VERBAND DER CHEMISCHEN INDUSTRIE e.V.

REACH Praxisführer zur Expositionsbewertung und zur Kommunikation in den Lieferketten
Beispiele zu Teil II: Expositionsszenarien und Kommunikation in den Lieferketten

Beispiel 1: Stoffsicherheitsbericht Acetonitril

Dieses Beispiel veranschaulicht die Stoffsicherheitsbeurteilung für einen Stoff, zu dem viele Daten vorliegen. Auch öffentlich verfügbare Daten wurden für die Beurteilung verwendet.

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Wichtiger Hinweis für den Leser:

Dieses Beispiel eines Stoffsicherheitsberichtes ist vom Verfasser in einer Arbeitsgruppe des VCI erstellt worden als Teil des gemeinsamen Projektes von Cefic/VCI zur Entwicklung von Instrumenten und Leitfäden – für die Stoffsicherheitsbeurteilung, den Stoffsicherheitsbericht und für Expositionsszenarien.

Das vorliegende Dokument gehört zum Teil II des „REACH Praxisführers zur Expositionsbewertung und zur Kommunikation in den Lieferketten“. Der Praxisführer besteht aus mehreren Teilen. Eine Übersicht finden Sie im Vorwort zu Teil I.

Eine Beschreibung der Inhalte und des Praxisführers steht auf der folgenden Internetseite zur Verfügung:

VCI: http://www.vci.de/default~cmd~shd~docnr~125022~lastDokNr~102474.htm

Alle zugehörigen Materialien (inklusive der Projektbeispiele zu Teil II und III) können von dieser Seite heruntergeladen werden. Sie finden hier zusätzlich Hinweise zu verwandten Themen und neuen Entwicklungen.

Die englischsprachigen Veröffentlichungen zum Praxisführer finden Sie auf der folgenden Internet-Seite:

CEFIC: http://cefic.org/templates/shwPublications.asp?HID=750

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Wenn bei der Ausarbeitung des Beispieles Schwerpunkte gesetzt worden sind, wird hierauf jeweils gesondert hingewiesen.

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Note

This Chemical Safety Report is an **example** CSR prepared for the Verband der Chemischen Industrie (VCI) CSA/CSR/eSDS Project. Publicly available data was used to prepare this example CSR. Data was obtained from the European Risk Assessment Report on acetonitrile (2002) and the IUCLID dataset on acetonitrile (2000), downloadable from the website of the European Chemicals Bureau. The editor is aware that the used data may be owned by other parties. However, the editor considers the question of data ownership not relevant, as this example CSR is prepared for educational purposes only, not for commercial or regulatory purposes.

For the purpose of the mentioned project several simplifications to real life data/situations were adopted (e.g. only two uses were assessed), with the aim to focus on the educational value of the mentioned project. This document should only be used for the purpose of the VCI CSA/CSR/eSDS project and resulting publications.

CHEMICAL SAFETY REPORT

Substance Name: **Acetonitrile**

EC Number: **200-835-2**

CAS Number: **75-05-8**

Editors: **Dr. Stefan Konietzny and Dr. Christoph Müller**

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CONTENTS

PART A

1 SUMMARY OF RISK MANAGEMENT MEASURES

Manufacture	
Use 0: Production of Acetonitrile	Adequate personal protection equipment (gloves, goggles, and coverall, see SDS for details), local exhaustive ventilation, decontamination procedures before maintenance, wide use of automatic systems for sampling, information to workers on risk.
Own use / Downstream Uses	
Use 1: Starting material/solvent in chemical synthesis	Adequate personal protection equipment (gloves, goggles, and coverall, see SDS for details), local exhaustive ventilation, decontamination procedures before maintenance, wide use of automatic systems for sampling, information to workers on risk. In addition, regular workplace measurements are carried out to show that DNELs are not exceeded.
Use 2: Analytical laboratories	Adequate personal protection equipment (gloves, goggles, and coverall, see SDS for details), local exhaustive ventilation, decontamination procedures before maintenance, wide use of automatic systems for sampling, information to workers on risk. In addition, regular workplace measurements are carried out to show that DNELs are not exceeded.

2 DECLARATION THAT RISK MANAGEMENT MEASURES ARE IMPLEMENTED

Risk management measures (RMM) necessary to control the risk of exposure to acetonitrile are implemented. Organisational measures, such as regular workplace measurements, are implemented to ensure RMM efficiency and compliance of exposure with OELs and DNELs.

3 DECLARATION THAT RISK MANAGEMENT MEASURES ARE COMMUNICATED

RMM are communicated via the safety data sheets (SDSs). As soon as SDSs are replaced by extended SDSs (eSDSs), RMMs will be communicated to downstream users through the eSDSs.

PART B

1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Acetonitrile is a synthetic organic substance with following characteristics and physical–chemical properties (see the IUCLID dataset for further details).

1.1 Name and other identifiers of the substance

Table 1: Substance identity

EC number:	200-835-2
EC name:	Acetonitrile
CAS number (EC inventory):	75-05-8
CAS number:	75-05-8
CAS name:	Acetonitrile
IUPAC name:	Acetonitrile
Annex I index number	608-001-00-3
Molecular formula:	CH_3CN
Molecular weight:	41.05 g/mol
Structural formula:	CH_3CN

1.2 Composition of the substance

Degree of purity: 100 % (for the purpose of this example, a purity of 100 % is assumed)

1.3 Physico-chemical properties

Table 2: Summary of physico- chemical properties

Property	**Value**	**Remarks**
Physical state at 20°C and 101.3 kPa	Liquid	--
Melting/freezing point	- 45.7 °C	--
Boiling point	81.6 °C	at 1013 hPa
Relative density	0.786	at 20 °C
Vapour pressure	98.64 hPa	at 25 °C
Surface tension	29.04 dynes/cm	at 20 °C
Water solubility	Very soluble	--
Partition coefficient n-octanol/water (log value)	- 0.34	--
Flash point	2 °C 5 °C	closed cup open cup
Flammability	highly flammable	--
Explosive properties	Explosive limits (lower to upper): 3.05 – 17.00 % (v/v)	--
Self-ignition temperature	524 °C	--
Oxidising properties	not oxidising	--
Granulometry	not applicable	substance is a liquid
Stability in organic solvents and identity of relevant degradation products	no information available	--
Dissociation constant	pKa = 29.1	--
Viscosity	0.316 mPa s	at 25 °C
Auto flammability	See *Self-ignition temperature* above	--
Reactivity towards container material	unsuitable working materials: various plastics and rubber	--
Thermal stability	heat sensitive: decomposition	--
Henry's Law constant	2.91 Pa m^3 mol^{-1}	--

2 MANUFACTURE AND USES

2.1 Manufacture (Use 0)

Acetonitrile is mainly obtained as a by-product of acrylonitrile synthesis, by a method known as the SOHIO (Standard Oil Company of Ohio) process, which involves a high temperature catalytic reaction between propylene and ammonia and produces crude acrylonitrile containing acetonitrile, hydrogen cyanide and carbon oxides as the main impurities. Acetonitrile is obtained from the reaction product, after cooling, by fractional distillation.

A production volume of 2000 tonnes / year is assumed for this CSR example.

The processes involved in the acetonitrile production can be categorized by the descriptor system as follows:

Use 0: Manufacturing:

Sector of use:	SU3 “Industrial Manufacturing”
Product category:	Not applicable
Process category:	PROC1 “Used in closed processes, no likelihood of exposure; industrial setting”
	PROC2 “Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting”
	PROC3 “Use in closed continuous batch process (synthesis or formulation); industrial setting”
	PROC8: “Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non dedicated facilities; industrial or non-industrial setting”
Article category:	Not applicable
Environmental release category:	Not applicable (environmental exposure assessment is based on measured data)

2.2 Identified uses

Acetonitrile is used as a starting material for the synthesis of many chemicals (pharmaceutical, pesticides, photographic film). Acetonitrile is widely used in research and analytical laboratories. It is used as a solvent in the analytical determination of a great number of chemicals by high performance liquid chromatography (HPLC). Other uses are possible. However, this example CSR focuses on the uses in synthesis and in analytical laboratories.

Use	**Approximate percentage**
Use 1: Starting material/solvent in chemical synthesis	65
Use 2: Analytical laboratories (HPLC)	35

The uses of acetonitrile in the above fields can be categorised according to VCI Use and Exposure Categories (UEC) Matrix as illustrated below, based on the following prerequisites:

- For acetonitrile only industrial, but not professional or consumer uses are considered.
- There is no oral exposure and dermal exposure is considered negligible, as acetonitrile is only handled by trained workers wearing protective gloves.
- Short- and long-term inhalation exposure is considered relevant.
- Environmental emissions assessed in this CSR are continuous. Therefore, short term exposure to the environment is not assessed.
- The relevant compartments are aquatic environments. There is no direct release to soil.

VCI UEC Matrix for the uses of acetonitrile:

	Industrial	Professional	Consumer
Human: Oral, Short-term	1	2	3
Human: Oral Long-term / repeated	4	5	6
Human: Dermal Short-term	7	8	9
Human: Dermal Long-term / repeated	10	11	12
Human: Inhalation Short-term	13	14	15
Human: Inhalation Long-term / repeated	16	17	18
Environment: Water, single instance / Short-term	19	20	21
Environment: Water, continuous	22	23	24
Environment: Air, single instance / Short-term	25	26	27
Environment: Air, continuous	28	29	30
Environment: Soil, single instance/ Short-term	31	32	33
Environment: Soil, continuous	34	35	36

Use descriptions:

Use 1: Starting material/solvent in chemical synthesis:

Acetonitrile is used as a solvent or raw material in the chemical industry (mainly pharmaceutical industry). In general, acetonitrile is handled in closed systems. General processing duties include operating general pharmaceutical production equipment (reaction vessel, pipes and pumps).

According to the use descriptor system this use can be categorised as follows:

Sector of use: SU3 “Industrial Manufacturing”

Product category: Not applicable (the substance is not used in consumer products)

Process categories: PROC1 “Used in closed processes, no likelihood of exposure; industrial setting”

PROC2 “Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting”

PROC3 “Use in closed continuous batch process (synthesis or formulation); industrial setting”

Article category: Not applicable

Environmental release category: Not applicable (environmental exposure assessment is based on measured data)

Use 2: Analytical laboratories

Acetonitrile is used in analytical laboratories as a mobile phase in HPLC analyses. In general, acetonitrile is handled in closed systems. In rare cases small amounts (< 1 L, <1 kg) might be directly handled in a fume cupboard. General processing duties include operating general equipment (vessels, pipes and pumps).

According to the use descriptor system this use can be categorised as follows:

Sector of use: SUM71.2 “Technical testing and analysis”

Product category: PC21 “Laboratory chemicals”

Process categories: PROC1 “Used in closed processes, no likelihood of exposure; industrial setting”

PROC2 “Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting”

PROC3 “Use in closed continuous batch process (synthesis or formulation); industrial setting”3

PROC8: “Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non dedicated facilities Industrial or non-industrial setting”

PROC9 “Transfer of substance of preparation into small containers (dedicated filling line, including weighing); industrial setting”

PROC15 “Use as a laboratory reagent; non-industrial setting”

Article category: Not applicable (no articles are manufactured in analytical laboratories)

Environmental release category: Not applicable (environmental exposure assessment is based on measured data)

2.3 Uses advised against

Acetonitrile as such or in preparations should not be placed on the market for professional or consumer use.

3 CLASSIFICATION AND LABELLING

3.1 Classification in Annex I of Directive 67/548/EEC

Classification

Classification and labelling according to the 28th ATP of Directive 67/548/EEC:

Classification:	F; R11 Highly flammable.
	Xn; R20/21/22 Harmful by inhalation, in contact with skin and if swallowed.
	Xi; R36 Irritating to eyes.
Labelling:	F; Xn
	R: 11-20/21/22-36
	S: (1/2-)16-36/37

Specific concentration limits

None

3.2 Self classification(s)

None: Substance is legally classified.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation

4.1.1 Abiotic degradation

4.1.1.1 Hydrolysis

The hydrolysis of acetonitrile is unimportant for the aquatic fate of this compound at the normal pH range of natural waters (see IUCLID 5 for study summary details). The half-life for acetonitrile in water has been estimated to be >150,000 years based on a hydrolysis rate constant at pH 7 and 25 ºC of $5.8.10^{-3}$ M^{-1} $hour^{-1}$ (see IUCLID 5 for study summary details).

4.1.1.2 Phototransformation/photolysis

Data on phototransformation are not required under REACH.

4.1.1.2.1 Phototransformation in air

A half life of 321 days can be assumed for acetonitrile in the atmosphere. For details, please refer to the IUCLID 5 dossier.

4.1.1.2.2 Phototransformation in water

No data available. As a worst case scenario, it is assumed that phototransformation of acetonitrile in water does not occur.

4.1.1.2.3 Phototransformation in soil

No data available. As a worst case scenario, it is assumed that phototransformation of acetonitrile in soil does not occur.

4.1.2 Biodegradation

4.1.2.1 Biodegradation in water

4.1.2.1.1 Screening tests

The test results are summarised in the following table:

Table 3: Screening tests for biodegradation in water

Method	Degradation rate	Remarks	Reference
River water Aerobic O_2 demand No further details available	100% 4 days	--	EU RAR (2002)
Activated sludge Aerobic O_2 demand No further details available	98% 28 days	--	EU RAR (2002)

4.1.2.2 Biodegradation in sediments

A test on the biodegradation in sediments is not needed, as the substance is readily biodegradable.

4.1.2.3 Biodegradation in soil

A test on the biodegradation in soil is not needed, as the substance is readily biodegradable.

4.1.2.4 Summary and discussion on biodegradation

Biodegradation in water:

According to the activated sludge test (98% degradation in 28 days) a DT_{50} of 5 days can be assumed.

Biodegradation in soil or sediment:

No biodegradation tests in soil or sediment are needed, as the substance is readily biodegradable.

Testing proposal:

A ready biodegradability test, according to the guidelines OECD 301 or EU C.4, is suggested to confirm that acetonitrile is readily biodegradable.

4.1.3 Summary and discussion on degradation

Table 4: Summary on degradation

Degradation rate in water	Hydrolysis is not a relevant degradation route for the substance.
Degradation rate in sediment	DT_{50} = 5 days
Degradation rate in soil	DT_{50} = 5 days
Degradation rate in air	DT_{50} = 321 days

Acetonitrile is considered ready biodegradable. However, an additional ready biodegradability test, according to the guidelines OECD 301 or EU C.4, is suggested to confirm the presented results.

4.2 Environmental distribution

4.2.1 Adsorption/desorption

The Koc was calculated using EUSES 2.0, for nonhydrophobics based on the logKow = - 0.34.

→ Koc = 6.97

logKoc = 0.843

4.2.2 Volatilisation

Acetonitrile is a volatile liquid with a vapour pressure of 98.64 hPa at 20 ºC and rapid volatilisation of this compound to the atmosphere is expected when released to the environment. The Henry's Law constant of 2.91 Pa m^3 mol^{-1} indicates that volatilisation of the substance from surface waters and moist soils is likely to be significant.
In one publication a decrease to 5 % of the original acetonitrile level in river water after 72 hours was reported (EU RAR, 2002)

4.2.3 Distribution modelling

See EUSES report in Appendix I.

4.3 Bioaccumulation

4.3.1 Aquatic bioaccumulation

4.3.1.1 Bioaccumulation estimation

Due to the low logKow of – 0.34, bioaccumulation is of no concern. Estimation of the bioconcentration factor (BCF) using EpiWin (v3.12) resulted in Log BCF = 0.5 (BCF = 3.162; see Appendix II).

4.3.1.2 Measured bioaccumulation data

No data available.

4.3.2 Terrestrial bioaccumulation

No data available. Summary and discussion of bioaccumulation

Due to the low logKow of – 0.34, bioaccumulation is of no concern. Estimation of the bioconcentration factor (BCF) using EpiWin (v3.12) resulted in Log BCF = 0.5 (BCF = 3.162; see Appendix II).

4.4 Secondary poisoning

As no bioaccumulation in organisms is anticipated (Log BCF = 0.5), secondary poisoning through the food chain is of no concern for acetonitrile.

5 HUMAN HEALTH HAZARD ASSESSMENT

5.1 Toxicokinetics (absorption, metabolism, distribution and elimination)

Extensive data on the toxicokinetics of acetonitrile is available. In vivo studies performed in animals covering the oral, inhalative, intra-peritoneal and intra-venous route are available. In vitro studies and human studies covering the inhalation route are available. The toxicokinetics of acetonitrile is well understood. For the purpose of this CSR a summary (Section 5.1.4) is considered to be sufficient. For details on study summaries and robust study summaries, reference is made to the IUCLID 5 registration dossier.

5.1.1 Non-human information

Please refer to the IUCLID 5 registration dossier for study summaries.

5.1.2 Human information

Please refer to the IUCLID 5 registration dossier for study summaries.

5.1.3 Other relevant information

Please refer to the IUCLID 5 registration dossier for study summaries.

5.1.4 Summary and discussion on toxicokinetics

Acetonitrile is well absorbed from the lungs, gastrointestinal tract and through the skin, although there are not available quantitative data.
Acetonitrile has a widespread distribution. It has been found in heart, lungs, liver, spleen, kidneys, stomach, intestines, skin, muscle, brain and testes. Free and conjugated hydrogen cyanide was also detected in all studied organs (Haguenoer et al., 1975). Following a single intravenous dose of 2-14C-acetonitrile to mice, the highest levels of radioactivity occurred in the liver and kidney at 5 min and levels declined over time. At 24 and 48 hours, acetonitrile derived radioactivity was detected in the gastrointestinal, thymus, liver and male reproductive organs. Covalent binding studies at 24 and 48 hours after treatment indicated that 40-50% of total radioactivity present in the liver was bound to the macromolecular fractions of the tissues. The radioactivity contents of other organs were, in large part (40-50% of total), present in the lipid fraction of the tissue (Ahmed et al., 1992).
There are no indications that repeated administrations of acetonitrile result in its accumulation in animal tissues.
Acetonitrile is metabolised to cyanide via cytochrome P450. Firstly, a cyanohydrin intermediate is formed and spontaneously decomposes in liberating free cyanide and possible formaldehyde.

