1. IDENTIFICATION OF THE SUBSTANCE / MIXTURE AND OF THE COMPANY / UNDERTAKING

1.1 Product identifier

Substance name : Acetonitrile

Index Number from Annex VI (Part 3) of Regulation (EC) No 1272/2008 : 608-001-00-3

Classification and Labelling Inventory Number : Not applicable

Authorisation Number : Not applicable

EC Number : 200-835-2

CAS Number : 75-05-8

REACH Registration Number : 01-2119471307-38-0035

1.2 Relevant identified uses of the substance or mixture and uses advised against

1.2.1 Identified uses

1.2.1.1 Industrial uses

Manufacture of substance
Pharmaceutical industry
Use as laboratory reagent
Printing and reproduction of recorded media - Photographic industry
Repackaging / dilution (azeotrope creation)

1.2.2 Uses advised against

Not for use in final Consumer Products, Plant Protection or Biocide products with wide dispersive indoor or outdoor uses (e.g. as auxiliary solvents in spray applications).

1.3 Details of the supplier of the safety data sheet

Only Representative:

Name :	NAM&NAM Europe GmbH
Address :	Emil-Figge-Str.80, 44227 Dortmund, Germany
Telephone number :	+49 (0)231 9742 4450
Telefax number :	+49 (0)231 9742 4451
E-mail address :	info@namandnam.eu

Importer in EU :

Name :	IVICT Europe GmbH
Address :	Kennedydamn 19, D-40476 Düsseldorf Germany
Telephone number :	+49-(0)211-4397-310
E-mail :	

Non-Community manufacturer :

Name : Tongsuh Petrochemical Corporation Ltd.

Address : 108-70, Sapyeong-ro, Nam-gu,
Ulsan, 44785
Republic of Korea

Telephone number : +82-(0)2-3215-0721

Telefax number : +82-(0)2-3215-0770

E-mail : tspcmail@tspc.co.kr

1.4 Emergency telephone number

+49-(0)211-4397-310 IVICT Europe GmbH (Germany)
+81-(0)3-6699-3284 Asahi Kasei Corporation (Japan)
+82-(0)52-259-7691
+82-(0)52-260-0178 Tongsuh Petrochemical Corporation Ltd. (Republic of Korea)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

2.1.1 Classification according to Regulation (EC) No. 1272/2008 [CLP/GHS]

Flammable Liquid Category 2
Acute Toxicity Oral Category 4
Acute Toxicity Dermal Category 4
Acute Toxicity Inhalation Category 4
Eye Irritation Category 2

2.2 Label elements

2.2.1 Labelling according to Regulation (EC) No 1272/2008 [CLP]

Hazard Pictograms

Signal word : **Danger**

Hazard statements :

H225 : Highly flammable liquid and vapour.
H332 : Harmful if inhaled.
H312 : Harmful in contact with skin.
H302 : Harmful if swallowed.
H319 : Causes serious eye irritation

Precautionary statements :

P210 : Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P280 : Wear protective gloves/protective clothing/eye protection/face protection.
P303+361+P352 IF ON SKIN (or hair), remove/take off immediately all contaminated clothing.

Wash with plenty of soap and water.

P304 : IF INHALED: (P340: Remove victim to fresh air and keep at rest in a position comfortable for breathing.)

P305+P351+P338: IF IN EYES, Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P313+P337: If eye irritation persists: Get medical advice/attention.

Notes :

Note D

For full text of P precautionary statements see section 16.

2.3 Other hazards

All known hazards are described by this Safety Data Sheet.

3. COMPOSITION / INFORMATION ON INGREDIENTS

3.1 Substance

Substance name : Acetonitrile

Index Number from Annex VI (Part 3) of Regulation (EC) No 1272/2008: 608-001-00-3
Classification and Labelling Inventory Number: Not applicable
Authorisation Number : Not applicable
EC Number : 200-835-2
CAS Number : 75-05-8
REACH Registration Number : 01-2119471307-38-####
Purity : ≥ 99.9 % v/v
Stabilisers : None
Impurities or other constituents contributing to substance classification: Not applicable

4. FIRST AID MEASURES

4.1 Description of first aid measures

First responders

Acetonitrile is harmful if inhaled, ingested or in contact with the skin. It is irritating to the eyes and can be harmful if adsorbed through the eyes. Acetonitrile is also extremely flammable. Odour is not reliably detected even above the recommended exposure levels.
Rescuers should not enter "hot zone" unless HAZMAT Trained and properly protected with positive pressure Self-contained Breathing Apparatus with Level A or B HAZMAT Chemical-protective equipment. Hot and cold zones should be defined with approved detection device. Remove patient from contaminated area as quickly as possible and begin decontamination. Persons performing decontamination must use proper PPE.
Decontamination of patient is essential by rinsing exposed areas, skin and hair, with a large amount of fresh water prior to commencing first aid or medical treatment. Avoid exposure of eyes, mouth and uncontaminated skin. Double bag all clothes and leather articles and dispose as contaminated hazardous chemical waste. Contaminated clothing is a fire hazard.

