 5 - 8 t/a.

Transport

Half of the production volume leaves the French production plant for transformation at other French or European processing sites. Adiponitrile is transported in dedicated containers or tanks. It is loaded under nitrogen. There is no vapour emission. On the processing site, the dedicated tanks are unloaded in nitrogen inerted stockers. Airtight pumps and piping link stockers and reactors.

3. ENVIRONMENT

3.1 Exposure assessment

3.1.0 General discussion

Release into the environment

As shown above, release into the environment of adiponitrile during production should be negligible, as no aqueous emissions occur. During transformation of the substance to hexamethylene diamine, emission with waste water appears to be possible, as it cannot be assumed that the waste water is incinerated at each processing site. Therefore, a worst case exposure scenario for processing will be developed below (see section 3.1.1).

Degradation

Hydrolysis

Adiponitrile is stable to hydrolysis at pH 4, 7 and 9 over 5 days at 50℃. Hydrolysis will not be an important fate process.

Biodegradation

A test result on ready biodegradation is available:

- MITI-I-Test (OECD GL 301 C): 53 - 66% degradation after 28 days (ThOD calculated for NH3-stage). There is not enough information available (e.g. lag-time) to determine whether the 10-day window criterion was fulfilled or not. In the absence of further data it has to be assumed that the 10-day window was not reached.

Adiponitrile has therefore to be considered as **inherently biodegradable** in the aquatic compartment. Furthermore, results from non standard tests are available which confirm this result.

Results from biodegradation simulation tests in WWTPs, in surface water and soil are not available and have to be estimated based on the above described screening test and the partition behaviour of Adiponitrile (EC, 1994):

compartment / medium	**biodegradation rate**
activated sludge (WWTP)	$k_{WWTP} = 0.3\ h^{-1}$
surface water	$k_{sw} = 0.014\ d^{-1}$
sediment	$k_{sed} = 0.014\ d^{-1}$
soil	$k_{soil} = 1.4\ d^{-1}$

Photooxidation

In the atmosphere, Adiponitrile will react with the photochemically produced hydroxyl radicals. Based upon atmospheric concentrations of $5 \cdot 10^5$ ·OH/cm^3 the atmospheric half-life of Adiponitrile has been estimated to be 11.6 days.

Distribution and accumulation

The Henry's law constant of $H = 7 \cdot 10^{-4}$ Pa.m^3/mol at 25 ℃ suggests that Adiponitrile is non volatile.
No test on soil adsorption has been performed. The low logPow-value of -0.32 suggests that the compound is highly mobile in soil and that it has no potential for accumulation in soil.
There are no experimental results on bioaccumulation available. The measured logPow of -0.32 indicates a low potential for bioaccumulation.
Based on the physical chemical properties of Adiponitrile, the hydrosphere is the preferred target compartment.

Elimination in WWTPs

Based on the above cited physical chemical properties (log H = -3; $logP_{ow}$ = -0.32), as well as the biodegradation rate of 0.3 h^{-1} in WWTP, the elimination through biodegradation and distribution can be estimated with the model SIMPLETREAT:

% to air	0
% to water	24
% to sludge	0
% degraded	76
% removal	76

3.1.1 Aquatic compartment (incl. sediment)

3.1.1.1 Production and transformation

As shown above, there are no aqueous releases during production. Releases during chemical transformation to hexamethylenediamine seem nevertheless to be possible.

In the Technical Guidance Document for New Chemicals (EC, 1993), a generic (i.e. non site-specific) exposure scenario ("use category document",UCD) for the release into surface water of intermediates during production and processing is proposed. This scenario reflects a realistic worst case situation:

Production volume: 100 000 t/a (highest volume indicated in IUCLID)
Release fraction during processing: 0.7% (default)
Yearly duration of operation: 300 days (default)
Removal in WWTP: 76% (SIMPLETREAT, see above)
Flow of receiving river: 60 m^3/s (default)

With these "worst case" default parameters, a **PEC_{local} of 108 µg/l** in surface water can be calculated.

With a release of 5 - 8 t/a as indicated by one producer/transformer and using the above scenario, a **PEC_{local} of 3.2 - 5.1 µg/l** in surface water can be calculated.

3.1.1.2 Monitoring data

Adiponitrile was not detected in surface water in Japan in 1978 (21 samples) at a detection limit of 10 **µ**g/l.

3.1.1.3 Sediment

Adiponitrile has a low tendency to partition to the sediment. It was not detected in sediment in Japan in 1978 (21 samples) at a detection limit of 0.1 - 0.3 mg/kg. Furthermore, as no experimental results with benthic organisms are available, there is no need for performing a risk assessment for this compartment.