Several studies have indicated that cyanide formed *in vivo* is subsequently conjugated with thiosulphate to form thiocyanate, which is eliminated in urine (Willhite, 1981; Willhite and Smith, 1981; Pozzani, 1959; Haguenoer et al., 1975; Silver et al., 1982; Ohkawa et al., 1972). Cyanide is responsible for the acetonitrile toxicity. The conversion of acetonitrile to cyanide proceeds at a slower rate than that of other nitriles (Ahmed & Farooqui, 1982). This explains the lower toxicity of acetonitrile comparing with other nitriles. Moreover the more rapid rate at which cyanide is produced in the mouse appears to account for the much greater sensitivity of this species to the toxic effects of acetonitrile.
The microsomal metabolism of acetonitrile to cyanide was found to be oxygen- and NADPHdependent, inactivated by heat and antagonised by NADH. Since the metabolism of acetonitrile is increased in animals pretreated with acetone, Freeman and Hayes (1987) suggested that acetonitrile is likely metabolised by the cytochrome P450j (LM3a, LMeb).
Elimination of acetonitrile occurs primarily through urinary excretion of the unchanged compound and free and bound hydrogen cyanide.
Pulmonary clearance of unchanged acetonitrile via exhalation is also an important pathway of elimination, especially at high exposure levels (Haguenoer et al., 1975).

5.2 Acute toxicity

5.2.1 Non-human information (according to EU-RAR, 2002)

Several studies have been carried out with different species and by different routes (see IUCLID 5 dossier for study summaries).

5.2.1.1 Acute toxicity: oral

Table 5: Acetonitrile acute oral toxicity results

Route	Species	LD50 / LC50	Reference
oral	Rat (Wistar-Nelson)	1,327-6,762 mg/kg bw	Pozzani et al. (1959)
oral	Guinea pig	140 mg/kg bw	Pozzani et al. (1959)
oral	Rat (SD) (14-day-old)	158 mg/kg bw	Kimmura et al. (1971)
oral	Rat (SD) (Young adult)	3,081 mg/kg bw	Kimmura et al. (1971)
oral	Rat (SD) (Older adult)	3,476 mg/kg bw	Kimmura et al. (1971)
oral	Mouse ddY	269 mg/kg bw	Tanii and Hashimoto (1984)
oral	Mouse (CD-1)	617 mg/kg bw	MPI Research (1998)

5.2.1.2 Acute toxicity: inhalation

Table 6: Acetonitrile acute inhalation toxicity results

Route	Species	LD50 / LC50	Reference
inhalation	Dog	13,440-26,880 mg/m^3 (4h)	Pozzani (1959)
inhalation	Rat Nelson	26,880 mg/m^3 (4h)	Pozzani (1959)
inhalation	Rat Nelson	12,685– 20,890 mg/m^3 (8h)	Pozzani (1959)
inhalation	Rabbit	4,751 mg/m^3 (4h)	Pozzani (1959)

inhalation	Guinea pig	9,500 mg/m^3 (4h)	Pozzani (1959)
inhalation	Mouse CD-1	4,524 mg/m^3 (1h)	Willhite (1981)
inhalation	Mouse CD-1	6,026 mg/m^3 (4h)	MPI Research (1998)

5.2.1.3 Acute toxicity: dermal

Table 7: Acetonitrile acute dermal toxicity results

Route	Species	LD50 / LC50	Reference
dermal	Rabbit	987.5 mg/Kg undiluted	Pozzani et al. (1959)
dermal	Rabbit	395 aqueous solution	Pozzani et al. (1959)
dermal	Rabbit	3,950 mg/Kg	Smyth and Carpenter (1948)
dermal	Rabbit	>2,000 mg/Kg	MPI Research (1997)

5.2.1.4 Acute toxicity: other routes

Table 8: Acetonitrile acute toxicity results for other routes

Route	Species	LD50 / LC50	Reference
intraperitoneal	Rat (Wistar or Nelson)	672-6,288 mg/kg bw undiluted	Pozzani et al. (1959)
intraperitoneal	Rat (Wistar or Nelson)	3,073-4,440 mg/kg bw saline	Pozzani et al. (1959)
intraperitoneal	Mouse (CD-1)	175 mg/kg bw	Willhite and Smith (1981)
intraperitoneal	Mouse	198 mg/kg bw	Pozzani et al. (1959)
intraperitoneal	Mouse (NMRI)	400 mg/kg bw	Zeller et al. (1969)
intraperitoneal	Mouse	521 mg/kg bw	Yoshikawa (1968)
intravenous	Rat-Wistar or Nelson	1,327 mg/kg bw	Pozzani et al. (1959)

5.2.2 Human information

Several cases of human intoxication with acetonitrile are reported in literature. Please refer to summaries in the IUCLID 5 registration dossier and see summary on acute toxicity below.

5.2.3 Other relevant information

None.

5.2.4 Summary and discussion of acute toxicity

Different animal species and individuals of the same species varied widely in susceptibility to acetonitrile in single-dose toxicity studies by various routes.
The range of oral LD50 values in mammals is between 140 and 6,762 mg/kg body weight. Mouse and Guinea pig seem to be the most sensitive species. These studies were performed without GLP information.

A study showed that acetonitrile was more toxic to immature rats (14-day-old) than to older rats given oral doses of 160-3,500 mg/kg. Another study reported that using male or female Wistar or Nelson albino rats, the males were more susceptible than the females; 6,762 mg/kg for females and 1,327 mg/kg for males, the route was by gavage. In a well-conducted study in mice, the oral LD50 of acetonitrile was calculated to be 617 mg/kg.
The main symptoms in animals appear to be prostration followed by seizures and convulsions. Animals exposed to acetonitrile via different routes of dosing always showed respiratory symptoms: rapid and irregular respiration, laboured or difficult breathing and intense dyspnea.
In humans, ingestion of 1 to 2 g acetonitrile/kg causes occasionally death (in infants). A dose of 570 mg/kg was estimated from a case of poisoning in a 26-year-old man, to be the dose that produced serious effects on human health without causing death.
→ R22; Harmful if swallowed.

A LD50 >2000 mg/kg was obtained in a well-conducted acute dermal toxicity study in rabbits.

Classification with R21 is proposed based on human data which reported symptoms and levels of cyanide in blood as result of paediatric accidental exposure to an acetonitrile-containing cosmetic.
→ R21; Harmful in contact with skin.

The 8-hour inhalation LC50 in male rats is 7,551 ppm (12,685 mg/m^3). Rabbits and mice were more sensitive than rats, with LC50 of 2,828 ppm (4,751 mg/m^3) and 2,693 ppm (4,524 mg/m^3), respectively and time of exposures of 4 hours for rabbits and 60 min for mice. A 4-hour exposure of dogs at concentrations up to and including 8,000 ppm (13,440 mg/m^3) produced no deaths, but deaths occured at concentrations of 16,000 and 32,000 ppm. (26,880 mg/m^3, 53,760 mg/m^3) Gross pathology indicated pulmonary haemorrhage and vascular congestion. In a well-conducted study of inhalation a LC50 3,587 ppm (6,026 mg/m^3) was obtained in mice.
The determination of blood cyanide and urinary thiocyanate should not be relied upon as evidence of brief inhalation to low concentrations of acetonitrile vapour. No blood cyanide was found in human subjects inhaling 40, 80 and 160 ppm vapour, and there was no correlation between thiocyanate excretion and acetonitrile concentration. The variability of subjective responses of humans to 40, 80 and 160 ppm acetonitrile vapour suggests that, even if a concentration of the solvent vapour were selected that would not endanger the health of the majority of workers, it might cause discomfort to some of them.
Symptoms and signs of acute acetonitrile intoxication include chest pain, tightness in the chest, nausea, emesis, tachycardia, hypotension, short and shallow respiration, headache, and seizures. The systemic effects appear to be largely attributable to the conversion of acetonitrile into cyanide. Blood cyanide and thiocyanate levels are elevated during acute intoxication. Two deaths after exposure to acetonitrile vapour in the workplace have been reported. Elevated tissue cyanide concentrations were found in postmortem examination of these cases.
The levels causing toxicity in man are unknown but, probably, they are very high due to the detection of high levels of cyanide at post-mortem examination (7,960 µg/l blood), whereas no significant change was detected in the blood or urine of volunteers exposed to 0.27 mg/l (160 ppm) acetonitrile for 4 hours. Taking into account all available data, classification as harmful by the inhalation route is appropriate.
→ R20; Harmful by inhalation.

5.3 Irritation

5.3.1 Skin

5.3.1.1 Non-human information

Several studies are available (see IUCLID 5 dossier for details). The study summarised below is considered as key study. The other studies did not lead to contradictory results.
MPI Research carried out a dermal irritation study of acetonitrile in rabbits in 1997. The study conforms to EPA/OECD Guidelines. Acetonitrile was applied to the skin of six male New Zealand white rabbits. A dose of 0.5 ml of acetonitrile was applied to one intact skin site on the back of each rabbit. The test article remained in contact with the skin for 4 hours. The test sites were evaluated for dermal irritation approximately 0.5-1, 24, 48 and 72 hours following patch removal and scored based on the Draize method. All scores at each observation interval were 0 for each animal. No signs of ill health or test article-related effects were observed during the study.

5.3.1.2 Human information

No information available.

5.3.2 Eye

5.3.2.1 Non-human information

Several studies are available (see IUCLID 5 dossier for details). The study summarised below is considered as key study. Other available studies did not report contradictory results.
MPI Research carried out an eye irritation study of acetonitrile in rabbits in 1997. The study conforms to EPA/OECD Guidelines. Acetonitrile (HPLC grade, 0.1 ml) was applied to the conjunctiva sac of six males New Zealand white rabbits without rinsing. The eye was held closed for one second and released, while the contralateral eye was treated in a similar way. The eyes were observed at 1, 24, 48 and 72 hours and 4, 7, 14 and 21 days after dosing, and scored by the Draize method. The mean scores for all animals over the period 24-72 hours were as follows: corneal opacity, 1.45; iris lesion, 0.83; conjunctiva redness, 3; conjunctiva oedema, 1.89. These effects were largely resolved in 21 days.

5.3.2.2 Human information

No information available.

5.3.3 Respiratory tract

5.3.3.1 Non-human information

In the inhalation studies available for acetonitrile, no irritation of the respiratory tract is reported at doses equal or similar to the relevant long term NOAEL of 100 ppm (refer to chapter 5.6.1.2 for details on derivation of the long term inhalative NOAEL).

5.3.3.2 Human information

Humans accidentally inhaling 500 ppm for brief periods, reported some nose and throat irritation; this dose has been estimated from the human poisoning cases (Admur,1959).

5.3.4 Other relevant information

None.

5.3.5 Summary and discussion of irritation

Two well-conducted irritation studies of acetonitrile in skin and eye indicated that acetonitrile is an eye irritant, but not a skin irritant.

→ R36: irritating to the eyes.

5.4 Corrosivity

The studies summarised in Section 5.3 indicate that acetonitrile is not corrosive to the skin or the eyes.

5.4.1 Non-human information

See statement under 5.4.

5.4.2 Human information

See statement under 5.4.

5.4.3 Other relevant information

None.

5.4.4 Summary and discussion of corrosion

See statement under 5.4.

5.5 Sensitisation

5.5.1 Skin

5.5.1.1 Non-human information

The results of studies on skin sensitisation are summarised in the following table (see IUCLID 5 dossier for a robust study summary):

Table 9: Skin sensitisation study summary

Species	Method, route	Result	Remarks	Reference
Guinea Pigs (Hartley) 10 male / 10 female	Buehler Test Vehicle: none; undiluted test material was used	On the grading scale used for this test, the observed reactions were not considered as indicating sensitisation.	--	Hill Top Research Inc. (1997)

5.5.1.2 Human information

No information available.

5.5.2 Respiratory system

5.5.2.1 Non-human information

In the inhalation studies available for acetonitrile, no sensitisation of the respiratory tract is reported at doses equal or similar the relevant long term NOAEL of 100 ppm (refer to section 5.6.1.2 for details on derivation of the long term inhalative NOAEL).

5.5.2.2 Human information

No information available.

5.5.3 Other relevant information

None.

5.5.4 Summary and discussion of sensitisation

5.5.4.1.1 Skin sensitisation

Negative results were obtained in a well-conducted Buehler test. Acetonitrile was shown to be a non-sensitiser.

5.5.4.1.2 Respiratory sensitisation

Inhalation studies do not indicate any sensitising potential of acetonitrile to the respiratory tract.

5.5.4.1.3 Justification for classification or non classification

No classification is proposed.

5.6 Repeated dose toxicity

5.6.1 Non-human information

5.6.1.1 Repeated dose toxicity: oral

No repeated dose oral toxicity study is available for acetonitrile.

An oral NOAEL can be derived from the inhalation NOAEL of 100 ppm (168 mg/m^3): Acetonitrile is metabolised to cyanide by all routes and cyanide is responsible for acetonitrile toxicity. In fact, similar symptoms were seen in humans regardless of the route of administration indicating that the route of administration does not appear to be a major factor contributing to toxicity. Therefore, the inhalation NOAEL of 168 mg/m^{3}can be converted to an oral NOAEL 54 mg/kg bw/day assuming that a 0.03 kg mouse breathes 0.027 litres of air per minute (USEPA, 1987), 6 hours exposure per day and 100 % absorption.

5.6.1.2 Repeated dose toxicity: inhalation

Several studies using a number of species investigated the repeated dose acetonitrile inhalation toxicity (see IUCLID 5 dossier for details). Mice appeared somewhat more susceptible to than rats. Mortality in a 13-week mouse study was complete at 1,600 ppm, and deaths of female extended down to the 400 ppm group.
In a 13-week study on rats, carried out by NTP, a NOAEL of 400 ppm was obtained given the haematology effects found in the superior doses. Later the NTP carried out an inhalation 2-year study established a 200 ppm NOAEL due to a slight anaemia observed in concentration of 400 ppm. Preliminary data from a not fully reported study (Coate, 1983, summarized in EPA, 1987 and IUCLID) showed no adverse effects at 200 ppm.
In a 13-week study, carried out by NTP in mice, a NOAEL of 100 ppm was obtained due to the forestomach lesions. However, a 2-year study carried out later by NTP concluded that these findings established an effect of prolonged acetonitrile exposure on the forestomach of mice, but the magnitude of the neoplastic findings were insufficient to attribute them to the chemical with any confidence. In addition, other effects seen in the 13-week study such as increased ratio of liver weight / body weight and increased absolute liver weight, were not seen when evaluated at either 15 or 24 months in a life time study. In the 13-week study there were no other findings. However, this study as well as the 2-year study lacked chemical biochemistry and haematology. Preliminary data from two unrelated not fully reported studies (Coate, 1983; Immuquest Labs-Inc., 1984, both summarised in EPA 1987 and IUCLID) showed a NOAEL of 100 ppm based on haematological data in B6C3F1 mice.
Dogs and monkeys exposed 7 hours / day, 3 days / week for 91 days at a mean acetonitrile vapour concentration of 350 ppm showed minor variations in body weight, haematocrit, and haemoglobin. Both, monkeys and dogs had pulmonary abnormalities.
Autopsy of monkeys noted cerebral haemorrhage and cloudy swelling of the kidney tubules was noted in two of the three exposed monkeys. Monkeys were more sensitive than dogs to the same dose of inhaled acetonitrile (350 ppm).

It has been noted that an intramuscular injection of 0.05 to 0.1 ml acetonitrile causes exophthalmia and thyroid hyperplasia in rabbits. The degree of exophthalmia could be related to the hyperplasia. Thyroid hyperplasia could also be induced by acetonitrile in rats and mice but did not develop phthalmia. Rats and mice showed considerable resistance to goitrogenic substances.

5.6.1.3 Repeated dose toxicity: dermal

No repeated dose dermal toxicity study is available for acetonitrile. For the purpose of the risk assessment, the systemic NOAEL is used with the assumption of 100% dermal penetration.

A dermal NOAEL can be derived from the inhalation NOAEL of 100 ppm: Acetonitrile is metabolised to cyanide by all routes and cyanide is responsible for acetonitrile toxicity. In fact, similar symptoms were seen in humans regardless of the route of administration indicating that the route of administration does not appear to be a major factor contributing to toxicity. Therefore, the inhalation NOAEL of 100 ppm (168 mg/m³) can be converted to a dermal NOAEL of 54 mg/kg bw/day assuming that a 0.03 kg mouse breathes 0.027 litres of air per minute (USEPA, 1987), 6 hours exposure per day and 100% absorption.

5.6.1.4 Repeated dose toxicity: other routes

No information available.

5.6.2 Human information

There is no information available on the effects of repeated exposure to acetonitrile in humans.