First Aid
Acetonitrile exposure can occur via inhalation, through contact with the eyes, or via ingestion of liquid. The rate of dermal adsorption is generally low but significant inhalation exposure may occur following dermal exposure as a result of the volatility of the liquid. Acetonitrile is slowly metabolised to cyanide, over many hours which can cause collapse and death several hours after exposure. Following decontamination specific first aid treatment can be given as follows:

Eye Contact: immediately flush eyes with copious amounts of water. Seek medical attention immediately. If symptomatic treat as inhalation.

Skin Contact: immediately flush the skin with copious amounts of water, whilst removing contaminated clothing and shoes. Treat any observed systemic toxicity as inhalation. Contaminated leather especially footwear should be discarded. Note: contaminated items could be a fire hazard so need to be placed in closed container and discarded. Provided prompt decontamination is carried out, small splashes on to skin should not give significant rise for concern.

Inhalation: remove exposed person to fresh air and keep warm and rested. If not breathing, ensure airway is clear and commence artificial respiration by mechanical means, **not mouth to mouth**. Use mouth to mask ventilation with one way valve to exhaust victim's exhaled air away from rescuer, or an Ambu bag or pressure demand valve with face mask. Commence administration of oxygen as soon as possible.
Administration of oxygen should be maintained until transfer to the care of a paramedic or doctor.

Ingestion: Seek immediate medical attention. If conscious rinse mouth with plenty of water without swallowing. Give activated charcoal slurry if conscious. Never give anything by mouth to an unconscious person. If breathing give oxygen and if not breathing begin artificial respiration following steps as with Inhalation.

See Section 11 for more detailed information on health effects.

4.2 Most important symptoms and effects, both acute and delayed

The earliest indicators of exposure to low concentrations of Acetonitrile vapour are a cooling sensation in the lungs and chest tightness. Commonly development of nausea and headaches can occur. At higher concentrations reddening of the eyes and skin is typical and after prolonged exposure or exposure to significant concentrations irritation of the throat/bronchioles, palpitations, salivation, breathing difficulties, numbness, weakness of arms and legs, giddiness, collapse and convulsions can occur. Effects will develop over many hours which can progress to significant cyanide poisoning effects where emergency medical response is required. The systemic effects appear to be largely attributable to the conversion of acetonitrile to cyanide.

4.3 Indication of any immediate medical attention and special treatment needed

CALL FOR IMMEDIATE MEDICAL ASSISTANCE and mention the likelihood of cyanide poisoning. Provide Safety Data Sheet and all other pertinent information to emergency medical team.

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

5.1.1 Suitable extinguishing media

Dry chemical powder foam, carbon dioxide and dry sand

5.1.2 Unsuitable extinguishing media

DO NOT USE WATER JET

5.2 Special hazards arising from the substance or mixture

Carbon oxides (CO and CO2); Nitrogen oxides (NO and NO2); Hydrogen cyanide (HCN)

5.3 Advice for fire fighters

Firefighters should wear appropriate protective equipment which includes a selfcontained breathing

apparatus (SCBA) with a full facepiece operated in positive pressure mode and full turnout gear. DO NOT FIGHT FIRE WHEN IT REACHES MATERIAL. Withdraw from fire and let it burn. Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. First move people out of line-ofsight of the scene and away from windows. Cool containers with water jet in order to prevent pressure build-up, auto-ignition or explosion.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Immediately contact emergency personnel. Keep unnecessary personnel away. Eliminate all ignition sources. Follow all fire-fighting procedures (section 5).Do not touch or walk through spilled material. Use suitable protective equipment (See Section 8: "Exposure controls/personal protection").
Wear splash goggles, full suit, vapour respirator or self-contained breathing apparatus (SCBA), chemical protective boots, gloves (Butyl rubber is suitable; Nitrile is not suitable). For large spills, suggested protective clothing might not be adequate. Consult a specialist in this situation.

6.2 Environmental precautions

Dispose of material in accordance with all applicable local and national regulations. Avoid contact of spilled material and runoff with soil and surface water.

Do not dump material into sewers, onto the ground, or into any body of water.

Follow EU legislation such as the Waste Framework Directive (75/442/EEC) and the Hazardous Waste Directive (91/689/EEC).

Empty containers may contain harmful, flammable/combustible residue or vapours. Do not cut, grind, drill, weld, re-use or dispose of containers unless precautions are taken against these hazards.