3.1.2 Terrestrial compartment

Direct releases to soil are not to expected. Indirect releases through atmospheric deposition and sewage sludge application can be considered as negligible.

3.1.3 Atmosphere

Due to the low vapour pressure (<1 Pa), the releases to the atmosphere during production and processing can be considered to be negligible.

3.1.4 Non compartment specific exposure relevant to the food chain (secondary poisoning)

As adiponitrile has a low potential for bioaccumulation ($\log P_{ow}$ = -0.38), a risk characterisation for secondary poisoning is not necessary.

3.1.5 Regional concentrations

As there exist only very few possible point sources, it is not opportune to determine a background concentration.

3.2 Effects assessment: Hazard identification and Dose (concentration) - response (effect) assessment

3.2.1 Aquatic compartment (incl. sediment)

Available effect data

In the following, the most relevant results from acute toxicity tests with aquatic organisms are presented:

vertebrates:

Lepomis macrochirus (static, nominal concentration)	96h-LC50	720 mg/l
Onchorynchus mykiss (static; nominal concentration)	96h-LC50	670 mg/l
Leuciscus idus (static, nominal concentration)	48h-LC50	384 mg/l

invertebrates:

Daphnia magna (effect: immobilization; static, nominal concentration)	24h-EC50	445 mg/l

plants:

Selenastrum capricornutum	72h-EC50	> 100 mg/l
	72h-NOEC	≥ 100 mg/l

(no effect on biomass or growth rate at 100 mg/l)

bacteria:

Pseudomonas putida (effect: inhibition of O2 consumption; nominal concentrations)	30min-EC10	408 mg/l

Other test results are available, which confirm the above reported values.

Determination of $PNEC_{aqua}$

Results from acute tests with species from 3 trophic levels are available. The lowest acute toxicity was recorded with fish (*Leuciscus idus:* 48h-LC50 = 384 mg/l), assuming that the EC50 for algae is not reached at that concentration. As results from long-term tests with fish and daphnids are not available, the assessment factor is set at F = 1000.

Therefore: **$PNEC_{aqua}$ = 384 000 / 1000 = 384 µg/l.**

Determination of $PNEC_{microorganisms}$

The procedure described in the TGD (EC, 1994) for a determination of a $PNEC_{microorganisms}$ is not very clear. On one hand the different sensitivities of standard tests are stated and the assessment factor is to be chosen in a range of 10 to 100. On the other hand an assessment factor of 10 is to be applied to the NOEC from the least sensitive test (OECD 209), rending the ranking of the different tests superfluous.

For Adiponitrile, only a 3h-NOEC with *Pseudomonas putida* is available. Awaiting the clarification of the above stated inconsistencies, an assessment factor of 100 is proposed for this kind of test result.

Therefore: $\mathbf{PNEC_{microorganisms} = 408 / 100 = 4.1\ mg/l.}$

Sediment

No experimental results with benthic organisms are available. As adiponitrile has a low tendency to partition to the sediment, there is no need for performing a risk assessment for this compartment.

3.2.2 Terrestrial compartment

Data on effects to terrestrial organisms are not available.

3.2.3 Atmosphere

No data are available.

3.2.4 Non compartment specific exposure relevant to the food chain (secondary poisoning)

As adiponitrile has a low potential for bioaccumulation (logPow = -0.38), a risk characterisation for secondary poisoning is not necessary.

3.3 Risk characterisation

3.3.1 Aquatic compartment (incl. sediment)

Waste water treatment plants

An evaluation of the inhibition to microorganisms in WWTPs would seem opportune only for those situations where adiponitrile-containing waste water is released to domestic treatment plants, excluding therefore the production and processing sites which usually have their own treatment plan.

Surface waters

For the potential releases during production and transformation of adiponitrile into surface water, the following PEC/PNEC ratio can be deduced:

$$\mathbf{PEC_{local\_aqua}/PNEC_{aqua}} = 108/\ 384 = \mathbf{0.28}$$

As PEC/PNEC < 1, the substance does not present a risk to the aquatic compartment.

Furthermore, using the releases indicated by one of the producers/transformers, a maximum PEC/PNEC ratio of 5.1/384 = 0.013 can be deduced.

Sediment

Adiponitrile has a low tendency to partition to the sediment. It was not detected in sediment in Japan in 1978 (21 samples) at a detection limit of 0.1 - 0.3 mg/kg. Furthermore, as no experimental results with benthic organisms are available, there is no need for performing a risk assessment for this compartment.

3.3.2 Terrestrial compartment

No immediate concern.

3.3.3 Atmosphere

No immediate concern.