5.6.3 Summary and discussion of repeated dose toxicity (key studies):

Table 10: Repeated dose toxicity studies

Endpoint	**Quantitative dose descriptor[1] (appropriate unit) or qualitative assessment**		**Associated relevant effect[2]**	**Remarks on study[3]**
	Local effect[4]	Systemic effect[5]		
Repeated dose toxicity [6] Sub-chronic Oral	--	--	--	--
Repeated dose toxicity [6] Sub-chronic (92 days) Inhalation	--	NOAEL = 168 mg/m³ (100 ppm)	Increased liver weight at 200 ppm	B6C3F1 mice exposed to acetonitrile vapours at 100, 200, 400, 800 and 1,600 ppm, 6 hours / day, 5 days / week
Repeated dose toxicity [6] Sub-chronic Dermal	--	--	--	--

[1] NOAEL (NOAEC), LOAEL ,bmdl05, bmd05, BMD(L)10 or any other dose descriptor; indicate whether this concerns a no or lowest observed effect level etc.

[2] In this column the relevant effect for which the dose descriptor is determined is provided

[3] This column is for indicating whether data were available, whether the substance is classified for this endpoint, for shortly describing specifics of the study (e.g. 28-d gavage rat, 5 d/wk or 2-gen diet rat, 7 d/wk), and for indicating (additional) uncertainty in available data

[4] Units are mg/m^3 for inhalation, and mg/cm^2 or ppm for dermal exposure

[5] Units are mg/m^3 for inhalation, mg/kg bw for oral dose and mg/m^2 for dermal exposure.

[6] These repeated exposure studies may also show relevant acute effects of the test substance; these should be accounted for under the endpoint acute toxicity

The repeated dose toxicity study relevant for risk assessment of acetonitrile is the sub-chronic (92-day) toxicity inhalation study. The determined NOAEL = 168 mg/m^3 (100 ppm).

5.7 Mutagenicity

Several *in vitro* and *in vivo* studies are available (see IUCLID 5 dossier for details).The information in bacteria indicates that acetonitrile is not mutagenic in Salmonella assay as well as when the assay is carried out employing a 20-minute preincubation period at 37°C. Acetonitrile induces mutations neither in chinese hamster ovary cells nor in mouse lymphoma L5178Y cells. These tests were conducted with and without S9 metabolic activation enzymes.
In cytogenetic tests with chinese hamster ovary cells, acetonitrile induced slight increase in sister chromatid exchanges without S9 and chromosomal aberrations with S9 for both endpoints; the increases were noted at the highest dose tested. In the SCE assay these increases were considered weak evidence of activity (increase at any single dose). In the chromosomal aberrations test the result was considered equivocal (absence of a statistically significant increase at any dose).
Positive results have been reported in assays, which measure the induction of aneuploid events. Acetonitrile was found to be a potent inducer of aneuploid. No point mutations or recombination in a diploid strain of *Saccharomyces cerevisae* were found, even with relatively high concentrations. Acetonitrile induced sex chromosomal aneuploid (both chromosome loss and chromosome gain) in oocytes of female *Drosophila melanogaster* fed an aqueous solution of the chemical either as larvae or as adults.
No induction of unscheduled DNA synthesis was observed in rat hepatocytes exposed *in vivo* or *in vitro* to acetonitrile.
In addition, weakly positive results were reported in a bone marrow micronucleus test with acetonitrile administered by intraperitoneal injection to male and female NMRI mice and a significant increase in micronucleated normochromatic erythrocytes was observed in peripheral blood samples from male mice treated with acetonitrile for 13 weeks; the frequency of micronucleated erythrocytes in female mice was not affected by exposure to acetonitrile. However, the interpretation of these findings is difficult, the i.p. study is the non-standard protocol and in the inhalation study, the association between exposure and micronuclei was weak in the absence of a strong dose-response relationship, in addition, no positive control group or bone marrow cytotoxicity was reported.
Negative results have been reported in a well-conducted Micronucleus test *in vivo* carried out on NMRI mice via intraperitoneal route.
In conclusion, acetonitrile did no induce gene mutations in bacteria, showed week clastogenic activity in cultured mammalian cells and was not clastogenic in a well-conducted *in vivo* micronucleus test.
No classification for this effect is proposed.

5.8 Carcinogenicity

Several studies are available (see IUCLID 5 dossier for details).

There was an increase in liver adenomas and carcinomas separately and jointly in male rats at the highest test level (400 ppm). This result was named as equivocal by NTP. However, this was not significant when compared with the dedicated controls or historical control ranges.
There were no exposure-related liver lesions in female rats.
There were no increases in the incidences of lung and liver neoplasms in exposed groups of mice that were considered related to acetonitrile exposure. However, the incidence of squamous hyperplasia of the epithelium of the forestomach was significantly increased at 15 months in 200 ppm females. At 2 years, the increased incidence was dose-related in all exposed male and female groups. These findings establish an effect of prolonged acetonitrile exposure on forestomach of mice, but the magnitude of the neoplastic findings is insufficient to attributethem to the chemical with any confidence.
In summary, the results of the NTP bioassay on acetonitrile do not indicate that acetonitrile was carcinogenic in laboratory rats or mice.
No classification for this effect is proposed.

5.9 Toxicity for reproduction

Several studies are available (see IUCLID 5 dossier for details).

5.9.1 Effects on fertility

In relation to fertility, there is no information available in humans and there are no animal studies specifically investigating such effects. However no changes were seen in (absolute or relative) weight of the cauda or testis and no effect on sperm motility in rats or mice exposed for 13 weeks with 100, 200 and 400 ppm to acetonitrile.
No classification is proposed.

5.9.2 Developmental toxicity

In a well-conducted study, rats exposed by inhalation to acetonitrile did not result in significant foetal effects, even at concentrations, which were overtly toxic to the dam. In this study, a maternal NOAEL of 1,200 ppm and a NOAEL of 1,200 ppm with respect to developmental toxicity were established.
In another inhalation developmental toxicity study in Sprague-Dawley rats, a NOAEL of 1,200 ppm was obtained for maternal toxicity and a NOAEL of 1,500 ppm for developmental toxicity. In two studies with pregnant rats that received acetonitrile by gavage no foetal abnormalities were reported.
In another study conducted in compliance with FDA GLP, pregnant rabbits administered 2, 15 or 30 mg/kg acetonitrile orally showed maternal toxicity at 15 and 30 mg/kg. The maternal toxicity at 15 mg/kg was expressed as a rebound effect on body weight gain after completion of the agent administration period. Embryotoxicity was observed only at the 30 mg/kg dose level. There were no treatment-related gross external, soft tissue or skeletal malformations or developmental variations.
Exposure of hamsters to 5,000 or 8,000 ppm acetonitrile on day 8 of gestation was shown to increase the incidences of resorptions and malformations including exencephaly encephalocele and rib fusions. Malformations identical to those noted following inhalation exposure occurred sporadically in a limited number of offspring after oral or intraperitoneal administration of 100-400 mg/kg acetonitrile.
In most of the available assays, teratogenicity was associated with maternal toxicity. However,

in the case of exposure of pregnant hamsters to acetonitrile, the study is the non-standard protocol and the interpretation of the findings is difficult.
In human, no association between solvent exposure and risk of malformation, birth weight or spontaneous abortion has been observed.No classification is proposed.

5.10 Derivation of DNEL(s) /DMELs

5.10.1 Overview of typical dose descriptors for all endpoints

In table 11 relevant information on the toxicity of acetonitrile are summarised. Two DNELs are derived:

- $DNEL_{acute}$
- $DNEL_{long\text{-}term}$

Table 11: Available dose-descriptor(s) per endpoint for acetonitrile as a result of its hazard assessment.

Endpoint		**Quantitative dose descriptor[1] (appropriate unit) or qualitative assessment**		**Associated relevant effect[2]**	**Remarks on study[3]**
		Local[4]	Systemic[5]		
Acute toxicity[6]	oral	--	LD_{50} = 140 – 6762 mg/kg bw	Mortality	Several studies in mammals, without GLP information
	dermal	--	LD_{50} = > 2000 mg/kg bw/day	None	Study performed in rabbits. Classification with R21, harmful in contact with skin is proposed based on human data
	inhalation	--	LC_{50} (rat) > 12000 mg/m^3 No observed effects in humans at 270 mg/m^3 (4 h; 159 ppm)	Mortality None	-- Human volunteer study. No significant change of cyanide in blood or urine
Irritation/Corrosivity	skin	Not corrosive. Not irritant.	NA[7]	Neither corrosion nor irritancy was observed.	Rabbit study

1 NOAEL (NOAEC), LOAEL , T25, BMD(L)10 or any other dose descriptor; indicate whether this concerns a no or lowest observed effect level etc
2 In this column the relevant effect for which the dose descriptor is determined is provided
3 This column is for indicating whether data were available, whether the substance is classified for this endpoint, for shortly describing specifics of the study (e.g. 28-d gavage rat, 5 d/wk or 2-gen diet rat, 7 d/wk), and for indicating (additional) uncertainty in available data
4 Local exposure: units are mg/m3 for inhalation, and mg/cm2 or ppm for dermal exposure
5 Systemic: units are mg/m3 for inhalation, and mg/kg bw/day for oral and dermal exposure
6 In general, sublethal toxicity is a more rational starting point for acute toxicity than mortality data; information on acute toxicity may also be derived from e.g. repeated dose toxicity studies or reproductive toxicity studies
7 Not applicable

Endpoint		Quantitative dose descriptor[1] (appropriate unit) or qualitative assessment		Associated relevant effect[2]	Remarks on study[3]
		Local[4]	Systemic[5]		
	eye	Not corrosive. Irritant.	NA	No corrosion was observed. According to the Draize method, Acetonitrile is irritant to the eyes.	Rabbit study
	resp. tract	Not corrosive and not irritant to the resp. tract.	NA	--	--
Sensitisation	skin	Not sensitising	NA	--	Buehler test
	resp. tract	Not sensitising to the resp. tract	NA	--	--
Repeated dose toxicity (Sub)-Chronic (derived on the basis of a sub-chronic mice and a chronic rat study)	oral	--	NOAEL = 54 mg/kg bw/day (calculated from inhalation NOAEL)	--	See inhalation study below.
	dermal	--	NOAEL = 54 mg/kg bw/day (calculated from inhalation NOAEL)	--	See inhalation study below.
	inhalation	--	NOAEL = 168 mg/m^3 (100 ppm)	Increased liver weight at 200 ppm.	B6C3F1 mice Exposed to acetonitrile vapours at 100, 200, 400, 800 and 1,600 ppm, 6 hours/day, 5 days/week
Mutagenicity	in vitro	--	Not mutagenic	--	Acetonitrile did not induce gene mutations in bacteria, showed weak clastogenic activity in cultured mammalian cells and was not clastogenic in a well-conducted in vivo micronucleus test.
	in vivo	--	Not mutagenic	--	
Carcinogenicity	oral	--	--	--	--
	dermal	--	--	--	--
	inhalation	--	Not carcinogenic	--	Acetonitrile was not carcinogenic in laboratory rats or mice.
Reproductive toxicity[8] fertility impairment	oral	NA	In relation to fertility, there is no information available in humans and there are no animal studies specifically investigating such effects. However, no changes were seen in (absolute or relative) weight of the cauda or testis and no effect on sperm motility in rats or mice exposed for 13 weeks with 100, 200 and 400 ppm to acetonitrile.		
	dermal	NA			
	inhalation	NA			
Reproductive toxicity developmental toxicity	oral	NA	In most of the available assays, developmental toxicity in rat and rabbit studies was associated with clear maternal toxicity. However, in the case of exposure of pregnant hamsters to acetonitrile (exposure to extreme		
	dermal	NA			

8 These repeated exposure studies may also show relevant acute effects of the test substance; these should be accounted for under the endpoint acute toxicity

Endpoint		Quantitative dose descriptor[1] (appropriate unit) or qualitative assessment		Associated relevant effect[2]	Remarks on study[3]
		Local[4]	Systemic[5]		
	inhalation	NA	concentration), the study is the non-standard protocol and the interpretation of the findings is difficult. In human, no association between solvent exposure and risk of malformation, birth weight or spontaneous abortion has been observed.		

5.10.2 Correction of dose descriptors if needed (for example route-to-route extrapolation), application of assessment factors and derivation of the endpoint specific DN(M)EL

For simplification, table 11 was adapted. Only systemic effects are considered, with the exception of irritant effects to the eyes, as no other relevant local effects occurred. Results are shown in table 12.

Derivation of $DNEL_{acute}$

For derivation of $DNEL_{acute}$ the human volunteer study was considered to represent the most relevant information: an exposure at a concentration of 270 mg/m^3 for 4 h showed no findings in the volunteers (NOEL ≥ 270 mg/m^3, equivalent to 159 ppm).
In accordance with Table R8.6, Guidance on Information Requirements and Chemical Safety Assessment, 2008, an assessment factor is 5 is applied for intraspecies variability for workers resulting in a **$DNEL_{acute}$ of 54 mg/m^3 (equivalent to 32 ppm**; 270 mg/m^3/5 = 54 mg/m^3, 159 ppm/5 = 32 ppm**)**.

The $DNEL_{acute}$ refers only to the inhalation route. It is not scientifically reasonable to convert the air concentration used in the human volunteer study into an oral or dermal dose. Therefore, no $DNEL_{acute}$ for the oral and dermal route is given. However, it should be noted that no acute findings were observed in the long-term studies with acetonitrile. This means that the $DNEL_{long\text{-}term}$ is also protective for acute oral and dermal exposure.

Derivation of $DNEL_{long\text{-}term}$

An inhalative NOAEL of 168 mg/m^3 (100 ppm) was obtained in a subchronic mouse study, the most sensitive animal species to acetonitrile toxicity. Based on the repeated dose toxicity information available, a NOAEL of 168 mg/m^3 (100 ppm) in mice is considered scientifically meaningful. The NOAEL of 168 mg/m^3 (100 ppm) is used to derive a $DNEL_{long\text{-}term}$.
Acetonitrile is not genotoxic, carcinogenic, toxic to reproduction or developmental toxic. Therefore, an assessment factor of 5 is considered for intraspecies variability and derivation of the $DNEL_{long\text{-}term}$ based on TRGS (BAuA, 1998,).

Considering the assessment factor of 5 and the NOAEL of 100 ppm, the **$DNEL_{long\text{-}term}$ is 34 mg/m^3 (corresponding to 20 ppm).**

Table 12: Corrected dose descriptor(s) per endpoint and endpoint-specific worst case DNEL(s)/DMEL(s) appropriate for all exposure patterns

Endpoint		**Most relevant quantitative dose descriptor[9] (appropriate unit)**	**Overall AF applied**	**Endpoint-specific DNEL/DMEL (appropriate unit)**
Acute toxicity	oral	LD_{50} = 140 – 6762 mg/kg bw Not used in the DNEL derivation.	--	Not relevant, see text above
	dermal	LD_{50} = > 2000 mg/kg bw Not used in the DNEL derivation.	--	Not relevant, see text above
	inhalation (4 h)	LC_{50} (rat) > 12000 mg/m³ No observed effects in humans at 270 mg/m³ (4 h; 159 ppm)	-- 5	-- **$DNEL_{acute}$ = 54 mg/m³(32 ppm)**
Repeated dose toxicity Chronic (derived on the basis of a sub-chronic mice and a chronic rat study)	oral	NOAEL = 54 mg/kg bw/day*	5	**$DNEL_{long\text{-}term}$ = 11 mg/kg bw/day**
	dermal	NOAEL = 54 mg/kg bw/day*	5	**$DNEL_{long\text{-}term}$ = 11 mg/kg bw/day**
	inhalation	NOAEL = 168 mg/m³ (100 ppm)	5	**$DNEL_{long\text{-}term}$ = 34 mg/m³ (20 ppm)**

* based on NOAEL of inhalation studies

6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES

6.1 Explosivity

Acetonitrile forms explosive mixtures in limits ranging from lower to upper: 3.0 – 17 % (v/v). Please see the IUCLID 5 dossier for study summary details.

6.2 Flammability

Acetonitrile is highly flammable. Please see the IUCLID 5 dossier for study summary details.

→ R11, highly flammable.

6.3 Oxidising potential

Acetonitrile is not oxidising. Please see the IUCLID 5 dossier for study summary details.

[9] NOAEL (NOAEC), LOAEL , T25, BMD10 etc or any other dose descriptor; indicate whether this concerns a no or lowest observed effect level etc

7 ENVIRONMENTAL HAZARD ASSESSMENT

7.1 Aquatic compartment (including sediment)

7.1.1 Toxicity data

7.1.1.1 Fish

7.1.1.1.1 Short-term toxicity to fish

Please see the IUCLID 5 dossier for study summary details. The results are summarised in the following table:

Table 13: Summary of short-term effects on fish

Species	Results	Remarks	Reference
Pimephales promelas (fresh water)	LC_{50} (96 h) > 100 mg/L (limit dose)	Nominal Static	Ewell et al. (1986)
Cyprinus carpio (fresh water)	LC_{50} (48 h) = 730 mg/L	--	Nishiuchi (1981)
Pimephales promeles (fresh water)	LC_{50} (96 h) = 1640 mg/L	Analytical monitoring Flow through	Centre for Lake Superior Environmental studies

The most relevant and sensitive value obtained in acute toxicity fish studies is an LC_{50} (48 h) = 730 mg/L. This value was used for risk assessment.

7.1.1.1.2 Long-term toxicity to fish

There are no data on the long-term toxicity to fish available.