6.3 Methods and material for containment and cleaning up

If emergency personnel are unavailable, contain spilt material. For small spills, add absorbent (soil may be used in the absence of other suitable materials) and use a non-sparking or explosion-proof means to transfer material to a sealable, appropriate container for disposal. For large spills, dyke spilt material or otherwise contain it to ensure runoff does not reach a waterway. Place spilt material in an appropriate container for disposal.

6.4 Reference to other sections

See Exposure Scenarios attached to this Safety Data Sheet for further details of exposure controls and disposal considerations.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Do not get in eyes, on skin or on clothing. Keep container closed. Use only with adequate ventilation. Do not breathe vapour or mist. Immediately remove contaminated clothing and thoroughly clean before reuse. Clothing and leather items such as shoes contaminated with this material are flammable. Place in a closed container and dispose properly. Keep away from heat, sparks and flame. To avoid fire or explosion, dissipate static electricity during transfer by earthing and bonding containers and equipment before transferring material. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Wash thoroughly after handling.

7.2 Conditions for safe storage, including any incompatibilities

Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).
Empty containers may contain harmful, flammable/combustible or explosive residue or vapours. Do not cut, grind, drill, weld or reuse containers unless adequate precautions are taken against these hazards. Keep away from incompatibles (see Section 10.5).
Packaging Materials: Use original container.

7.3 Specific end uses(s)

Industrial uses :

The use of acetonitrile in industrial and pharmaceutical applications is performed outdoors or indoors in a closed batch and continuous processes where opportunity for exposure arises when performing specific activities such as sampling, loading, transferring and other tasks. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures. Dermal exposure should be controlled by the use of appropriate
PPE (gloves and clothing with long sleeves and long legs) and good industrial hygiene and inhalation exposure should be controlled by the use of appropriate respiratory protection in order to minimise exposure. For operations with potential exposure to workers, use of respiratory protection or local exhaust ventilation (LEV) will be required to ensure that risks to workers are adequately controlled with acceptable margins of safety.

Professional uses :

The use of acetonitrile at non industrial sites (professional uses) is performed indoors in a closed batch and continuous processes where opportunity for exposure arises when performing specific activities such as sampling, loading, transferring and other tasks. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures. Dermal exposure should be controlled by the use of appropriate
PPE (gloves and clothing with long sleeves and long legs) and good industrial hygiene and inhalation exposure should be controlled by the use of appropriate respiratory protection in order to minimise exposure. For operations with further potential exposure to workers, use of local exhaust ventilation (LEV) may also be advised to ensure that risks to workers are adequately controlled with acceptable margins of safety.

Refer to attached exposure scenarios for requirements for specific uses and processes.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1 Control parameters

8.1.1 Occupational exposure limits

Country	Exposure Limit	Legal Basis
ACGIH	Limit value - 8h TWA 34 mg/m3 (20 ppm)	2010
EU IOEL	Limit value - 8h TWA 40 ppm (skin) - 8h TWA 70 mg/m³	EU OEL (Europe, 12/2009).
Germany	Limit value - 8h TWA 34 mg/m3 (20 ppm) skin	MAKs
UK OEL	Limit value - 8h TWA 40 ppm - STEL 60 ppm	

8.1.2 Recommended monitoring procedures

Use absorption on tubes to trap acetonitrile from the air, desorption, and subsequent analysis by gas chromatography.

8.1.3 Occupational exposure limits and/or biological limits for air contaminants

None identified

8.1.4 DNEL values

8.1.4.1 Workers

Acute Local and Systemic Effects Inhalation 40.6 ppm(68 mg/m3)
Long-term Systemic Effects Dermal 32.2 mg/kg bw/day
Long-term Local and Systemic Effects Inhalation 40.6ppm (68 mg/m3)

8.1.4.2 General population

Acute Systemic Effects Inhalation 131.3 ppm (220 mg/m3)
Acute Systemic Effects Oral 0.6 mg/kg bw/day
Acute Local Effects Inhalation 13.1 ppm (22 mg/m3)
Long-term Local and Systemic Effects Inhalation 2.9 ppm (4.8 mg/m3)

8.1.5 PNEC values

Compartment	PNEC	Remarks
Aquatic (freshwater)	10 mg/L	Assessment factor

8.2 Exposure controls

Recommended Monitoring Procedures : Recommended Monitoring Procedures: Personal, workplace atmosphere monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

8.2.1 Appropriate engineering controls

Provide local exhaust ventilation or other engineering controls to maintain any air contaminant below their occupational exposure limits.

8.2.2 Individual protection measures, such as personal protective equipment (PPE)

Personal Protective Measurers

Eye/face Protection : Avoid contact with eyes. Wear chemical splash goggles.

Skin Protection: Do not get on skin or clothing. Wear chemical protective clothing and footwear that cannot be penetrated by chemicals. Note: contaminated items could be a fire hazard so need to be placed in closed container and discarded.