3.3.4 Non compartment specific exposure relevant to the food chain (secondary poisoning)

No immediate concern.

4. HUMAN EXPOSURE

4.1. Human Health (toxicity)

4.1.1. Exposure assessment

4.1.1.0. General discussion

Adiponitrile is obtained by the reaction of butadiene on cyanhydric acid. Because of the high toxicity of the raw materials used a full containment system (closed system) is in place. At the French production site, all the by-products synthesized during the reaction are incinerated. Adiponitrile is an intermediate for the synthesis of hexamethylene diamine (diamino-1,6 hexane) which is used in the manufacture of Polyamide 6-6.

4.1.1.1. Occupational exposure

Production
At the French production site, sampling is made 3 times a day by 3 different operators corresponding to 3 eight hours shifts. Sampling is made automatically. All the atmosphere exposure controls carried out up to now were below the detection level (< 0.1 mg/m^3) at the Adiponitrile sampling location indicating no actual exposure to Adiponitrile. A continuous monitoring of the raw material emissions i.e. cyanhydric acid also demonstrated a non-exposure to the products used.
During maintenance specific procedures are adopted to protect people. The synthesis is stopped every 2 years. If a partial interruption is necessary (pump maintenance for instance) similar procedures are applied. Cleaning water is drained for incineration. Should a spillage occur at any place of the plant (even if rain water is contaminated), the products are drained at the ground level and collected before incineration so that no environmental release may occur.

At a German production site, exposure measurements at workplace, even if relatively few values are available, showed exposure levels mainly below 0.10 ppm (TWA) (personal communication).

In the USA, a large number of exposure measurements (1980-1996) at workplace for several job classes at different areas in two plants also demonstrated low exposure levels below 0.1 ppm (personal communication, details of measurement-results have been provided)

Processing
Adiponitrile is an intermediate for the synthesis of hexamethylene diamine (diamino-1,6 hexane). Adiponitrile in the presence of an hydrogen catalyst is reduced to hexamethylene diamine. The whole process is performed in a closed system. **All the available Adiponitrile is transformed during the reaction.** Consequently no Adiponitrile emissions occur during the process.

Monitoring results are available from one European site. Adiponitrile is monitored 12 times a year. In 1995, the highest measured concentration was 0.06 ppm. Between January and August 1996, the highest measured concentration was 0.05 ppm.

4.1.1.2. Consumer exposure

The only identified use of Adiponitrile is as intermediate for the production of hexamethylène diamine which is used for the manufacture of Polyamide 6-6. Consequently consumer exposure is not relevant.

4.1.1.3. Indirect exposure via the environment

The only identified possible route of exposure via the environment is through drinking water processed from surface water. Assuming a worst-case concentration in surface water of 108 µg/l (see section 3.1.1.1), no elimination during processing of drinking water, a daily intake of 0.22 mg/d can be deduced with a dinking water consumption of 2 l/d. This would amount to 0.003 mg/kg bw/d, assuming a body-weight of 70 kg.

4.1.2. Effects assessment:

Hazard identification and dose (concentration) - response (effect) assessment

4.1.2.1 Animal data

Toxico-kinetics, metabolism and distribution

Adiponitrile when given orally to rats was rapidly absorbed and reached the tissues within one hour. The biological half-life was 21 hours. Adiponitrile did not appear to accumulate in any tissue; no detectable amounts of Adiponitrile were found in tissues analyzed 96 hours after dosing. Maximum excretion via the kidney occurred during 24-48 hours.
In guinea pigs Adiponitrile was metabolized to HCN and excreted in the urine as thiocyanate.

Acute toxicity

Acute oral toxicity LD50 in fasted and non fasted rat is respectively 138 and 300 mg/kg. The reported LD50 in rabbit is about 20 mg/kg.
Acute inhalation toxicity LC50 in rat is 1.71 mg/l/4h.
Acute dermal toxicity LD50 in rats or rabbits is above 2000 mg/kg.

Irritation

Adiponitrile is not considered as skin irritant in rabbit. It is considered as a slight irritant to the eye.

Sensitization

Results in guinea pigs did not show any sensitization potential.

Repeated dose toxicity

Rat	2 years	0.5, 5 and 50 ppm in drinking water	No NOEL determined
Rabbit	6 to 36 adm.	25, 10 mg/kg (orally)	No NOEL determined
Rat	6h/d, 5d/w, 4w	0 up to 0.49 mg/l (inhalation)	NOEL female 0.064mg/l NOEL male 0.033 mg/l
Rat	6h/d, 5d/w, 13w	0 up to 0.099 mg/l (inhalation)	NOEL 0.030 mg/l

Observations in these studies showed decreases in hemoglobin concentration and increases in urine and plasma thiocyanates indicating exposure to a cyano-compound. Neither gross nor microscopic lesions referrable to adiponitrile exposure were observed in any test animals. Males were more adversely and earlier affected by cyanide toxicity than females.