7.1.1.2 Aquatic invertebrates

7.1.1.2.1 Short-term toxicity to aquatic invertebrates

Please see the IUCLID 5 dossier for study summary details. The results are summarised in the following table:

Table 14: Summary of short-term effects on invertebrates

Species	Results	Remarks	Reference
Asellus intermedius (fresh water crustacean)	EC_{50} (96 h) >100 mg/L	Nominal Static	Ewell et al. (1996)
Daphnia magna (fresh water crustacean)	LC_{50} (24 h) > 10,000 mg/L	Nominal Static	Bringmann and Kuhn (1977)
Dapnia pulex (fresh water crustacean)	LC_{50} (18 h) = 5,838 mg/L	Nominal Static	Bownan et al. (1981)
Dapnia magna (fresh water crustacean)	LC_{50} (96 h) > 100 mg/L	Nominal Static	Ewell et al. (1986)
Gammarus fasciatus (fresh water crustacean)	LC_{50} (96 h) > 100 mg/L	Nominal Static	Ewell et al., (1986)
Culex restuans (insect larvae)	LC_{50} (18 h) = 6,420 mg/L	Nominal Static	Bownan et al., (1981)
Dugesia tigrina flatworus (Phatyhelminthe)	LC_{50} (96 h) > 100 mg/L	Nominal Static	Ewell et al., (1986)
Helisoma trivolvis (fresh water snail)	LC_{50} (96 h) > 100 mg/L	Nominal Static	Ewell et al. (1986)
Hyalella azteca (fresh water crustacean)	LC_{50} (18 h) = 6,565 mg/L	Nominal Static	Bowman et al. (1981)
Lumbriculus variegatus (segmented worm)	EC_{50} (96 h) > 100 mg/L	Nominal Static	Ewell et al., (1976)
Palaemonetes kadiakensis (fresh water crustacea)	EC_{50} (18 h) = 5,170 mg/L	Nominal Static	Bowman et al., (1981)

The most relevant and sensitive value obtained in acute toxicity invertebrate studies is an EC_{50} (18 h) = 5,170 mg/L. This value was used for risk assessment.

7.1.1.2.2 Long-term toxicity to aquatic invertebrates

There are no data on the long-term toxicity to aquatic invertebrates available.

7.1.1.3 Algae and aquatic plants

Please see the IUCLID 5 dossier for study summary details. The results are summarised in the following table:

Table 15: Summary of effects on algae and aquatic plants

Species	**Results (TT = toxicity threshold for inhibition of cell multiplication)**	**Remarks**	**Reference**
Microcystis aeruginosa (blue-green algae)	TT = 520 mg/L	Inhibition of cell multiplication	Bringmann and Kühn (1978)
Scenedesmus quadricauda (green algae)	TT = 7300 mg/L	Inhibition of cell multiplication	Bringmann and Kühn (1977)

The most relevant and sensitive value obtained in acute toxicity algae studies is a TT = 520 mg/L. This value was used for risk assessment.

7.1.1.4 Sediment organisms

There are no data available. The PNEC for sediment is derived via the equilibrium partitioning method based on the $PNEC_{aquatic}$ (see section 7.1.2.1)

7.1.1.5 Other aquatic organisms

There are no data on other aquatic organisms available.

7.1.2 Calculation of Predicted No Effect Concentration (PNEC)

7.1.2.1 PNEC water

The lowest L(E)C_{50} figure is the 48 h LC_{50} on *Cyprinus carpio*, 730 mg/l. The TTs for algae are in the same range. Therefore, it seems appropriate in this assessment to consider 730 mg/l as the lowest end of the acute toxicity range for aquatic organisms. This range covers three taxonomic groups, fish, invertebrates and algae, and taking into account the lack of chronic figures, the recommendations of the TGD (2003) suggest the application of the factor 1,000 to the lowest end of the acute toxicity range (730 mg/l), obtaining a PNEC for aquatic organisms of 0.73 mg/l.

$$PNEC_{aquatic\ organisms} = \text{lowest end acute toxicity range}/1{,}000 = 0.73\ mg/l$$

The data set only includes freshwater species. Therefore, in absence of data on saltwater species the above PNEC can be used for both, freshwater and marine environments.

7.1.2.2 PNEC sediment

An estimation of the PNEC sediment can be performed according to the equilibrium partitioning method according to the following equation:

$$PNEC_{sediment} = (K_{susp\text{-}water} / RHO_{susp}) * PNEC_{water} * 1000$$

According to EUSES: $K_{susp\text{-}water} = 1.07\ m^3/m^3$

According to the "R16" Guidance document (2008) equation R16-23: RHO_{susp} = 1150 kg/m^3

→ $PNEC_{sediment}$ = (1.07 / 1150) * $PNEC_{water}$ * 1000 = 0.68 mg/kg

This estimation indicates that there is no concern for the sediment compared to the aquatic compartment and that therefore no further testing of the toxicity of acetonitrile to sediment organisms is necessary.

7.2 Terrestrial compartment

As acetonitrile is readily biodegradable and is not directly applied to soil, it is assumed that the substance will not enter the terrestrial environment and therefore no testing of soil organisms is required. Due to the low tendency to adsorb to solid matter and the resulting low tendency to adsorb to sewage sludge which might be deposited onto soil, the indirect exposure of soil to acetonitrile via sewage sludge is also of no concern.

7.2.1 Calculation of Predicted No Effect Concentration (PNEC_soil)

The $PNEC_{soil}$ can be estimated via the equilibrium partitioning method:

$PNEC_{soil} = (K_{soil\text{-}water} / RHO_{soil}) * PNEC_{water} * 1000$

According to EUSES: $K_{soil\text{-}water}$ = 0.405 m^3 /m^3

According to the "R16" Guidance document equation R16-23: RHO_{soil} = 1700 kg/m^3

→ $PNEC_{soil}$ = (0.405 / 1700) * $PNEC_{water}$ * 1000 = 0.173 mg/kg

This estimation indicates that there is no concern for the soil compared to the aquatic compartment and that therefore no further testing of the toxicity of acetonitrile to soil organisms is necessary.

7.3 Atmospheric compartment

The highest PEC_{air} as calculated in EUSES (v2.03) is 3.2 * 10^{-9} mg/m^3 which is ca. 10 orders of magnitude below the long term inhalative DNEL of 34 mg/m^3. This comparison indicates that exposure of atmospheric biota to acetonitrile via the atmosphere is of no concern.

There is no structural alert in the structure of acetonitrile to expect effects on global warming, ozone depletion in the stratosphere, ozone formation in the troposphere or acidification.

7.4 Microbiological activity in sewage treatment systems

7.4.1 Toxicity to aquatic micro-organisms

Several studies are available (please see the IUCLID 5 registration dossier for study summaries). The results are summarised in the following table:

Table 16: Summary of effects on micro-organisms

Species	Results	Remarks	Reference
Chillmonas paramecium (Protozoa)	TT = 942 mg/L	Inhibition of cell multiplication	Bringmann and Kühn (1981)
Entosiphon sulcatum (Protozoa)	TT = 1810 mg/L	Inhibition of cell multiplication	Bringmann and Kühn (1981)
Pseudomona putida (Bacteria)	TT = 680	Inhibition of cell multiplication	Bringmann and Kühn (1981)
Uronema parduzci (Protozoa)	TT = 5825	Inhibition of cell multiplication	Bringmann and Kühn (1981)
Nirosomas (Bacteria)	IC_{50} = 73 mg/L	Inhibition of ammonia consumption	Blum and Speece (1991)
Aerobic microorganisms	IC_{50} = 7500 mg/L	Inhibition of oxygen uptake AFNOR and ETAD	Blum and Speece (1991)
Methanogenic bacteria	IC_{50} = 28000 mg/L	Inhibition of gas production	Blum and Speece (1991)

The recommendations of Guidance document "R10" (2008) suggest the application of the factor 10 to the EC_{50} and one to the NOEC if the test has been performed with nitrifying bacteria and a factor of 100 for the EC_{50} obtained using respiration inhibition or similar endpoints. However, the amount of information available for acetonitrile is clearly higher than that usually available, covering most significant bacterial population and several protozoan species. Nitrifying bacteria seem to be particularly sensitive under laboratory conditions, considering all the available information. Therefore, the weight of evidence justifies use of factor 1 on the IC_{50} reported for nitrifying bacteria. The value obtained in this way for the most sensitive test on nitrifying bacteria, 73 mg/l, agrees with the application of the factor 100 to the inhibition of oxygen uptake by aerobic heterotrophs, which produces a figure of 75 mg/l, and with the derivation expected from the Pseudomona data. Thus a $PNEC_{microorganisms}$ of 73 mg/l is proposed in this assessment.

$PNEC_{microorganisms}$ = 73 mg/l

This value is more than 10 times lower than the lowest toxicity threshold reported for protozoa and therefore is considered appropriate to cover the potential effects on this taxonomic group.

7.4.2 PNEC for sewage treatment plant

The $PNEC_{STP}$ is derived on the basis of the $PNEC_{microorganisms}$ (see section 7.4.1)

$PNEC_{STP}$ = 73 mg/l

7.5 Non compartment specific effects relevant for the food chain (secondary poisoning)

Due to the low logKow of – 0.34 and based on the estimation of the BCF-factor (LogBCF = 0.5), no bio-accumulation is expected for acetonitrile and consequently secondary poisoning via the food chain is of no concern.

7.5.1 Toxicity to birds

It is unlikely that a secondary poisoning risk exists for acetonitrile as acetonitrile is

- readily biodegradable, and

- has a low potential for bioaccumulation ($logK_{ow}$ = -0.34 which is far below 3 and estimated BCF-factor LogBCF = 0.5)).

7.5.2 Toxicity to mammals

This point is covered by the extensive data provided in section 5.

7.5.3 Calculation of $PNEC_{oral}$ (secondary poisoning)

There is no concern for secondary poisoning and therefore no $PNEC_{oral}$ (secondary poisoning) is derived.

7.6 Conclusion on the environmental classification and labelling

No classification due to the environmental effects is necessary for acetonitrile. Please also refer to Chapter 3 for details on the classification and labelling of acetonitrile according to Annex I to Directive 67/548/EEC.

8 PBT AND VPVB ASSESSMENT

8.1 Assessment of PBT/vPvB Properties – Comparison with the Criteria of Annex XIII

8.1.1 Persistence Assessment

Acetonitrile is readily biodegradable. Therefore, acetonitrile is not regarded as persistent.

8.1.2 Bioaccumulation Assessment

Acetonitrile has a logKow of -0.34, i.e. far below the threshold value of 4.5 for which bio-accumulation is expected. The BCF-factor was estimated at logBCF = 0.5. Therefore, acetonitrile is not regarded as bio-accumulative.

8.1.3 Toxicity Assessment

Acetonitrile is not classified as toxic according to Annex I to 67/548/EEC and the data on toxicity provided herein.

8.1.4 Summary and overall Conclusions on PBT or vPvB Properties

Acetonitrile is no PBT or vPvB substance.

8.2 Emission Characterisation

Not needed as acetonitrile is neither PBT nor vPvB.

9 EXPOSURE ASSESSMENT

Table 17: Overview on exposure scenarios and coverage of substance life cycle

Number and title	Manufacture	Preparation making	Industrial and/or wide disperse use	Consumer use	Article service life	Waste stage
Use 0: Production	X	-	-	-	-	X
Use 1: Starting material/solvent in chemical synthesis	-	-	X	-	-	X
Use 2: Analytical laboratories (HPLC)	-	-	X	-	-	X

9.1 Use 0: Production of Acetonitrile

9.1.1 Exposure scenario

Description of process:

Acetonitrile is mainly obtained as a by-product of acrylonitrile manufacture via propylene ammoxidation. This process, named as SOHIO, is carried out in a closed system and involves temperatures of 400 - 500 ºC. After cooling, the reaction product is absorbed in water and the resulting solution is fractionally distilled. The column bottoms, consisting of acetonitrile and water, are azeotropically distilled. The distillate is dried at 70 ºC and redistilled to produce technical acetonitrile.
The plants are outdoors, taking advantage of natural ventilation or, if indoor, local exhaustive ventilation is available. In this situation, significant exposures would be accidental. The likelihood of such exposure increases during activities involving breaching of the closed system such as maintenance operations, repair of equipment, transferring and quality control sampling of acetonitrile. The process is continuous and automated. Filling operations consist of filling railway tank cars with gas exhaust pipes for purification.

The processes involved in the acetonitrile production can be categorized by the descriptor system as follows:

Sector of use: SU3 “Industrial Manufacturing”

Product category: Not applicable

Process category: PROC1 “Used in closed processes, no likelihood of exposure; industrial setting”

PROC2 “Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting”

PROC3 “Use in closed continuous batch process (synthesis or formulation); industrial setting”

PROC8: “Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non dedicated facilities Industrial or non-industrial setting”

Article category: Not applicable

Environmental release category: Not relevant; environmental exposure assessment is based on measured data

9.1.1.1 Risk management measures

9.1.1.1.1 Risk management measures related to workers

Acetonitrile is produced and processed in plants with R45 substances (acrylonitrile, butadiene) present and therefore, all the operations in which there is a potential for exposure are carried out with special care to minimise the risk to the workers.
Measures to prevent exposure comprise the use of adequate personal protection equipment (gloves, goggles, and coverall), local exhaustive ventilation, decontamination procedures before maintenance, wide use of automatic systems for sampling, information to workers on risk, etc.
In addition, regular workplace measurements are carried out to show that the DNELs derived are not exceeded. This ensures the safety of the worker in the production plant.

9.1.1.1.2 Risk management measures related to environment

Do not allow to directly enter the environment.

Any potential releases to air or water should be avoided.

Use scrubbers to reduce emission to air.

9.1.1.1.3 Waste related measures

Any wastes and cleaning solutions that can contain residues of acetonitrile are incinerated.

9.1.2 Exposure estimation

9.1.2.1 Worker exposure

Measured air concentration data are available for the production of acetonitrile. The data show that exposures are lower than 0.1 ppm. Exposures rose to 1.1 ppm in one site (mean value in this period: 0.5 ppm). In the subsequent years the situation returned to concentrations below 0.1 ppm.
Considering the risk management measures described above and the closed production processes, the dermal exposure is considered to be negligible. Therefore, no further assessment is performed.

In summary, exposure to 0.1 ppm represents a worst-case exposure scenario and will be used for purposes of risk characterisation. This concentration is much lower than the $DNEL_{acute}$ of 32 ppm (54 mg/m^3) and the $DNEL_{long\text{-}term}$ of 20 ppm (34 mg/m^3).

In addition to the measured data, model calculations were performed using ECETOC TRA. The following table gives an overview on the scenarios assessed in relation to the process categories according to the descriptor system:

Table 18: ECETOC TRA scenarios (Use 0)

No.	Process category according to descriptor system	Exposure Scenario acc. to ECETOC TRA (non-dispersive uses)
1	PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"	Use in a closed continuous process
2	PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"	Use in a continuous process (with process sampling)
3	PROC3 "Use in closed continuous batch process (synthesis or formulation); industrial setting"	Use in a closed batch process i.e. where no opportunity for breaching arises, including product transfers and sampling
4	PROC8: "Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non dedicated facilities Industrial or non-industrial setting"	Filling containers with the substance or its preparations

The following table summarises the output of the ECETOC TRA inhalative exposure estimation for the scenarios listed above.

Table 19: Model calculations with ECETOC TRA (Use 0)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [ppm]
Non-dispersive	Use in a closed continuous process	1 - 4 hours	Yes	0.006
Non-dispersive	Use in a continuous process (with process sampling)	1 - 4 hours	Yes	12.000
Non-dispersive	Use in a closed batch process i.e. where no opportunity for breaching arises, including product transfers and sampling	1 - 4 hours	Yes	12.000
Non-dispersive	filling containers with the substance or its preparations	15 mins - 1 hour	Yes	10.000

The model calculations show estimated exposures in the range of 0.006 to 12 ppm for the different scenarios/work steps. The estimated exposures are higher than measured workplace concentrations. However, the air concentrations are below the $DNEL_{acute}$ of 32 ppm (54 mg/m^3) and the $DNEL_{long\text{-}term}$ of 20 ppm (34 mg/m^3).

9.1.2.2 Indirect exposure of humans via the environment

Indirect exposure of humans to acetonitrile via the environment can be excluded during the production process, as the manufacturing takes place under strictly controlled conditions in closed systems. As described in chapters 4.3, 4.4 and 5.1, there is no tendency for acetonitrile to bioaccumulate and, therefore, there is no risk of indirect exposure of humans.

9.1.2.3 Environmental exposure

Environmental exposure was assessed using EUSES 2.0.3 and is summarised in the tables below. For details please refer to the EUSES report attached to this document.

Table 20: Duration, frequency and amounts related to emissions from production

Information type	Data field	Explanation
Annual amount used per site	2000 kg/y	--
Emission days per site	292 d/y	This figure was set in the EUSES calculation overriding the default value, based on the assumption of an average utilisation of 80%. This figure is considered to represent a worst case scenario.
Other determinants related to duration, frequency and amount	--	--

Table 21: Technical fate of substance and losses from process to waste, waste water and air

Information type	Data field	Explanation
Fraction of applied amount lost from process to waste gas	0.01 kg/kg	Based on data available in EU RAR (2002)
Fraction of applied amount lost from process to waste water (after internal recycling of substance, if any)	0.003 kg/kg	Based on data available in EU RAR (2002)
Fraction of applied amount lost from process to waste (after internal recycling of substance, if any)	not relevant	The fraction lost to waste is not relevant for release estimations, as measured release data is available and the exposure of the environment to acetonitrile through waste is negligible as waste is incinerated
Fraction of applied amount leaving the site with products	0 kg/kg	--
Fraction consumed in process	not relevant	The fraction consumed in process is not relevant, as real life release data exists

Table 22: Predicted Exposure Concentrations (PECs); regional PECs are negligible compared to local PECs

Compartments	Local concentration	PEC[1] (local+regional)	Justification
Surface water (in mg/L)	0.125		--
Fresh water sediment (in mg/kgwwt)	0.117		--
Sea water (mg/L)	0.0125		--
Marine sediment (mg/kgwwt)	0.0117		--
Agricultural soil total (averaged over 30 days; mg/kgwwt)	0.0163		--
STP (mg/L)	1.25		
Groundwater (mg/L)	0.0214		--
Grassland total (averaged over 180 days; mg/kgwwt)	$3.31 * 10^{-3}$		
Air (mg/m^3)	0.019		--

[1] Regional PECs are negligible compared to local PECs (see EUSES report). Therefore, no summation of local and regional PECs was performed.