Hands : Wear gloves that cannot be penetrated by chemicals. (Butyl rubber gloves are appropriate, breakthrough time >240 minutes. Nitrile gloves are not appropriate.)) The correct choice of protective gloves depends upon the chemicals being handled, the conditions of work and use, and the condition of the gloves (even the best chemically resistant glove will break down after repeated chemical exposures). Most gloves provide only a short time of protection before they must be discarded and replaced. Because specific work environments and material handling practices vary, safety procedures should be developed for each intended application. Gloves should therefore be chosen in consultation with the supplier/manufacturer and with a full assessment of the working conditions.

Respiratory Protection: Use only with adequate ventilation. Do not breathe vapour or mist. Use appropriate respiratory protection if there is the potential to exceed the exposure limit(s). If the exposure limit is exceeded, use an approved supplied-air respirator. Ventilation and other forms of engineering controls are the preferred means for controlling chemical exposures. Respiratory protection may be needed for non-routine or emergency situations.

Respirator selection and use should be based on contaminant type, form and concentration. Follow applicable regulations and good Industrial Hygiene practice.

Other protection: Ensure that eyewash stations and safety showers are close to the workstation location.

Hygiene Measures: Wash hands, forearms and face thoroughly after handling this material and before eating, smoking, using lavatory and at the end of the day. Appropriate techniques should be used to remove potential contaminated clothing. Wash contaminated clothing before reusing. Dispose of contaminated leather articles.

8.2.3 Environmental exposure controls

Avoid contact of spilled material with the soil. Contain any spilled material so that it does not enter a waterway.
Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental legislation. In some cases, fume scrubbers, filters or engineering modifications to process equipment will be necessary to reduce emissions to acceptable levels.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Appearance	Liquid, Clear, Colourless
Odour:	faint, like ether
Odour threshold:	170 ppm
pH:	6.0~7.5(5% aqueous solution)
Melting/freezing point:	~ 45.7ºC
Boiling point:	81.6 at 101325 Pa
Flash point:	closed cup: 12.8 , open cup: 5 to 6
Evaporation rate:	Not available
Flammability:	Not applicable.

Upper / lower flammability or explosive limits:	3 vol % in air	16 % vol in air
Vapour pressure:	98.64 hPa at 20 ℃	
Relative vapour density:	1.42 (air = 1)	
Relative density:	0.79 at 20 ℃	
Solubility:	Water 1,000,000 mg/L at 25 ℃	
Partition coefficient; n-octanol/water:	Log Kow -0.34 -0.54 at 25 ℃	
Auto-ignition temperature:	524℃	
Decomposition temperature:	Not available	
Viscosity:	0.35 mPa · s at 20 ℃	
Explosive properties:	Not available	
Oxidising properties:	Not available	

9.2 Other information

Conductivity : 60000 pS/m
Molecular weight : 41.05 g/moleSurface tension; 29.04 mN/m at 20 ℃

10. STABILITY AND REACTIVITY

10.1 Reactivity

Not reactive under normal handling and storage.

10.2 Chemical stability

Stable under recommended storage and handling conditions. (See Section 7 "Handling and Storage")

10.3 Possibility of hazardous reactions

Hazardous polymerization will not occur.

10.4 Conditions to avoid

Avoid all possible sources of ignition (spark or flame). Take precautionary measures against static discharges.

10.5 Incompatible materials

Incompatible with acids, bases, nitrating agents, nitrogen-fluorine compounds oxidizers, perchlorates, sulphites.

10.6 Hazardous decomposition products

Decomposition products may include the following materials: carbon oxides (CO, CO2), nitrogen oxides (NO, NO2 etc.), Hydrogen cyanide (HCN).

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

Acute Oral Toxicity	LD50 rat 1.68 - 8.53 mL/kg LD50 mouse 617 mg/kg
Acute Dermal Toxicity	LD50 rabbit >2000 mg/kg
Acute Inhalation Toxicity	LC50 mouse 3587 ppm/4 hr (6.022 mg/L) LC50 rat 16,000 ppm/4 hr (26.8 mg/L)

Skin Irritation/Corrosivity : Non-irritating in rabbits. Not corrosive.
Serious eye irritation/damage : Severely Irritating in rabbits.
Respiratory Sensitization : No information is available.
Skin Sensitization : Negative in guinea pigs (Buehler Test).

Germ Cell Mutagenicity : Acetonitrile does not induce gene mutations in bacteria, gave negative responses in all mammalian cell gene mutation assays and has produced only marginal effects in chromosome aberration assays in vitro - equivocal results in presence of metabolic activation but negative in absence of activation. Reliable in vivo micronucleus studies have shown marginal or negative results. The potential of acetonitrile to interfere with chromosome segregation in D. melanogaster has been demonstrated both in vitro and in vivo systems. Not classified as a germ cell mutagen.