Mutagenicity

Salmonella typhimurium reverse mutation assay, Mouse Lymphoma assay(OECD 476), and Unscheduled DNA Synthesis (OECD 482) were negative in both presence or absence of appropriate metabolic activation system. In vivo mammalian Bone Marrow Cytogenetic assay (OECD 475) was negative as well.

Carcinogenicity

A two year oral rat study (drinking water) does not report tumor observation. Detailed data was not available; it was reported as such in the used documentation.

Toxicity for reproduction.

Fertility in female rat after inhalation exposure to 13, 31 or 104 mg/m^3, 6h/d for 22 days is not affected. Similar exposure of male rats for 74 days did not affect the fertility. Oral administration of 0, 30, 50 and 80 mg/kg/d on day 6 to 19 of pregnancy of rats did not induce teratogenic response. NOEL for offspring is 80 mg/kg/d

4.1.2.2 Human data

Because skin damage has been reported Adiponitrile will be considered as irritant in human.

4.1.3 Risk characterisation

4.1.3.0. General aspects

Oral and inhalation acute toxicity is reported in animal assays. Few reported human cases of skin irritation lead to consider Adiponitrile as irritant although such effects on acute dermal exposure are not observed in animals. Adiponitrile is considered as toxic and irritant accordingly.
A NOEL of 0.03 mg/l was derived from repeated dose toxicity tests (inhalation route).
No genotoxic effects were observed in any systems up to the maximum possible dose. No effects were observed on either male or female fertility. No teratogenic response was observed in treated females up to maternal toxic dose.
A TLV (TWA) of 2 ppm (8.8 mg/m^3) is recommended by the ACGIH.

4.1.3.1 Workers

Production and use of Adiponitrile is performed in a closed system. Very low exposure is confirmed by the atmosphere exposure controls which are below 0.1 mg/m^3. Under these conditions, the ratio to the TLV is greater than 20. Keeping in mind that the TLV (TWA) is calculated using safety factors of about 100, when referring to the NOEL of 0.03 mg/l (90d-inhalation), the margin of safety, compared to that level should be about 2000. Moreover, all effects observed at low doses are reversible when exposure stops. It is concluded that there is at present no need for further information and / or testing and for risk reduction measures beyond those which are being applied already.

4.1.3.2. Consumers

Consumer exposure is not relevant (see 4.1.1.2)

4.1.3.3 Man exposed indirectly via the environment

The estimated worst-case exposure of 0.003 mg/kg/d through drinking water is several orders of magnitude lower than the lowest determined NOEL and therefore, no risk can be deduced for the indirect exposure of man via the environment.

4.2 Human health (physico-chemical properties)

4.2.1. Exposure assessment

No specific exposure information available (closed system).

4.2.2 Effect assessment

4.2.2.1 Explosivity

Explosivity limits in the air : 1.7 to 5.0 %

4.2.2.2. Flammability

Auto inflammability is 500℃.

4.2.2.3. Oxidizing potential

No data

In addition Adiponitrile has a flash point of 159℃ and is of low volatility.

4.2.3 Risk characterisation

4.2.3.1 Workers

Synthesis or use conditions (closed system) and physico-chemical properties are such that no adverse effects are expected.

4.2.3.2. Consumers

Not applicable

4.2.3.3 Man exposed indirectly via the environment

Not applicable

5. RESULTS

Environment

Adiponitrile represents, based on the present data configuration, no concern to the environment. A PEC/PNEC ratio of 0.28, based on a "worst case" release scenario could be deduced for the aquatic

compartment. Based on the physical-chemical properties, the releases to soil and the atmosphere are considered to be negligible.

Human Health

Based on the toxicological data and human observations Adiponitrile is considered as an acutely toxic and irritant material. The available data shows that 1,4-Dicyanobutane is only produced and transformed in closed systems, and therefore present a low exposure potential to workers. Exposure measurements in several plants confirm the negligible exposure. Consequently, Adiponitrile presents no concern to humans.

6. References

- US-EPA, 1996, SIDS Data summary for Dicyanobutane (Adiponitrile), draft summary, May 15, 1996
- EC (European Comission), 1994, Risk Assessment of Existing Substances; Technical Guidance Document; Doc XI/919/94
- EC (European Comission), 1993, Risk Assessment of Notified New Substances; Technical Guidance Document