9.2 Use 1: Starting material/solvent in chemical synthesis

9.2.1 Exposure scenario

Description of process:

Acetonitrile is used as a solvent or raw material in the chemical industry (mainly pharmaceutical industry). In general, acetonitrile is handled in closed systems. General processing duties include operating general pharmaceutical production equipment (reaction vessel, pipes and pumps).

According to the use descriptor system this use can be categorised as follows:

Sector of use: SU3 "Industrial Manufacturing"

Product category: Not relevant (the substance is not used in consumer products)

Process categories: PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"

PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"

PROC3 "Use in closed continuous batch process (synthesis or formulation); industrial setting"

Article category: Not relevant (the substance should not be present in articles in relevant amounts)

Environmental release category: Not relevant; environmental exposure assessment is based on measured data

9.2.1.1 Risk management measures

9.2.1.1.1 Risk management measures related to workers

Measures to prevent exposure comprise the use of adequate personal protection equipment (gloves, goggles, and coverall), local exhaustive ventilation, decontamination procedures before maintenance, wide use of automatic systems for sampling, information to workers on risk, etc.
In addition, regular workplace measurements are carried out to show that the DNELs derived are not exceeded. This ensures the safety of the worker in the production plant.

9.2.1.1.2 Risk management measures related to environment

Do not allow to directly enter the environment.

Any potential releases to air or water should be avoided.

Waste waters should be directed to an STP.

Use scrubbers to reduce emission to air.

9.2.2 Exposure estimation

9.2.2.1 Worker exposure

Measured air concentration data are available for the use of acetonitrile as starting material/solvent.

- Measurement during extraction processes showed air concentrations in the range of < 0.0001 to 2.7 ppm.
- Measurements were conducted in a company that distributes acetonitrile. Samples were collected in the close vicinity of the drum filling installation during filling operations and showed air concentrations of 774 µg/m^3 and 136.6 µg/m^3 (0.46 – 0.08 ppm). It was stated that the operator was wearing an air-cap with pressurised air during filling operations.
- Air concentration during laboratory work and process work was 10 ppm. The pattern of use has been reported as non-dispersive and the pattern of control as dilution ventilation.
- Workplace measurement in the pharmaceutical industry showed air concentrations of acetonitrile in the range "not detected" up to 16.8 ppm.
- Data from Germany (MEGA database, BIA) collected in different companies (plastic and pharmaceuticals) and research laboratories gave a 95th percentile of 7.3 ppm.

Considering the risk management measures described above and the closed production processes, the dermal exposure is considered to be negligible. Therefore, no further assessment is performed.

By analysing all measured exposure data together, a long-term exposure level of 7.3 ppm is estimated a reasonable worst-case situation and it will be used for risk characterisation purposes. In addition to the measured data, model calculations were performed using ECETOC TRA. The following table gives an overview on the scenarios assessed in relation to the process categories according to the descriptor system:

Table 23: ECETOC TRA scenarios (Use 1)

No.	Process category according to descriptor system	Exposure Scenario acc. to ECETOC TRA (non-dispersive uses)
1	PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"	Use in a closed continuous process
2	PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"	Use in a continuous process (with process sampling)
3	PROC3 "Use in closed continuous batch process (synthesis or formulation); industrial setting"	Use in a closed batch process i.e. where no opportunity for breaching arises, including product transfers and sampling

The following table summarises the output of the ECETOC TRA inhalative exposure estimation for the scenarios listed above.

Table 24: Model calculations with ECETOC TRA (Use 1)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [ppm]
Non-dispersive	Use in a closed continuous process	1 - 4 hours	Yes	0.006
Non-dispersive	Use in a continuous process (with process sampling)	1 - 4 hours	Yes	12.000
Non-dispersive	Use in a closed batch process i.e. where no opportunity for breaching arises, including product transfers and sampling	1 - 4 hours	Yes	12.000

The model calculations show estimated exposures in the range of 0.006 to 12 ppm for the different scenarios/work steps. The exposures are comparable to concentrations detected in workplace measurements.

9.2.2.2 Indirect exposure of humans via the environment

Indirect exposure of humans to acetonitrile via the environment can be excluded during the use as starting material/solvent as these processes take place under strictly controlled conditions in closed systems. As described in chapters 4.3, 4.4 and 5.1, there is no tendency for acetonitrile to bioaccumulate and, therefore, there is no risk of indirect exposure of humans.

9.2.2.3 Environmental exposure

Environmental exposure was assessed using EUSES 2.0.3 and is summarised in the tables below. For details please refer to the EUSES report attached to this document.

Table 25: Duration, frequency and amounts related to emissions from use as a starting material/solvent in chemical synthesis production

Information type	Data field	Explanation
Fraction of tonnage for application	0.65	--
Annual amount used per site (fraction of the main local source)	520 t/y (0.4)	--
Emission days per site	292 d/y	This figure was set in the EUSES calculation overriding the default value, based on the assumption of an average utilisation of 80%. This figure is considered to represent a worst case situation
Other determinants related to duration, frequency and amount	--	--

Table 26: Technical fate of substance and losses from process to waste, waste water and air

Information type	Data field	Explanation
Fraction of applied amount lost from process to waste gas	0.03 kg/kg	Based on data available in EU RAR (2002)
Absolute amount released to air per day	53 kg/day	calculated
Fraction of applied amount lost from process to waste water (after internal recycling of substance, if any)	0.06 kg/kg	Based on data available in EU RAR (2002)
Absolute amount released to waste water per day	107 kg/day	calculated
Fraction of applied amount lost from process to waste (after internal recycling of substance, if any)	not relevant	The fraction lost to waste is not relevant for release estimations, as measured release data is available and the exposure of the environment to acetonitrile through waste is negligible as waste and cleaning solutions are incinerated
Fraction of applied amount leaving the site with products	0 kg/kg	--
Fraction consumed in process	not relevant	The fraction consumed in process is not relevant, as real life release data exists

Table 27: Predicted Exposure Concentrations (PECs); regional PECs are negligible compared to local PECs

Compartments	Local concentration	PEC[1] (local+regional)	Justification
Surface water (in mg/L)	0.649		--
Fresh water sediment (in mg/kgwwt)	0.606		--
Sea water (mg/L)	0.0649		--
Marine sediment (mg/kgwwt)	0.0606		--
Agricultural soil total (averaged over 30 days; mg/kgwwt)	0.0777		--
STP (mg/L)	6.49		
Groundwater (mg/L)	0.0816		--
Grassland total (averaged over 180 days; mg/kgwwt)	$7.04 * 10^{-3}$		--
Air (mg/m^3)	0.0149		--

[1] Regional PECs are negligible compared to local PECs (see EUSES report). Therefore, no summation of local and regional PECs was performed.

9.3 Use 2: Analytical laboratories

9.3.1 Exposure scenario

Description of process:

Acetonitrile is used in analytical laboratories as a mobile phase in HPLC analyses. In general, acetonitrile is handled in closed systems. In rare cases small amounts (< 1 L, <1 kg) might be directly handled in a fume cupboard. General processing duties include operating general equipment (vessels, pipes and pumps).

According to the use descriptor system this use can be categorised as follows:

Sector of use: SUM71.2 “Technical testing and analysis”

Product category: PC21 “Laboratory chemicals”

Process categories: PROC1 “Used in closed processes, no likelihood of exposure; industrial setting”

PROC2 “Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting”

PROC3 “Use in closed continuous batch process (synthesis or formulation); industrial setting”3

PROC8: “Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non dedicated facilities Industrial or non-industrial setting”

PROC9 “Transfer of substance of preparation into small containers (dedicated filling line, including weighing); industrial setting”

PROC15 “Use as a laboratory reagent; non-industrial setting”

Article category: Not relevant (no articles are manufactured in analytical laboratories)

Environmental release category: Not relevant; environmental exposure assessment is based on measured data

9.3.1.1 Risk management measures

9.3.1.1.1 Risk management measures related to workers

Measures to prevent exposure comprise the use of adequate personal protection equipment (gloves, goggles, and coverall), local exhaustive ventilation, decontamination procedures before maintenance, information to workers on risk, etc.
In addition, regular workplace measurements are carried out to show that the DNELs derived are not exceeded. This ensures the safety of the worker in the production plant.

9.3.1.1.2 Risk management measures related to environment

Do not allow to directly enter the environment.

Any potential releases to air or water should be avoided.

Waste waters should be directed to an STP.

Use scrubbers to reduce emission to air.

9.3.2 Exposure estimation

9.3.2.1 Worker exposure

Workplace measurements are available for the use of acetonitrile in analytical laboratories. Data show that exposures around 4.76 – 7.3 ppm could be obtained in research laboratories in which acetonitrile is used in chromatography.
Considering the risk management measures described above and the closed production processes the dermal exposure is considered to be negligible. Therefore, no further assessment is performed.

The exposure level of 7.3 ppm is used for risk characterisation purposes.

In addition to the measured data, model calculations were performed using ECETOC TRA. The following table gives an overview on the scenarios assessed in relation to the process categories according to the descriptor system:

Table 28: ECETOC TRA scenarios (Use 2)

No.	Process category according to descriptor system	Exposure Scenario acc. to ECETOC TRA (non-dispersive uses)
1	PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"	Use in a closed continuous process
2	PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"	Use in a continuous process (with process sampling)
3	PROC3 "Use in closed continuous batch process (synthesis or formulation); industrial setting"	Use in a closed batch process i.e. where no opportunity for breaching arises, including product transfers and sampling
4	PROC8: "Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non dedicated facilities Industrial or non-industrial setting" PROC9 "Transfer of substance of preparation into small containers (dedicated filling line, including weighing); industrial setting"	Filling containers with the substance or its preparations
5	PROC15 "Use as a laboratory reagent; non-industrial setting"	Use as a laboratory reagent

The following table summarises the output of the ECETOC TRA inhalative exposure estimation for the scenarios listed above.

Table 29: Model calculations with ECETOC TRA (Use 2)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [ppm]
Non-dispersive	Use in a closed continuous process	1 - 4 hours	Yes	0.006
Non-dispersive	Use in a continuous process (with process sampling)	1 - 4 hours	Yes	12.000
Non-dispersive	Use in a closed batch process i.e. where no opportunity for breaching arises, including product transfers and sampling	1 - 4 hours	Yes	12.000
Non-dispersive	filling containers with the substance or its preparations	15 mins - 1 hour	Yes	10.000
Non-dispersive	Use as a laboratory reagent	1 - 4 hours	Yes	6.000

The model calculations show estimated exposures in the range of 0.006 to 12 ppm for the different scenarios/work steps. The exposures are close to concentrations detected in workplace measurements.

9.3.2.2 Indirect exposure of humans via the environment

Indirect exposure of humans to acetonitrile via the environment can be excluded during the use in analytical laboratories as the waste of analytical laboratories has to be disposed of according to the national regulations (e.g. incineration). As described in chapters 4.3, 4.4 and 5.1, there is no tendency for acetonitrile to bioaccumulate and, therefore, there is no risk of indirect exposure of humans.

9.3.2.3 Environmental exposure

Environmental exposure was assessed using EUSES 2.0.3 and is summarised in the tables below. For details please refer to the EUSES report attached to this document (Annex I).

Table 30: Duration, frequency and amounts related to emissions from use as a starting material/solvent in chemical synthesis production

Information type	Data field	Explanation
Fraction of tonnage for application	0.35	--
Annual amount used per site (Fraction of the main local source)	280 t/y (0.4)	--
Emission days per site	292 d/y	This figure was set in the EUSES calculation overriding the default value, based on the assumption of an average utilisation of 80%. This figure is considered to represent a worst case situation.
Other determinants related to duration, frequency and amount	--	--

Table 31: Technical fate of substance and losses from process to waste, waste water and air

Information type	Data field	Explanation
Fraction of applied amount lost from process to waste gas	0.025 kg/kg	Based on data available in EU RAR (2002)
Absolut amount released to air per day	24 kg/day	calculated
Fraction of applied amount lost from process to waste water (after internal recycling of substance, if any)	0.02 kg/kg	Based on data available in EU RAR (2002)
Absolute amount released to waste water per day	19.2	calculated
Fraction of applied amount lost from process to waste (after internal recycling of substance, if any)	not relevant	The fraction lost to waste is not relevant for release estimations, as measured release data is available and the exposure of the environment to acetonitrile through waste is negligible as waste is incinerated
Fraction of applied amount leaving the site with products	0 kg/kg	--
Fraction consumed in process	not relevant	The fraction consumed in process is not relevant, as real life release data exists

Table 32: Predicted Exposure Concentrations (PECs); regional PECs are negligible compared to local PECs

Compartments	Local concentration	PEC[1] (local+regional)	Justification
Surface water (in mg/L)	0.117		--
Fresh water sediment (in mg/kgwwt)	0.109		--
Sea water (mg/L)	0.0117		--
Marine sediment (mg/kgwwt)	0.0109		--
Agricultural soil total (averaged over 30 days; mg/kgwwt)	0.0143		--
STP (mg/L)	1.16		
Groundwater (mg/L)	0.0161		--
Grassland total (averaged over 180 days; mg/kgwwt)	$1.75 * 10^{-3}$		--
Air (mg/m^3)	$6.66 * 10^{-3}$		--

[1] Regional PECs are negligible compared to local PECs (see EUSES report). Therefore, no summation of local and regional PECs was performed.

9.4 Regional exposure concentrations

Regional exposure concentrations are negligible. Please refer to the EUSES report in the attachment for details (Annex I).

10 RISK CHARACTERISATION

10.1 Use 0: Production of Acetonitrile

10.1.1 Human health

10.1.1.1 Risk Characterisation for Workers

Table 33: Quantitative risk characterisation for workers based on measured data

Route		ES 0- exposure concentrations (EC)	Leading toxic end point / Critical effect	DNEL	Risk characterisation ratio
Inhalation - systemic/ combined routes	**Acute**	0.1 ppm	--	32 ppm	0.003
	Long term		increased liver weight	20 ppm	0.005

Table 34: Quantitative risk characterisation for workers based on modelled data in terms of generic exposure scenarios

UEC Matrix Element	Process Categories	Estimated Exposure [ppm]	LEV	Duration of activity	DNEL	Risk characterisation ratio
13 Inhalation Short-term	PROC1	0.006	yes	1 – 4 h	32 ppm	0.0002
	PROC2	12.0	yes	1 – 4 h		0.38
	PROC3	12.0	yes	1 – 4 h		0.38
	PROC8	10.0	yes	15 min – 1 h		0.31
16 Inhalation Long-term / repeated	PROC1	0.006	yes	1 – 4 h	20 ppm	0.0003
	PROC2	12.0	yes	1 – 4 h		0.6
	PROC3	12.0	yes	1 – 4 h		0.6
	PROC8	10.0	yes	15 min – 1 h		0.5

Conclusion (i): the substance is of no immediate concern for man.

10.1.1.2 Indirect exposure of humans via the environment

Not relevant, see chapter 9.1.2.2.

10.1.2 Environment

10.1.2.1 Risk Characterisation (PEC/PNEC)

Table 35: Quantitative risk characterisation for environmental compartments

UEC Matrix Element	Compartments	Local PEC	PNEC	PEC/PNEC
22 Environment: Water, continuous	**Surface water (in mg/L)**	0.125	0.73	0.171
	Fresh water sediment (in mg/kgwwt)	0.117	0.682	0.171
	Sea water (mg/L)	0.0125	0.073	0.171
	Marine sediment (mg/kgwwt)	0.0117	0.0682	0.171
	Agricultural soil total (averaged over 30 days; mg/kgwwt)	0.0163	0.176	0.0929
	STP (mg/L)	1.25	7.3	0.171
28 Environment Air, continuous	**Air (mg/m^3)**	0.019	34 ($DNEL_{long\text{-}term}$)	0.006

Conclusion (i): the substance is of no immediate concern for the environment.

The risk for the environment is considered to be acceptable for all relevant compartments, as all PEC/PNEC values are below the trigger value of 1.

10.2 Use 1: Starting material/solvent in chemical synthesis

10.2.1 Human health

10.2.1.1 Risk Characterisation for workers

Table 36: Quantitative risk characterisation for workers based on measured data

Route		ES 1-exposure concentrations (EC)	Leading toxic end point / Critical effect	DNEL	Risk characterisation ratio
Inhalation - systemic/ combined routes	**Acute**	7.3 ppm	--	32 ppm	0.23
	Long term		increased liver weights	20 ppm	0.37

Table 37: Quantitative risk characterisation for workers based on modelled data in terms of generic exposure scenarios

UEC Matrixelement	Process Categories	Estimated Exposure [ppm]	LEV	Duration of activity	DNEL	Risk characterisation ratio
13 Inhalation Short-term	PROC1	0.006	yes	1 – 4 h	32 ppm	0.0002
	PROC2	12.0	yes	1 – 4 h		0.38
	PROC3	12.0	yes	1 – 4 h		0.38
16 Inhalation Long-term / repeated	PROC1	0.006	yes	1 – 4 h	20 ppm	0.0003
	PROC2	12.0	yes	1 – 4 h		0.6
	PROC3	12.0	yes	1 – 4 h		0.6

The results of the modelled data show, that the use of acetonitrile as a starting material in chemical synthesis can be considered to be of acceptable risk, when the RMM LEV and limited duration of activity are followed.