Carcinogenicity : In a NTP inhalation study with rats and mice an increase in liver adenomas and carcinomas was observed at 400 ppm (the highest dose) in male rats but was not statistically significant compared to controls. No exposure related liver lesions were observed in female rats. There were no exposure related increases in the incidence of lung or liver neoplasms in mice. In summary, the results of the NTP bioassay on acetonitrile do not indicate that acetonitrile was carcinogenic in laboratory rats or mice. Acetonitrile is not classified as carcinogenic by IARC, NTP or the EU CLP.

Reproductive Toxicity : No reproductive or developmental effects were seen below maternally lethal doses in the following reliable animal studies: reproductive/developmental toxicity

screening (rat, inhalation); organ histopathology and sperm motility (chronic rat and mouse, inhalation); developmental (rat, inhalation and gavage; rabbit, gavage); 2 −generation reproduction (rat, inhalation) or structural analogue acrylonitrile. No classified as toxic to reproduction.

STOT − single exposure : Animal studies do not demonstrate target organ effects. Not classified for specific target organ toxicity.

STOT − repeat exposure : NOAECs in reliable chronic rodent inhalation studies are based on mortality (NOAEC in 104 week inhalation study was 400 ppm for rats and 200 ppm for mice). These studies did not demonstrate target organ effects, clinically or by histopathology, with the exception of forestomach lesions in the mice. Mice exhibited forestomach lesions at all exposure levels; however the role that inhalation exposure plays in the occurrence of these lesions is not known and may be minor compared to ingestion as a result of grooming of contaminated fur and/or mucociliary clearance. Not classified for specific target organ toxicity.

11.2 Other Information

Routes of Exposure :
Dermal, eye, inhalation and ingestion

Potential Health Effects :

Eye Contact: Causes severe eye irritation.

Skin Contact: Contact is not expected to result in irritation. Harmful in contact with skin. Prolonged or repeated contact can defat the skin and lead to irritation and/or dermatitis. Effects may be delayed.
Inhalation: Harmful by inhalation. Effects may be delayed
Ingestion: Harmful if swallowed. May cause headache, weakness, dizziness, shortness of breath, cyanosis, rapid heart beat, unconsciousness and possible death. Effects may be delayed.

Symptoms related to the physical, chemical and toxicological characteristics:
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 to cyanide. There are human case reports of severe intoxication and death following exposure to high concentrations of acetonitrile vapour.

Delayed and immediate effects as well as chronic effects from short and long−term exposure:
Upon absorption and metabolism acetonitrile immediately begins a slow release of cyanide, which can continue for several hours. The toxic effects and associated clinical signs of cyanide poisoning may therefore be delayed. There is no evidence of chronic toxicity from the experimental animal data or human case studies.

Interactive effects: No applicable data is available on interactive effects.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Acute Toxicity to Fish	The acute toxicity of acetonitrile to fish has been studied in several freshwater species. Reported LC50 values range from 730 mg/L to 7050 mg/L. 96−hour LC50 1640 mg/L Pimephales promelas (Fathead minnow). 48−hour TLm 730 mg/L Oryzias latipes (Medaka, high−eyes) 48−hour LC50 >1000 mg/L Oryzias latipes (Medaka, high−eyes)
Acute Toxicity to Aquatic Invertebrates 48 hr	LC50 values range from 400 mg/L to 8250 mg/L. T LC50 521 mg/L Artemia salina larvae
Acute Toxicity to Algae	48−hr EC50 in the green algae Raphidocelis subcapitata 7943 mg/L. 72 hr ErC50(growth rate) 9696 mg/L marine algae (Phaeodactylum tricornutum)
Chronic Toxicity to Fish	21 −day NOEC >102 mg/L Oryzias latipes
Chronic toxicity to Aquatic	21−day NOEC (reproduction) 160 mg/L − > 960 mg/L Daphnia

magna.Invertebrates

12.2 Persistence and degradability

Readily biodegradable in water. Hydrolysis is unimportant to the aquatic fate.
Aerobic biodegradation is expected to be the major loss process in soil and water; volatilization may become competitive in shallow water.

12.3 Bioaccumulative potential

No experimental data on bioaccumulation are available for acetonitrile.
Calculated values based on Kow are in the range of 0.3 − 0.4. Based on these results, low Kow values and high water solubility very low bioaccumulation potential is expected.

12.4 Mobility in soil

Estimated Koc values for acetonitrile range from 0.3 − 16 and indicate a low potential for adsorption to soils.

12.5 Results of PBT and vPvB assessment

The data show that the properties of acetonitrile do not meet the specific criteria detailed in REACH Annex XIII or do not allow a direct comparison with all the criteria in Annex XIII but nevertheless indicate that acetonitrile would not have these properties and the substance is not considered a PBT/vPvB.

12.6 Other adverse effects

Not applicable

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Dispose of contents/container in accordance with local/regional/national/international regulations.
Avoid contact of spilled material and runoff with soil and surface waterways. Consult an environmental professional to determine if local, regional or national regulations would classify spilled or contaminated materials as hazardous waste. Use only approved transporters, recyclers, treatment, storage or disposal facilities. Comply with all local, regional and national laws pertaining to waste management.
Consult your local or regional authorities.

14. TRANSPORT INFORMATION

	14.1 UN Number	14.2 UN Proper Shipping Name	14.3 Hazard Class(s)	14.4 Packing Group	14.5 Environmental Hazards
EU ADR/RID	1648	Acetonitrile	3	PG II	−
IMDG	1648	Acetonitrile	3	PG II	−
ICAO/IATA	1648	Acetonitrile	3	PG II	−

14.6 Special precautions for user

EmS FIRE SCHEDULE : F−E (Non−water−reactive flammable liquids)
EmS SPILLAGE SCHEDULE : S−D (Flammable liquids)

14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

Ship Type 2. Pollution category Z.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations / legislation specific for the substance or mixture

International Inventories

International Inventories

AUSTRALIAN INVENTORY (AICS)	: Listed.
CANADA INVENTORY (DSL)	: Listed
CHINA INVENTORY (IECS)	: Listed
EU INVENTORY (EINECS/ELINCS)	: Listed
JAPAN INVENTORY (ENCS)	: Listed
KOREA INVENTORY (ECL)	: Listed.
PHILIPPINE INVENTORY (PICCS)	: Listed
UNITED STATES (TSCA)	: Listed.

TA Luft: 5.2.5

Classification of Substances Hazardous to Water (WGK): 2

15.2 Chemical safety assessment

A chemical safety assessment has been performed.

16. OTHER INFORMATION

16.1 Classification information

Full text of abbreviated P statements

P210: Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233: Keep container tightly closed.
P240: Ground/bond container and receiving equipment.
P241: Use explosion-proof electrical/ventilating/lighting/equipment.
P242: Use only non-sparking tools.
P243: Take precautionary measures against static discharge.
P261: Avoid breathing dust/fume/gas/mist/vapours/spray.
P270: Do not eat, drink or smoke when using this product.
P271: Use only outdoors or in a well-ventilated area.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P301: IF SWALLOWED: (P330: Rinse mouth.)
P303+361+P352 IF ON SKIN (or hair), remove/take off immediately all contaminated clothing. Wash with plenty of soap and water.
P304: IF INHALED: (P340: Remove victim to fresh air and keep at rest in a position comfortable for breathing.)
P305+P351+P338: IF IN EYES, Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P313+P337: If eye irritation persists: Get medical advice/attention.
P312: Call a POISON CENTER or doctor/physician if you feel unwell.
P313+P337: If eye irritation persists: Get medical advice/attention.
P322: Specific measures (see first aid measures on this label).
P363: Wash contaminated clothing before reuse.
P370+P378: In case of fire, use water fog, foam, dry chemical or carbon dioxide for extinction.
P501: Dispose of contents/container only to approved transporters, recyclers, treatment, storage or disposal facilities. Comply with all local, regional and national laws pertaining to waste management.

NOTICE: This Material Safety Data Sheet is based upon data considered to be accurate at the time of its preparation. Despite our efforts, it may not be up to date or applicable to the circumstances of any particular case. We are not responsible for any damage or injury resulting from abnormal use, from any failure to follow appropriate practices or from hazards inherent in the nature of the product.

16.2 Abbreviations and acronyms

BCF	Bioconcentration factor
CLP	Classification, labelling and packaging (Regulation (EC) 1272/2008)
DNEL	Derived no effect level
DSD	Dangerous Substances Directive 67/548/EEC
ECHA	European Chemicals Agency
EC50	Median effect concentration
LC50	Median lethal concentration
NOAEL	No observed adverse effect level
PBT	Persistent, bioaccumulative and toxic
PNEC	Predicted no effect concentration
REACH	Registration, evaluation, authorisation and restriction of chemicals (Regulation (EC) 1907/2006)
STOT	Specific target organ toxicity
STP	Sewage treatment plant
vPvB	Very persistent and very bioaccumulative

16.3 Further information

This Safety Data Sheet has been prepared in accordance with Commission Regulation (EU) No 453/2010. The information provided is based on data considered to be accurate at the time of document preparation. The information given is designed only as guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. Information relates only to the specific material and processes designated in the text and may not be valid for other materials or processes. Responsibility cannot be accepted for damage or injury resulting from hazards inherent to the product, from abnormal use, or from failure to follow appropriate practices.

16.4 Indication of changes

Revision Indicator : Conversion to REACH format with CLP/GHS Classification. All Sections revised.