Conclusion (i): the substance is of no immediate concern for man.

10.2.1.2 Indirect exposure of humans via the environment

Not relevant, see chapter 9.2.2.2

10.2.2 Environment

10.2.2.1 Risk Characterisation (PEC/PNEC)

Table 38: Quantitative risk characterisation for environmental compartments

UEC Matrix Element	Compartments	Local concentration	PNEC	PEC/PNEC
22 Environment: Water, continuous	**Surface water (in mg/L)**	0.649	0.73	0.889
	Fresh water sediment (in mg/kgwwt)	0.606	0.682	0.889
	Sea water (mg/L)	0.0649	0.073	0.889
	Marine sediment (mg/kgwwt)	0.0606	0.0682	0.889
	Agricultural soil total (averaged over 30 days; mg/kgwwt)	0.0777	0.176	0.442
	STP (mg/L)	6.49	7.3	0.889
28 Environment Air, continuous	**Air (mg/m^3)**	0.0149	34 ($DNEL_{long\text{-}term}$)	0.00045

The risk for the environment is considered to be acceptable for all relevant compartments, as all PEC/PNEC values are below the trigger value of 1. However, users of acetonitrile may need to perform their own exposure assessment to ensure that their emissions to the environment lead to PECs below the relevant PNECs.

The highest PEC/PNEC ratio for this exposure scenario is 0.889. This PEC/PNEC ratio corresponds to a release to waste water of 107 kg/day. Hence, a release below 120 kg/day, corresponding to a PEC/PNEC < 1, should result in an acceptable risk for the environment, provided that the defaults in EUSES are comparable to the real life situation assessed and that waste waters are directed to an STP.

Conclusion (i): the substance is of no immediate concern for the environment.

10.3 Use 2: Analytical laboratories

10.3.1 Human health

10.3.1.1 Risk Characterisation for workers

Table 39: Quantitative risk characterisation for workers based on measured data

Route		ES 2-exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Inhalation - systemic/ combined routes	**Acute**	7.3 ppm	--	32 ppm	0.23
	Long term		increased liver effects	20 ppm	0.37

Table 40: Quantitative risk characterisation for workers based on modelled data in terms of generic exposure scenarios

UEC Matrixelement	Process Categories	Estimated Exposure [ppm]	LEV	Duration of activity	DNEL	Risk characterisation ratio
13 Inhalation Short-term	PROC1	0.006	yes	1 – 4 h	32 ppm	0.0002
	PROC2	12.0	yes	1 – 4 h		0.38
	PROC3	12.0	yes	1 – 4 h		0.38
	PROC8	10.0	yes	15 min – 1 h		0.31
	PROC9	10.0	yes	15 min – 1 h		0.31
	PROC15	6.0	yes	1 – 4 h		0.19
16 Inhalation Long-term / repeated	PROC1	0.006	yes	1 – 4 h	20 ppm	0.0003
	PROC2	12.0	yes	1 – 4 h		0.6
	PROC3	12.0	yes	1 – 4 h		0.6
	PROC8	10.0	yes	15 min – 1 h		0.5
	PROC9	10.0	yes	15 min – 1 h		0.5
	PROC15	6.0	yes	1 – 4 h		0.3

The results of the modelled data show, that the use of acetonitrile in analytical laboratories can be considered to be of acceptable risk, when the RMM LEV and limited duration of activity are followed.

Conclusion (i): the substance is of no immediate concern for man.

10.3.1.2 Indirect exposure of humans via the environment

not relevant, see chapter 9.3.2.2

10.3.2 Environment

10.3.2.1 Risk Characterisation (PEC/PNEC)

Table 41: Quantitative risk characterisation for environmental compartments

UEC Matrix Element	Compartments	Local concentration	PNEC	PEC/PNEC
22 Environment: Water, continuous	**Surface water (in mg/L)**	0.117	0.73	0.16
	Fresh water sediment (in mg/kgwwt)	0.109	0.682	0.16
	Sea water (mg/L)	0.0117	0.073	0.16
	Marine sediment (mg/kgwwt)	0.0109	0.0682	0.16
	Agricultural soil total (averaged over 30 days; mg/kgwwt)	0.0143	0.176	0.0813
	STP (mg/L)	1.16	7.3	0.16
28 Environment Air, continuous	**Air (mg/m^3)**	$6.66 * 10^{-3}$	34 ($DNEL_{long\text{-}term}$)	0.0002

The risk for the environment is considered to be acceptable for all relevant compartments, as all PEC/PNEC values are below the trigger value of 1. However, users of acetonitrile may need to perform their own exposure assessment to ensure that their emissions to the environment lead to PECs below the relevant PNECs.

The highest PEC/PNEC ratio for this exposure scenario is 0.16. This PEC/PNEC ratio corresponds to a release to waste water of 19.2 kg/day. Hence, a release below 120 kg/day, corresponding to a PEC/PNEC < 1, should result in an acceptable risk for the environment, provided that the defaults in EUSES are comparable to the real life situation assessed and that waste waters are directed to an STP.

Conclusion (i): the substance is of no immediate concern for the environment.

10.4 Overall exposure (combined for all relevant emission/release sources)

10.4.1 Human health (combined for all exposure routes)

The scenarios displayed in the worker exposure scenario chapters are comparable for each use, i.e. the scenario in the manufacturing plant is similar to the scenario “use of acetonitrile as starting material/solvent”. The workplace measurements show that the use of acetonitrile in analytical laboratories results is similar worker exposure as the use “starting material/solvent”.

Considering the work pattern in the manufacturing plant, in the plant using acetonitrile as starting material/solvent and in analytical laboratories and the non-relevance of indirect exposure it can be excluded that workers are exposed to acetonitrile from more than one emission source.

The workplace measurements show that the manufacturing of acetonitrile, the use of acetonitrile as starting material/solvent and the use in analytical laboratories results in acceptable exposure.

Conclusion (i): overall the substance is of no immediate concern for man.

10.4.2 Environment (combined for all emission sources)

Combined exposure through the use of acetonitrile which is produced by the company responsible for this CSR might be possible. However, the assumption in the exposure estimation that a local source may use a fraction of up to 40% of the total amount sold for a specific use, is considered to be a conservative worst case approach to cover emissions from more than one source located in close proximity to each other.

Conclusion (i): overall the substance is of no immediate concern for the environment.

Appendix I: EUSES 2.0.3 Report

The following default values were replaced in the EUSES calculation:

- For all scenarios the use of an STP was assumed for the marine compartment.
- Release fractions were set on the basis of information available in the European Union Risk Assessment Report (2002) as follows:

Scenario	Release fraction Air	Release Fraction Water
Production	0.01	0.003
Synthesis	0.03	0.06
Analytical Laboratory	0.025	0.02

- The number of emission days was set to 292 days for all scenarios, based on the assumption of an average utilisation of 80%. This figure is considered to represent a worst case situation.

NAME	REFERENCE	VALUE	UNITS	STATUS
IDENTIFICATION OF THE SUBSTANCE				
GENERAL NAME	ACETONITRILE	ACETONITRILE		S
CAS-NO	75-05-8	75-05-8		S
EC-NOTIFICATION NO.	608-001-00-3	608-001-00-3		S
EINECS NO.	200-835-2	200-835-2		S
MOLECULAR WEIGHT	41.05	41.05	[G.MOL-1]	S

NAME	REFERENCE	VALUE	UNITS	STATUS
PHYSICO-CHEMICAL PROPERTIES				
MELTING POINT	-45.7	-45.7	[OC]	S
BOILING POINT	81.6	81.6	[OC]	S
VAPOUR PRESSURE AT TEST TEMPERATURE	98.64	98.64	[HPA]	S
VAPOUR PRESSURE AT 25 [OC]	9.86E+03	9.86E+03	[PA]	O
WATER SOLUBILITY AT TEST TEMPERATURE	1E+05	1E+05	[MG.L-1]	S
WATER SOLUBILITY AT 25 [OC]	1E+05	1E+05	[MG.L-1]	O
OCTANOL-WATER PARTITION COEFFICIENT	-0.34	-0.34	[LOG10]	S
HENRY'S LAW CONSTANT	4.05	4.05	[PA.M3.MOL-1]	O

NAME	REFERENCE	VALUE	UNITS	STATUS
ENVIRONMENT-EXPOSURE				
RELEASE ESTIMATION				
TONNAGE OF SUBSTANCE IN EUROPE	2E+03	2E+03	[TONNES.YR-1]	O
REGIONAL PRODUCTION VOLUME OF SUBSTANCE	2E+03	2E+03	[TONNES.YR-1]	O
ENVIRONMENT-EXPOSURE				
RELEASE ESTIMATION				
[1 "PRODUCTION", IC=15/UC=55]				
INDUSTRY CATEGORY	15/0 OTHERS	15/0 OTHERS		D
USE CATEGORY	55/0 OTHERS	55/0 OTHERS		D
FRACTION OF TONNAGE FOR APPLICATION	1	1	[-]	O
ENVIRONMENT-EXPOSURE				
RELEASE ESTIMATION				
[PRODUCTION]				
USE SPECIFIC EMISSION SCENARIO	NO	NO		D
EMISSION TABLES	A1.1 (GENERAL TABLE), B1.6 (GENERAL TABLE)			
		A1.1 (GENERAL TABLE), B1.6 (GENERAL TABLE)	S	
EMISSION SCENARIO	NO SPECIAL SCENARIO SELECTED/AVAILABLE			
		NO SPECIAL SCENARIO SELECTED/AVAILABLE	S	
MAIN CATEGORY PRODUCTION	III MULTI-PURPOSE EQUIPMENT			
		III MULTI-PURPOSE EQUIPMENT		D
FRACTION OF TONNAGE RELEASED TO AIR	0.05	0.01	[-]	S
FRACTION OF TONNAGE RELEASED TO WASTE WATER	3E-03	3E-03	[-]	S
FRACTION OF TONNAGE RELEASED TO SURFACEWATER	0	0	[-]	O
FRACTION OF TONNAGE RELEASED TO INDUSTRIAL SOIL	1E-04	1E-04	[-]	O
FRACTION OF TONNAGE RELEASED TO AGRICULTURAL SOIL	0	0	[-]	O
FRACTION OF THE MAIN LOCAL SOURCE	1	1	[-]	O
NUMBER OF EMISSION DAYS PER YEAR	300	292	[-]	S
LOCAL EMISSION TO AIR DURING EPISODE	333	68.5	[KG.D-1]	O
LOCAL EMISSION TO WASTEWATER DURING EPISODE	20	20.5	[KG.D-1]	O
INTERMITTENT RELEASE	NO	NO		D
ENVIRONMENT-EXPOSURE				
RELEASE ESTIMATION				
[2 "STARTING MATERIAL/SOLVENT IN CHEMICAL SYNTHESIS", IC=3/UC=41]				
INDUSTRY CATEGORY	3 CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS			
		3 CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS	S	
USE CATEGORY	41 PHARMACEUTICALS			
		41 PHARMACEUTICALS		S
FRACTION OF TONNAGE FOR APPLICATION	0.65	0.65	[-]	O

NAME	REFERENCE	VALUE	UNITS	STATUS
ENVIRONMENT-EXPOSURE				
RELEASE ESTIMATION				
[INDUSTRIAL USE]				
USE SPECIFIC EMISSION SCENARIO	NO	NO		D
EMISSION TABLES	A3.3 (IC-SPECIFIC), B3.2 (GENERAL TABLE)			
		A3.3 (IC-SPECIFIC), B3.2 (GENERAL TABLE)	S	
EMISSION SCENARIO	NO SPECIAL SCENARIO SELECTED/AVAILABLE			
		NO SPECIAL SCENARIO SELECTED/AVAILABLE	S	
MAIN CATEGORY INDUSTRIAL USE	IC INTERMED. STORED OFF-SITE/DEDICATED EQUIP.			
		IC INTERMED. STORED OFF-SITE/DEDICATED EQUIP.	D	
FRACTION OF TONNAGE RELEASED TO AIR	1E-03	0.03	[-]	S
FRACTION OF TONNAGE RELEASED TO WASTE WATER	7E-03	0.06	[-]	S
FRACTION OF TONNAGE RELEASED TO SURFACEWATER	0	0	[-]	O
FRACTION OF TONNAGE RELEASED TO INDUSTRIAL SOIL	1E-04	1E-04	[-]	O
FRACTION OF TONNAGE RELEASED TO AGRICULTURAL SOIL	0	0	[-]	O
FRACTION OF THE MAIN LOCAL SOURCE	0.4	0.4	[-]	O
NUMBER OF EMISSION DAYS PER YEAR	130	292	[-]	S
LOCAL EMISSION TO AIR DURING EPISODE	4	53.4	[KG.D-1]	O
LOCAL EMISSION TO WASTEWATER DURING EPISODE	28	107	[KG.D-1]	O
INTERMITTENT RELEASE	NO	NO		D
ENVIRONMENT-EXPOSURE				
RELEASE ESTIMATION				
[3 "ANALYTICAL LABORATORIES", IC=2/UC=34]				
INDUSTRY CATEGORY	2 CHEMICAL INDUSTRY: BASIC CHEMICALS			
		2 CHEMICAL INDUSTRY: BASIC CHEMICALS	S	
USE CATEGORY	34 LABORATORY CHEMICALS			
		34 LABORATORY CHEMICALS		S
FRACTION OF TONNAGE FOR APPLICATION	0.35	0.35	[-]	S
ENVIRONMENT-EXPOSURE				
RELEASE ESTIMATION				
[INDUSTRIAL USE]				
USE SPECIFIC EMISSION SCENARIO	NO	NO		D
EMISSION TABLES	A3.2 (GENERAL TABLE), B3.2 (GENERAL TABLE)			
		A3.2 (GENERAL TABLE), B3.2 (GENERAL TABLE)	S	
EMISSION SCENARIO	NO SPECIAL SCENARIO SELECTED/AVAILABLE			
		NO SPECIAL SCENARIO SELECTED/AVAILABLE	S	
FRACTION OF TONNAGE RELEASED TO AIR	0.25	0.025	[-]	S
FRACTION OF TONNAGE RELEASED TO WASTE WATER	0.65	0.02	[-]	S
FRACTION OF TONNAGE RELEASED TO SURFACEWATER	0	0	[-]	O
FRACTION OF TONNAGE RELEASED TO INDUSTRIAL SOIL	1E-03	1E-03	[-]	O
FRACTION OF TONNAGE RELEASED TO AGRICULTURAL SOIL	0	0	[-]	O
FRACTION OF THE MAIN LOCAL SOURCE	0.4	0.4	[-]	O
NUMBER OF EMISSION DAYS PER YEAR	70	292	[-]	S
LOCAL EMISSION TO AIR DURING EPISODE	1E+03	24	[KG.D-1]	O
LOCAL EMISSION TO WASTEWATER DURING EPISODE	2.6E+03	19.2	[KG.D-1]	O
INTERMITTENT RELEASE	NO	NO		D