ANNEX TO THE SDS

The exposure scenario section is extracted from the CSR.

9. EXPOSURE ASSESSMENT

Overview of the exposure assessment
Acetonitrile is a simple organic nitrile produced as a coproduct in the manufacture of acrylonitrile by catalytic ammoxidation of propylene. Acetonitrile is commonly used as a solvent in industrial and laboratory settings. It is generally used as a process solvent or for cleaning equipment.
Acetonitrile may also be used as a building block for certain active pharmaceutical ingredients (APIs), agrochemical products, and vitamins/nutrition products. Certain other small scale uses exist such as uses in photographic/printing processes.
There are no proposed consumer uses for acetonitrile. Staff associated with manufacture, use, sampling and maintenance are fully trained and receive detailed instructions on the safe handling and use of acetonitrile and will wear appropriate protective equipment. No exposure of the general population is expected.
For the environmental assessment in cases where tier 1 assessments were not sufficient to demonstrate safe use only the second tier is presented in order to prevent multiple tiers of superseded data being present.
Where safe use could not be demonstrated in tier 2 maximum emission limits were set.

Table 58. Overview on exposure scenarios and coverage of substance life cycle

ES number	Identified uses				Resulting Life Cycle Stage		Linked to Identified Use	Sector of Use (SU)	Preparation Category (PC)	Process Category (PROC)	Article Category (AC)	Environmental release Category (ERC)
	Manufacture	Formulation	End use	Consumer use	Service life (for articles)	Waste stage						
ES 1 Manufacture	Y	N	N	N	N/A	N/A		SU3 SU8 SU9	PC19 PC20 PC35 PC40	PROC1 PROC2 PROC3 PROC4 PROC8a PROC8b PROC9	N/A	ERC1
ES 2 Industrial Uses	Y	N	N	N	N/A	N/A		SU3 SU8 SU9	PC19 PC20 PC35 PC40	PROC1 PROC2 PROC3 PROC4 PROC8a PROC8b PROC9	N/A	ERC6a ERC6b ERC7
ES3 Pharmaceutical, fine chemical and active substance manufacture uses	Y	N	Y	N	N/A	N/A		SU9 SU0-2	PC19 PC21 PC29	PROC1 PROC2 PROC3 PROC4 PROC8a PROC8b PROC9	N/A	ERC4 ERC6a
ES4 Professional use of acetonitrile as a laboratory reagent	N	N	Y	N	N/A	N/A		SU0-2	PC21 PC40	PROC3 PROC15	N/A	ERC8a
ES5 Photographic/ printing uses	N	N	Y	N	N/A	N/A		SU0-2	PC30	PROC3 PROC15	AC1	ERC8a
ES6 Repackaging/ dilution (Azeotrope creation)	N	Y	N	N	N/A	N/A		SU10	PC21 PC40	PROC3 PROC5 PROC9	N/A	ERC2

9.1. Exposure scenario 1 – Manufacture of acetonitrile

9.1.1. Exposure scenario

Acetonitrile is a co-product in the manufacture of acrylonitrile by catalytic ammoxidation of propylene.

Sector of Use:
SU3: Industrial manufacturing.
SU8: Manufacture of bulk, large scale chemicals (including petroleum products).
SU9: Manufacture of fine chemicals.

Product Categories:
PC19: Intermediates.
PC20: Products such as pH regulators, flocculants, precipitants, neutralisation (specifically Azeotrope breaking)
PC35: Washing, cleaning products (including solvent based products).
PC40: Extraction agent.

Process Categories:
PROC1: Use in closed process, no likelihood of exposure.
PROC2: Use in closed, continuous process with occasional controlled exposure.
PROC3: Use in closed batch process (synthesis or formulation). Industrial setting.
PROC4: Use in batch and other process (synthesis) where opportunity for exposure arises.
PROC8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at nondedicated
facilities. Industrial setting.
PROC8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities. Industrial setting.
PROC9: Transfer of substance or preparation into small containers at dedicated facilities.

Environmental Release Category:
ERC1: Manufacture of substances.

9.1.1.1. Description of activities and processes covered in the exposure scenario

Acetonitrile is manufactured and processed at industrial sites in closed continuous processes with either no likelihood of exposure or with only occasional opportunity for exposure in controlled conditions e.g. during maintenance, sampling or discharge of the material.
The industrial manufacture or use of Acetonitrile is conducted outdoors in closed batch and continuous processes at large scale industrial plants. Some smaller scale batch processing may be performed indoors.
There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required outdoors, except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. The bulk transfer of Acetonitrile, following manufacture is conducted outside at dedicated facilities using a closed system processes with a vapour return to closed vessels
e.g. from external terminal tanks via road or rail tankers, barges or ships to large scale bulk storage vessels.
There is also potential exposure to workers during transfer of acetonitrile when filling smaller vessels for further
use (e.g. drumming) at dedicated facilities. This is usually conducted outside but under cover from precipitation.
Workers involved in the production, handling, sampling and transfer of Acetonitrile are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.
For operations with potential inhalation exposure to workers, use of respiratory protection or local exhaust ventilation (LEV) will be required to ensure that risks to workers are adequately controlled with acceptable margins of safety.