NAME	REFERENCE	VALUE	UNITS	STATUS
ENVIRONMENT-EXPOSURE				
RELEASE ESTIMATION				
TOTAL REGIONAL EMISSIONS TO COMPARTMENTS				
TOTAL REGIONAL EMISSION TO AIR	757	210	[KG.D-1]	O
TOTAL REGIONAL EMISSION TO WASTEWATER	1.03E+03	215	[KG.D-1]	O
TOTAL REGIONAL EMISSION TO SURFACE WATER	258	53.7	[KG.D-1]	O
TOTAL REGIONAL EMISSION TO INDUSTRIAL SOIL	2.82	2.82	[KG.D-1]	O
TOTAL REGIONAL EMISSION TO AGRICULTURAL SOIL	0	0	[KG.D-1]	O
ENVIRONMENT-EXPOSURE				
DEGRADATION AND TRANSFORMATION				
CHARACTERIZATION OF BIODEGRADABILITY	NOT BIODEGRADABLE			
		READILY BIODEGRADABLE		S
DEGRADATION CALCULATION METHOD IN STP	FIRST ORDER, STANDARD OECD/EU TESTS			
		FIRST ORDER, STANDARD OECD/EU TESTS	D	
RATE CONSTANT FOR BIODEGRADATION IN STP	0	24	[D-1]	O
RATE CONSTANT FOR BIODEGRADATION IN SURFACE WATER	0	0.0462	[D-1] (12[OC])	O
RATE CONSTANT FOR BIODEGRADATION IN BULK SOIL	6.93E-07	0.0231	[D-1] (12[OC])	O
RATE CONSTANT FOR BIODEGRADATION IN AERATED SEDIMENT	6.93E-07	0.0231	[D-1] (12[OC])	O
RATE CONSTANT FOR HYDROLYSIS IN SURFACE WATER	6.93E-07	6.93E-07	[D-1] (12[OC])	O
RATE CONSTANT FOR PHOTOLYSIS IN SURFACE WATER	6.93E-07	6.93E-07	[D-1]	O
ENVIRONMENT-EXPOSURE				
SEWAGE TREATMENT				
LOCAL STP [1 "PRODUCTION", IC=15/UC=55][PRODUCTION]				
OUTPUT				
FRACTION OF EMISSION DIRECTED TO AIR BY STP	7.08	1.55	[%]	O
FRACTION OF EMISSION DIRECTED TO WATER BY STP	92.8	12.1	[%]	O
FRACTION OF EMISSION DIRECTED TO SLUDGE BY STP	0.0859	0.0656	[%]	O
FRACTION OF THE EMISSION DEGRADED IN STP	0	86.2	[%]	O
CONCENTRATION IN UNTREATED WASTEWATER	10	10.3	[MG.L-1]	O
CONCENTRATION OF CHEMICAL (TOTAL) IN THE STP-EFFLUENT	9.28	1.25	[MG.L-1]	O
CONCENTRATION IN EFFLUENT EXCEEDS SOLUBILITY	NO	NO		O
CONCENTRATION IN DRY SEWAGE SLUDGE	21.7	17.1	[MG.KG-1]	O
PEC FOR MICRO-ORGANISMS IN THE STP	9.28	1.25	[MG.L-1]	O
ENVIRONMENT-EXPOSURE				
SEWAGE TREATMENT				
LOCAL STP [2 "STARTING MATERIAL/SOLVENT IN CHEMICAL SYNTHESIS", IC=3/UC=41][INDUSTRIAL USE]				
OUTPUT				
FRACTION OF EMISSION DIRECTED TO AIR BY STP	7.08	1.55	[%]	O
FRACTION OF EMISSION DIRECTED TO WATER BY STP	92.8	12.1	[%]	O
FRACTION OF EMISSION DIRECTED TO SLUDGE BY STP	0.0859	0.0656	[%]	O
FRACTION OF THE EMISSION DEGRADED IN STP	0	86.2	[%]	O
CONCENTRATION IN UNTREATED WASTEWATER	14	53.4	[MG.L-1]	O
CONCENTRATION OF CHEMICAL (TOTAL) IN THE STP-EFFLUENT	13	6.49	[MG.L-1]	O
CONCENTRATION IN EFFLUENT EXCEEDS SOLUBILITY	NO	NO		O
CONCENTRATION IN DRY SEWAGE SLUDGE	30.4	88.7	[MG.KG-1]	O
PEC FOR MICRO-ORGANISMS IN THE STP	13	6.49	[MG.L-1]	O
ENVIRONMENT-EXPOSURE				
SEWAGE TREATMENT				
LOCAL STP [3 "ANALYTICAL LABORATORIES", IC=2/UC=34][INDUSTRIAL USE]				
OUTPUT				
FRACTION OF EMISSION DIRECTED TO AIR BY STP	7.08	1.55	[%]	O
FRACTION OF EMISSION DIRECTED TO WATER BY STP	92.8	12.1	[%]	O
FRACTION OF EMISSION DIRECTED TO SLUDGE BY STP	0.0859	0.0656	[%]	O
FRACTION OF THE EMISSION DEGRADED IN STP	0	86.2	[%]	O
CONCENTRATION IN UNTREATED WASTEWATER	1.3E+03	9.59	[MG.L-1]	O
CONCENTRATION OF CHEMICAL (TOTAL) IN THE STP-EFFLUENT	1.21E+03	1.16	[MG.L-1]	O
CONCENTRATION IN EFFLUENT EXCEEDS SOLUBILITY	NO	NO		O
CONCENTRATION IN DRY SEWAGE SLUDGE	2.83E+03	15.9	[MG.KG-1]	O
PEC FOR MICRO-ORGANISMS IN THE STP	1.21E+03	1.16	[MG.L-1]	O

NAME	REFERENCE	VALUE	UNITS	STATUS
ENVIRONMENT-EXPOSURE				
DISTRIBUTION				
LOCAL SCALE				
[1 "PRODUCTION", IC=15/UC=55][PRODUCTION]				
CONCENTRATION IN AIR DURING EMISSION EPISODE	0.0927	0.019	[MG.M-3]	O
ANNUAL AVERAGE CONCENTRATION IN AIR, 100 M FROM POINT SOURCE	0.0762	0.0152	[MG.M-3]	O
CONCENTRATION IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	0.928	0.125	[MG.L-1]	O
ANNUAL AVERAGE CONCENTRATION IN SURFACE WATER (DISSOLVED)	0.763	0.0998	[MG.L-1]	O
LOCAL PEC IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	0.931	0.125	[MG.L-1]	O
ANNUAL AVERAGE LOCAL PEC IN SURFACE WATER (DISSOLVED)	0.766	0.1	[MG.L-1]	O
LOCAL PEC IN FRESH-WATER SEDIMENT DURING EMISSION EPISODE	0.87	0.117	[MG.KGWWT-1]	O
CONCENTRATION IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	0.0928	0.0125	[MG.L-1]	O
ANNUAL AVERAGE CONCENTRATION IN SEA WATER (DISSOLVED)	0.0763	9.98E-03	[MG.L-1]	O
LOCAL PEC IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	0.0931	0.0125	[MG.L-1]	O
ANNUAL AVERAGE LOCAL PEC IN SEA WATER (DISSOLVED)	0.0766	1E-02	[MG.L-1]	O
LOCAL PEC IN MARINE SEDIMENT DURING EMISSION EPISODE	0.087	0.0117	[MG.KGWWT-1]	O
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 30 DAYS	0.0451	0.0163	[MG.KGWWT-1]	O
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 180 DAYS	0.03	5.16E-03	[MG.KGWWT-1]	O
LOCAL PEC IN GRASSLAND (TOTAL) AVERAGED OVER 180 DAYS	0.0219	3.31E-03	[MG.KGWWT-1]	O
LOCAL PEC IN GROUNDWATER UNDER AGRICULTURAL SOIL	0.125	0.0214	[MG.L-1]	O
ENVIRONMENT-EXPOSURE				
DISTRIBUTION				
LOCAL SCALE				
[2 "STARTING MATERIAL/SOLVENT IN CHEMICAL SYNTHESIS", IC=3/UC=41][INDUSTRIAL USE]				
CONCENTRATION IN AIR DURING EMISSION EPISODE	1.11E-03	0.0149	[MG.M-3]	O
ANNUAL AVERAGE CONCENTRATION IN AIR, 100 M FROM POINT SOURCE	3.96E-04	0.0119	[MG.M-3]	O
CONCENTRATION IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	1.3	0.649	[MG.L-1]	O
ANNUAL AVERAGE CONCENTRATION IN SURFACE WATER (DISSOLVED)	0.463	0.519	[MG.L-1]	O
LOCAL PEC IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	1.3	0.649	[MG.L-1]	O
ANNUAL AVERAGE LOCAL PEC IN SURFACE WATER (DISSOLVED)	0.466	0.519	[MG.L-1]	O
LOCAL PEC IN FRESH-WATER SEDIMENT DURING EMISSION EPISODE	1.22	0.606	[MG.KGWWT-1]	O
CONCENTRATION IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	0.13	0.0649	[MG.L-1]	O
ANNUAL AVERAGE CONCENTRATION IN SEA WATER (DISSOLVED)	0.0463	0.0519	[MG.L-1]	O
LOCAL PEC IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	0.13	0.0649	[MG.L-1]	O
ANNUAL AVERAGE LOCAL PEC IN SEA WATER (DISSOLVED)	0.0466	0.0519	[MG.L-1]	O
LOCAL PEC IN MARINE SEDIMENT DURING EMISSION EPISODE	0.122	0.0606	[MG.KGWWT-1]	O
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 30 DAYS	0.0356	0.0777	[MG.KGWWT-1]	O
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 180 DAYS	0.0146	0.0196	[MG.KGWWT-1]	O
LOCAL PEC IN GRASSLAND (TOTAL) AVERAGED OVER 180 DAYS	3.19E-03	7.04E-03	[MG.KGWWT-1]	O
LOCAL PEC IN GROUNDWATER UNDER AGRICULTURAL SOIL	0.0605	0.0816	[MG.L-1]	O
ENVIRONMENT-EXPOSURE				
DISTRIBUTION				
LOCAL SCALE				
[3 "ANALYTICAL LABORATORIES", IC=2/UC=34][INDUSTRIAL USE]				
CONCENTRATION IN AIR DURING EMISSION EPISODE	0.278	6.66E-03	[MG.M-3]	O
ANNUAL AVERAGE CONCENTRATION IN AIR, 100 M FROM POINT SOURCE	0.0533	5.33E-03	[MG.M-3]	O
CONCENTRATION IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	121	0.116	[MG.L-1]	O
ANNUAL AVERAGE CONCENTRATION IN SURFACE WATER (DISSOLVED)	23.1	0.0932	[MG.L-1]	O
LOCAL PEC IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	121	0.117	[MG.L-1]	O
ANNUAL AVERAGE LOCAL PEC IN SURFACE WATER (DISSOLVED)	23.1	0.0933	[MG.L-1]	O
LOCAL PEC IN FRESH-WATER SEDIMENT DURING EMISSION EPISODE	113	0.109	[MG.KGWWT-1]	O
CONCENTRATION IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	12.1	0.0116	[MG.L-1]	O
ANNUAL AVERAGE CONCENTRATION IN SEA WATER (DISSOLVED)	2.31	9.32E-03	[MG.L-1]	O
LOCAL PEC IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	12.1	0.0117	[MG.L-1]	O
ANNUAL AVERAGE LOCAL PEC IN SEA WATER (DISSOLVED)	2.31	9.33E-03	[MG.L-1]	O
LOCAL PEC IN MARINE SEDIMENT DURING EMISSION EPISODE	11.3	0.0109	[MG.KGWWT-1]	O
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 30 DAYS	3.31	0.0143	[MG.KGWWT-1]	O
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 180 DAYS	1.35	3.87E-03	[MG.KGWWT-1]	O
LOCAL PEC IN GRASSLAND (TOTAL) AVERAGED OVER 180 DAYS	0.297	1.75E-03	[MG.KGWWT-1]	O
LOCAL PEC IN GROUNDWATER UNDER AGRICULTURAL SOIL	5.62	0.0161	[MG.L-1]	O

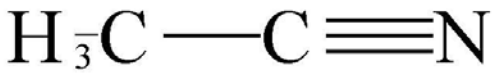
NAME	REFERENCE	VALUE	UNITS	STATUS
ENVIRONMENT-EXPOSURE				
DISTRIBUTION				
REGIONAL AND CONTINENTAL SCALE				
CONTINENTAL				
CONTINENTAL PEC IN SURFACE WATER (DISSOLVED)	7.7E-06	1.11E-07	[MG.L-1]	O
CONTINENTAL PEC IN SEA WATER (DISSOLVED)	7.02E-06	4.99E-09	[MG.L-1]	O
CONTINENTAL PEC IN AIR (TOTAL)	6.08E-06	1.35E-07	[MG.M-3]	O
CONTINENTAL PEC IN AGRICULTURAL SOIL (TOTAL)	2.98E-06	3.09E-08	[MG.KGWWT-1]	O
CONTINENTAL PEC IN PORE WATER OF AGRICULTURAL SOILS	1.24E-05	1.28E-07	[MG.L-1]	O
CONTINENTAL PEC IN NATURAL SOIL (TOTAL)	2.98E-06	4.69E-08	[MG.KGWWT-1]	O
CONTINENTAL PEC IN INDUSTRIAL SOIL (TOTAL)	2.98E-06	4.69E-08	[MG.KGWWT-1]	O
CONTINENTAL PEC IN SEDIMENT (TOTAL)	6.4E-06	9E-08	[MG.KGWWT-1]	O
CONTINENTAL PEC IN SEA WATER SEDIMENT (TOTAL)	5.91E-06	4.09E-09	[MG.KGWWT-1]	O
ENVIRONMENT-EXPOSURE				
DISTRIBUTION				
REGIONAL AND CONTINENTAL SCALE				
REGIONAL				
REGIONAL PEC IN SURFACE WATER (DISSOLVED)	3.02E-03	1.42E-04	[MG.L-1]	O
REGIONAL PEC IN SEA WATER (DISSOLVED)	2.72E-04	1.12E-05	[MG.L-1]	O
REGIONAL PEC IN AIR (TOTAL)	3.7E-05	4.53E-06	[MG.M-3]	O
REGIONAL PEC IN AGRICULTURAL SOIL (TOTAL)	2.43E-05	1.37E-06	[MG.KGWWT-1]	O
REGIONAL PEC IN PORE WATER OF AGRICULTURAL SOILS	1.01E-04	5.71E-06	[MG.L-1]	O
REGIONAL PEC IN NATURAL SOIL (TOTAL)	1.81E-05	1.57E-06	[MG.KGWWT-1]	O
REGIONAL PEC IN INDUSTRIAL SOIL (TOTAL)	1.36E-04	6.34E-05	[MG.KGWWT-1]	O
REGIONAL PEC IN SEDIMENT (TOTAL)	2.51E-03	1.15E-04	[MG.KGWWT-1]	O
REGIONAL PEC IN SEA WATER SEDIMENT (TOTAL)	2.29E-04	9.2E-06	[MG.KGWWT-1]	O
ENVIRONMENT-EXPOSURE				
BIOCONCENTRATION				
BIOCONCENTRATION FACTOR FOR EARTHWORMS	0.845	0.845	[L.KGWWT-1]	O
BIOCONCENTRATION FACTOR FOR FISH	1.41	1.41	[L.KGWWT-1]	O

NAME	REFERENCE	VALUE	UNITS	STATUS
ENVIRONMENT - EFFECTS				
MICRO-ORGANISMS				
TEST SYSTEM	RESPIRATION INHIBITION, EU ANNEX V C.11, OECD 209			
		INHIBITION OF NITRIFICATION, ISO-9509	S	
EC50 FOR MICRO-ORGANISMS IN A STP	??	73	[MG.L-1]	S
EC10 FOR MICRO-ORGANISMS IN A STP	??	??	[MG.L-1]	D
NOEC FOR MICRO-ORGANISMS IN A STP	??	??	[MG.L-1]	D
PNEC FOR MICRO-ORGANISMS IN A STP	??	7.3	[MG.L-1]	O
ASSESSMENT FACTOR APPLIED IN EXTRAPOLATION TO PNEC MICRO	??	10	[-]	O
ENVIRONMENT - EFFECTS				
FRESH_WATER ORGANISMS				
LC50 FOR FISH	??	730	[MG.L-1]	S
L(E)C50 FOR DAPHNIA	??	5E+03	[MG.L-1]	S
EC50 FOR ALGAE	??	1000	[MG.L-1]	S
LC50 FOR ADDITIONAL TAXONOMIC GROUP	??	??	[MG.L-1]	D
NOEC FOR FISH	??	??	[MG.L-1]	D
NOEC FOR DAPHNIA	??	??	[MG.L-1]	D
NOEC FOR ALGAE	??	??	[MG.L-1]	D
NOEC FOR ADDITIONAL TAXONOMIC GROUP	??	??	[MG.L-1]	D
PNEC FOR AQUATIC ORGANISMS	??	0.73	[MG.L-1]	O
PNEC FOR AQUATIC ORGANISMS, INTERMITTENT RELEASES	??	7.3	[MG.L-1]	O
ENVIRONMENT - EFFECTS				
MARINE ORGANISMS				
LC50 FOR FISH (MARINE)	??	??	[MG.L-1]	D
L(E)C50 FOR CRUSTACEANS (MARINE)	??	??	[MG.L-1]	D
EC50 FOR ALGAE (MARINE)	??	??	[MG.L-1]	D
LC50 FOR ADDITIONAL TAXONOMIC GROUP (MARINE)	??	??	[MG.L-1]	D
NOEC FOR FISH (MARINE)	??	??	[MG.L-1]	D
NOEC FOR CRUSTACEANS (MARINE)	??	??	[MG.L-1]	D
NOEC FOR ALGAE (MARINE)	??	??	[MG.L-1]	D
NOEC FOR ADDITIONAL TAXONOMIC GROUP (MARINE)	??	??	[MG.L-1]	D
PNEC FOR MARINE ORGANISMS	??	0.073	[MG.L-1]	O
ENVIRONMENT - EFFECTS				
FRESH-WATER SEDIMENT ORGANISMS				
LC50 FOR FRESH-WATER SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
EC10 FOR FRESH-WATER SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
EC10 FOR FRESH-WATER SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
EC10 FOR FRESH-WATER SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
NOEC FOR FRESH-WATER SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
NOEC FOR FRESH-WATER SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
NOEC FOR FRESH-WATER SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
PNEC FOR FRESH-WATER SEDIMENT-DWELLING ORGANISMS	??	0.682	[MG.KGWWT-1]	O
ENVIRONMENT - EFFECTS				
MARINE SEDIMENT ORGANISMS				
LC50 FOR MARINE SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
EC10 FOR MARINE SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
EC10 FOR MARINE SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
EC10 FOR MARINE SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
NOEC FOR MARINE SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
NOEC FOR MARINE SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
NOEC FOR MARINE SEDIMENT ORGANISM	??	??	[MG.KGWWT-1]	D
PNEC FOR MARINE SEDIMENT ORGANISMS	??	0.0682	[MG.KGWWT-1]	O

NAME	REFERENCE	VALUE	UNITS	STATUS
ENVIRONMENT - EFFECTS				
TERRESTRIAL ORGANISMS				
LC50 FOR PLANTS	??	??	[MG.KGWWT-1]	D
LC50 FOR EARTHWORMS	??	??	[MG.KGWWT-1]	D
EC50 FOR MICROORGANISMS	??	??	[MG.KGWWT-1]	D
LC50 FOR OTHER TERRESTRIAL SPECIES	??	??	[MG.KGWWT-1]	D
NOEC FOR PLANTS	??	??	[MG.KGWWT-1]	D
NOEC FOR EARTHWORMS	??	??	[MG.KGWWT-1]	D
NOEC FOR MICROORGANISMS	??	??	[MG.KGWWT-1]	D
NOEC FOR ADDITIONAL TAXONOMIC GROUP	??	??	[MG.KGWWT-1]	D
NOEC FOR ADDITIONAL TAXONOMIC GROUP	??	??	[MG.KGWWT-1]	D
PNEC FOR TERRESTRIAL ORGANISMS	??	0.176	[MG.KGWWT-1]	O
EQUILIBRIUM PARTITIONING USED FOR PNEC IN SOIL?	YES	YES		O
ENVIRONMENT - EFFECTS				
BIRDS AND MAMMALS				
DURATION OF (SUB-)CHRONIC ORAL TEST	28 DAYS	28 DAYS		D
NOEC VIA FOOD FOR SECONDARY POISONING	??	??	[MG.KG-1]	O
PNEC FOR SECONDARY POISONING OF BIRDS AND MAMMALS	??	??	[MG.KG-1]	O

NAME	REFERENCE	VALUE	UNITS	STATUS
ENVIRONMENT - RISK CHARACTERIZATION				
LOCAL [1 "PRODUCTION", IC=15/UC=55][PRODUCTION]				
RCR FOR THE LOCAL FRESH-WATER COMPARTMENT	??	0.171	[-]	O
RCR FOR THE LOCAL FRESH-WATER COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE LOCAL MARINE COMPARTMENT	??	0.171	[-]	O
RCR FOR THE LOCAL MARINE COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE LOCAL FRESH-WATER SEDIMENT COMPARTMENT	??	0.171	[-]	O
RCR FOR THE LOCAL MARINE SEDIMENT COMPARTMENT	??	0.171	[-]	O
RCR FOR THE LOCAL SOIL COMPARTMENT	??	0.0929	[-]	O
RCR FOR THE LOCAL SOIL COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE SEWAGE TREATMENT PLANT	??	0.171	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION				
LOCAL [2 "STARTING MATERIAL/SOLVENT IN CHEMICAL SYNTHESIS", IC=3/UC=41][INDUSTRIAL USE]				
RCR FOR THE LOCAL FRESH-WATER COMPARTMENT	??	0.889	[-]	O
RCR FOR THE LOCAL FRESH-WATER COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE LOCAL MARINE COMPARTMENT	??	0.889	[-]	O
RCR FOR THE LOCAL MARINE COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE LOCAL FRESH-WATER SEDIMENT COMPARTMENT	??	0.889	[-]	O
RCR FOR THE LOCAL MARINE SEDIMENT COMPARTMENT	??	0.889	[-]	O
RCR FOR THE LOCAL SOIL COMPARTMENT	??	0.442	[-]	O
RCR FOR THE LOCAL SOIL COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE SEWAGE TREATMENT PLANT	??	0.889	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION				
LOCAL [3 "ANALYTICAL LABORATORIES", IC=2/UC=34][INDUSTRIAL USE]				
RCR FOR THE LOCAL FRESH-WATER COMPARTMENT	??	0.16	[-]	O
RCR FOR THE LOCAL FRESH-WATER COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE LOCAL MARINE COMPARTMENT	??	0.16	[-]	O
RCR FOR THE LOCAL MARINE COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE LOCAL FRESH-WATER SEDIMENT COMPARTMENT	??	0.16	[-]	O
RCR FOR THE LOCAL MARINE SEDIMENT COMPARTMENT	??	0.16	[-]	O
RCR FOR THE LOCAL SOIL COMPARTMENT	??	0.0813	[-]	O
RCR FOR THE LOCAL SOIL COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE SEWAGE TREATMENT PLANT	??	0.16	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION				
REGIONAL				
RCR FOR THE REGIONAL FRESH-WATER COMPARTMENT	??	1.95E-04	[-]	O
RCR FOR THE REGIONAL FRESH-WATER COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE REGIONAL MARINE COMPARTMENT	??	1.54E-04	[-]	O
RCR FOR THE REGIONAL MARINE COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O
RCR FOR THE REGIONAL FRESH-WATER SEDIMENT COMPARTMENT	??	1.69E-04	[-]	O
RCR FOR THE REGIONAL MARINE SEDIMENT COMPARTMENT	??	1.35E-04	[-]	O
RCR FOR THE REGIONAL SOIL COMPARTMENT	??	7.81E-06	[-]	O
RCR FOR THE REGIONAL SOIL COMPARTMENT, STATISTICAL METHOD	??	??	[-]	O

Appendix II: EpiWin calculation



```
SMILES : CC(#N)
CHEM   :
MOL FOR: C2 H3 N1
MOL WT : 41.05
------------------------------ EPI SUMMARY (v3.12) --------------------------
 Physical Property Inputs:
    Water Solubility (mg/L):   ------
    Vapor Pressure (mm Hg) :   ------
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   ------
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   ------

KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): -0.15

SMILES : CC(#N)
CHEM   :
MOL FOR: C2 H3 N1
MOL WT : 41.05
-------+-----+---------------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
-------+-----+---------------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]                 | 0.5473  |  0.5473
 Frag  |  1  |  -C#N    [cyano, aliphatic attach]          |-0.9218  | -0.9218
 Const |     |  Equation Constant                          |         |  0.2290
-------+-----+---------------------------------------------+---------+--------
                                                          Log Kow   =  -0.1455


MPBPWIN (v1.41) Program Results:
================================
SMILES : CC(#N)
CHEM   :
MOL FOR: C2 H3 N1
MOL WT : 41.05
----------------------- SUMMARY MPBPWIN v1.41 --------------------


Boiling Point:    71.84 deg C (Adapted Stein and Brown Method)

Melting Point:  -95.87 deg C (Adapted Joback Method)
Melting Point:  -71.71 deg C (Gold and Ogle Method)
Mean Melt Pt :  -83.79 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  -83.79 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
  (Using BP: 71.84 deg C (estimated))
  (MP not used for liquids)
    VP:  125 mm Hg (Antoine Method)
    VP:  119 mm Hg (Modified Grain Method)
    VP:  139 mm Hg (Mackay Method)
  Selected VP:  122 mm Hg (Mean of Antoine & Grain methods)
```

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	1	-CN (cyano)	119.16	119.16
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		339.32
RESULT- corr		BOILING POINT in deg Kelvin		345.00
		BOILING POINT in deg C		71.84

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	1	-CN (cyano)	59.89	59.89
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		177.29
		MELTING POINT in deg C		-95.87

Water Sol from Kow (WSKOW v1.41) Results:

Water Sol: 9.327e+004 mg/L

SMILES : CC(#N)
CHEM :
MOL FOR: C2 H3 N1
MOL WT : 41.05

WSKOW v1.41 Results

Log Kow (estimated) : -0.15
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.15

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
Nitrile	-0.265

Log Water Solubility (in moles/L) : 0.356
Water Solubility at 25 deg C (mg/L): 9.327e+004

WATERNT Program (v1.01) Results:

Water Sol (v1.01 est): 2.2266e+005 mg/L

SMILES : CC(#N)
CHEM :
MOL FOR: C2 H3 N1
MOL WT : 41.05

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	-0.3213	-0.3213
Frag	1	-CδN [cyano, aliphatic attach]	0.8064	0.8064
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = 0.7343
Water Solubility (mg/L) at 25 dec C =2.2266e+005

```
ECOSAR Program (v0.99h) Results:
================================
SMILES : CC(#N)
CHEM   :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C2 H3 N1
MOL WT : 41.05
Log Kow: -0.15  (KowWin estimate)
Melt Pt:
Wat Sol: 2.847E+004 mg/L  (calculated)

ECOSAR v0.99h Class(es) Found
-----------------------------
Neutral Organics
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	4111.439
Neutral Organics	: Fish	96-hr	LC50	3194.066
Neutral Organics	: Fish	14-day	LC50	4111.439
Neutral Organics	: Daphnid	48-hr	LC50	2950.148
Neutral Organics	: Green Algae	96-hr	EC50	1629.648
Neutral Organics	: Fish	30-day	ChV	290.967
Neutral Organics	: Daphnid	16-day	EC50	59.067
Neutral Organics	: Green Algae	96-hr	ChV	47.037
Neutral Organics	: Fish (SW)	96-hr	LC50	258.728
Neutral Organics	: Mysid Shrimp	96-hr	LC50	4274.092
				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	1160.229

```
 Note:  * = asterisk designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000


HENRY (v3.10) Program Results:
==============================

       Bond Est :  3.06E-005 atm-m3/mole
       Group Est:  3.46E-005 atm-m3/mole

SMILES : CC(#N)
CHEM   :
MOL FOR: C2 H3 N1
MOL WT : 41.05
--------------------------- HENRYWIN v3.10 Results --------------------------
----------+-------------------------------------------+---------+----------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION         | COMMENT |  VALUE
----------+-------------------------------------------+---------+----------
 HYDROGEN |   3  Hydrogen to Carbon (aliphatic) Bonds |         | -0.3590
 FRAGMENT |   1  C-CN                                 |         |  3.2624
----------+-------------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE |  TOTAL  |  2.903
----------+-------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 3.06E-005 atm-m3/mole
                                = 1.25E-003 unitless

--------+-------------------------------------------+-----------+--------
```

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	1 CH3-CN	EXPERIMENTAL	2.85
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	2.85

HENRYs LAW CONSTANT at 25 deg C = 3.46E-005 atm-m3/mole
= 1.41E-003 unitless

Henrys LC [VP/WSol estimate using EPI values]:
HLC: 7.065E-005 atm-m3/mole
VP: 122 mm Hg
WS: 9.33E+004 mg/L

BIOWIN (v4.02) Program Results:

SMILES : CC(#N)
CHEM :
MOL FOR: C2 H3 N1
MOL WT : 41.05

---------- BIOWIN v4.02 Results ----------

Biowin1 (Linear Model Prediction) : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks
Biowin5 (MITI Linear Model Prediction) : Biodegrades Fast
Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast
Ready Biodegradability Prediction: YES

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Cyanide / Nitriles [-C#N]	0.3070	0.3070
MolWt	*	Molecular Weight Parameter		-0.0195
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		1.0350

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Cyanide / Nitriles [-C#N]	4.6440	4.6440
MolWt	*	Molecular Weight Parameter		-0.5830
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.9992

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Cyanide / Nitriles [-C#N]	-0.0824	-0.0824
MolWt	*	Molecular Weight Parameter		-0.0907
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		3.0261

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Cyanide / Nitriles [-C#N]	-0.0652	-0.0652
MolWt	*	Molecular Weight Parameter		-0.0592
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.7233

```
Result Classification:   5.00 -> hours      4.00 -> days     3.00 -> weeks
 (Primary & Ultimate)    2.00 -> months     1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Cyanide / Nitriles [-C#N]	0.0717	0.0717
Frag	1	Methyl [-CH3]	0.0004	0.0004
MolWt	*	Molecular Weight Parameter		-0.1221
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.6621

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Cyanide / Nitriles [-C#N]	0.2340	0.2340
Frag	1	Methyl [-CH3]	0.0194	0.0194
MolWt	*	Molecular Weight Parameter		-1.1851
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.8312

```
A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast
```

```
AOP Program (v1.91) Results:
============================
SMILES : CC(#N)
CHEM   :
MOL FOR: C2 H3 N1
MOL WT : 41.05
------------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS -------------------
Hydrogen Abstraction       =   0.0258 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =   0.0258 E-12 cm3/molecule-sec
   HALF-LIFE =   413.931 Days (12-hr day; 1.5E6 OH/cm3)
------------------- SUMMARY (AOP v1.91): OZONE REACTION ----------------------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NOT Available


PCKOC Program (v1.66) Results:
==============================

                   Koc (estimated): 4.5


SMILES : CC(#N)
CHEM   :
MOL FOR: C2 H3 N1
MOL WT : 41.05
--------------------------- PCKOCWIN v1.66 Results ---------------------------

         First Order Molecular Connectivity Index  ..... :  1.414
         Non-Corrected Log Koc  ........................ :  1.3755
         Fragment Correction(s):
```

```
                *   Nitrile/Cyanide  (-C≡N) ..............  : -0.7223
        Corrected Log Koc  ................................ :  0.6532

                      Estimated Koc:  4.5


HYDROWIN Program (v1.67) Results:
=================================
SMILES : CC(#N)
CHEM   :
MOL FOR: C2 H3 N1
MOL WT : 41.05
--------------------------- HYDROWIN v1.67 Results ---------------------------

 Currently, this program can NOT estimate a hydrolysis rate constant for
               the type of chemical structure entered!!

 ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
   and Specific Alkyl Halides can be estimated!!  For more information,
    (Click OVERVIEW in Help  or  see the User's Guide)

             *****   CALCULATION NOT PERFORMED   *****


BCF Program (v2.15) Results:
============================
SMILES : CC(#N)
CHEM   :
MOL FOR: C2 H3 N1
MOL WT : 41.05
--------------------------------- Bcfwin v2.15 ---------------------------------
Log Kow  (estimated)  :  -0.15
Log Kow (experimental):  not available from database
Log Kow used by BCF estimates:  -0.15

Equation Used to Make BCF estimate:
   Log BCF = 0.50

      Correction(s):                   Value
       Correction Factors Not Used for Log Kow < 1

   Estimated Log BCF =  0.500  (BCF = 3.162)



                          Volatilization From Water
                          =========================

Chemical Name:

Molecular Weight    :  41.05 g/mole
Water Solubility    :  -----
Vapor Pressure      :  -----
Henry's Law Constant:  3.46E-005 atm-m3/mole  (estimated by Group SAR Method)

                            RIVER            LAKE
                          ---------        ---------
Water Depth     (meters):   1                1
Wind Velocity    (m/sec):   5                0.5
Current Velocity (m/sec):   1                0.05

      HALF-LIFE (hours) :   11.5             179.1
      HALF-LIFE (days ) :   0.479            7.464


STP Fugacity Model:  Predicted Fate in a Wastewater Treatment Facility
======================================================================
   (using 10000 hr Bio P,A,S)
PROPERTIES OF:
```

```
-------------
Molecular weight (g/mol)                              41.05
Aqueous solubility (mg/l)                             0
Vapour pressure (Pa)                                  0
                (atm)                                 0
                (mm Hg)                               0
Henry 's law constant (Atm-m3/mol)                    3.46E-005
Air-water partition coefficient                       0.00141504
Octanol-water partition coefficient (Kow)             0.707946
Log Kow                                               -0.15
Biomass to water partition coefficient                0.941589
Temperature [deg C]                                   25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
          -Primary tank       0.04        18.80       10000.00
          -Aeration tank      0.04        18.80       10000.00
          -Settling tank      0.04        18.80       10000.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                              g/h              mol/h          percent

Influent                    1.00E+001         2.4E-001        100.00

Primary sludge              2.51E-002         6.1E-004          0.25
Waste sludge                1.48E-001         3.6E-003          1.48
Primary volatilization      1.65E-002         4.0E-004          0.16
Settling volatilization     4.42E-002         1.1E-003          0.44
Aeration off gas            1.25E-001         3.0E-003          1.25

Primary biodegradation      1.76E-003         4.3E-005          0.02
Settling biodegradation     5.17E-004         1.3E-005          0.01
Aeration biodegradation     6.82E-003         1.7E-004          0.07

Final water effluent        9.63E+000         2.3E-001         96.33

Total removal               3.67E-001         8.9E-003          3.67
Total biodegradation        9.10E-003         2.2E-004          0.09


STP Fugacity Model:  Predicted Fate in a Wastewater Treatment Facility
=======================================================================
   (using Biowin/EPA draft method)
PROPERTIES OF:
-------------
Molecular weight (g/mol)                              41.05
Aqueous solubility (mg/l)                             0
Vapour pressure (Pa)                                  0
                (atm)                                 0
                (mm Hg)                               0
Henry 's law constant (Atm-m3/mol)                    3.46E-005
Air-water partition coefficient                       0.00141504
Octanol-water partition coefficient (Kow)             0.707946
Log Kow                                               -0.15
Biomass to water partition coefficient                0.941589
Temperature [deg C]                                   25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
          -Primary tank       36.87         0.02          10.00
          -Aeration tank     368.69         0.00           1.00
          -Settling tank     368.69         0.00           1.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                              g/h              mol/h          percent

Influent                    1.00E+001         2.4E-001        100.00

Primary sludge              2.13E-002         5.2E-004          0.21
Waste sludge                1.21E-002         3.0E-004          0.12
Primary volatilization      1.40E-002         3.4E-004          0.14
Settling volatilization     3.62E-003         8.8E-005          0.04
Aeration off gas            1.32E-002         3.2E-004          0.13
```

Primary biodegradation	1.49E+000	3.6E-002	14.93
Settling biodegradation	4.24E-001	1.0E-002	4.24
Aeration biodegradation	7.23E+000	1.8E-001	72.28
Final water effluent	7.90E-001	1.9E-002	7.90
Total removal	9.21E+000	2.2E-001	92.10
Total biodegradation	9.15E+000	2.2E-001	91.46

Level III Fugacity Model (Full-Output):

Chem Name :
Molecular Wt: 41.05
Henry's LC : 3.46e-005 atm-m3/mole (Henrywin program)
Vapor Press : 122 mm Hg (Mpbpwin program)
Log Kow : -0.15 (Kowwin program)
Soil Koc : 0.29 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	13.3	9.93e+003	1000
Water	43.9	360	1000
Soil	42.7	720	1000
Sediment	0.0808	3.24e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	7.84e-010	9.19	1.32e+003	0.306	43.9
Water	1.83e-009	834	433	27.8	14.4
Soil	6.43e-008	406	0	13.5	0
Sediment	1.67e-009	0.171	0.016	0.00569	0.000532

Persistence Time: 329 hr
Reaction Time: 790 hr
Advection Time: 564 hr
Percent Reacted: 41.7
Percent Advected: 58.3

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 9934
Water: 360
Soil: 720
Sediment: 3240
Biowin estimate: 3.026 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004