9.1.1.2. Operational conditions related to frequency, duration and amount of use

Table 59: Duration, frequency and amount (for industrial use)

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	8500 tonnes/y	Tonnage produced per year
Emission days per site	300 d/y	Information from ESVOC SPERC 1.1.v1

9.1.1.3. Operational conditions and risk management measures related to product characteristics

Table 60: Characteristics of the substance

Information type	Data field	Explanation
Physical state	Liquid	See section 1.3
For solids: Categorisation of dust grades	Not applicable	
Concentration of substance in preparation	99.9%	
Concentration after dilution for use (if relevant)	Not applicable	
Risk management measures related to the design of product		Acetonitrile is manufactured and processed at industrial sites in closed continuous processes with either no likelihood of exposure or with only occasional opportunity for exposure in contolled conditions e.g. during maintenance, sampling or discharge of the material. Exposure to acetonitrile is likely during charging, sampling or discharge of the material. Workers involved in these tasks are professional, well-trained in these procedures and occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

9.1.1.4. Operational conditions related to available dilution capacity and characteristics of exposed humans

Table 61: Operational conditions related to respiration and skin contact

Information type	Data field	Explanation
Respiration volume under conditions of use	10 m^3/d	Default for Light work *(Guidance Section R 8.4.2)*
Room size and ventilation rate	m^3 ; exchange per hour	*If room size and general ventilation is employed to control risk, explain the background of the values assumed.*
Area of skin contact with the substance under conditions of use	0 cm^2	Exposure to acetonitrile is only possible during charging, sampling or discharge of the material and filling of tankers/barges/bulk storage vessels.
Body weight	70 kg	Default for workers

9.1.1.5. Other operational conditions of use

Table 62: Technical fate of substance and losses from process/use to waste, waste water and air

Information type	Data field	Explanation
Fraction of applied amount lost from process/use to waste gas,	0.005	ESVOC SPERC 1.1.v1 release factor
Fraction of applied amount lost from process/use to waste water	0.01	ESVOC SPERC 1.1.v1 release factor
Fraction of applied amount lost from process/use to waste	0	Loss of acetonitrile to waste is not foreseen.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

9.1.1.6. Risk management measures

The manufacture of acetonitrile is performed outdoors in closed and continuous processes. Some smaller scale batch processing may be performed indoors with LEV.
There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. The bulk production of acetonitrile is transported to an external terminal (tankers, barges, ships, large scale bulk storage vessels) for filling into vessels via a closed system with a vapour
return. Workers involved in the production of acetonitrile, handling, sampling and transfer of materials are welltrained
in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

Table 63: Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) should be required for indoor industrial use.
Personal protective equipment (PPE)		
Information type	**Data field**	**Explanation**
Type of PPE (gloves, respirator, faceshield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves
Other risk management measures related to workers		
Training to workers to ensure goodpractise methods.	Effectiveness in terms of residual exposure	Workers involved in the production, handling, sampling and transfer of materials are well-trained.
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	Removal from liquid waste stream.	Facilities producing acetonitrile will most likely have on-site waste-water treatment facilities. For this risk assessment the default EUSES calculated removal rates for readily biodegradable substances were used.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	Varies depending on system.	Worst case estimated production releases are considered below and have been determined to be safe for the environment.
Air emission abatement	No specific air abatement measures	No specific air emission abatement included for the purposes of this risk assessment.
Resulting amount waste gas released to environment	142 kg/day	Based on the closed and highly contained production systems this amount is considered to be a vast overestimation.
Onsite waste treatment	Removal from liquid waste stream.	Facilities producing acetonitrile will most likely have on-site waste-water treatment facilities. For this risk assessment the default EUSES calculated removal rates for readily biodegradable substances were used.
Municipal or other type of external waste water treatment	No	Waste water from acetonitrile production will be emitted to surface water following on-site waste water treatment.
Effluent (of the waste water treatment plant) discharge rate	2000 m^3/d	Default: 2000 m^3/d
Recovery of sludge for agriculture or horticulture	No	Facilities which produce acetonitrile are likely to have dedicated waste water treatment facilities. Sludge from these facilities would not be spread on land.

9.1.1.7. Waste related measures

Table 61: Fraction of substance in waste and waste management measures.

Information type	Data field	Explanation
Amount of substances in waste water resulting from identified uses covered in the exposure scenario	283 kg/d	Based on worst case emission to waste waters from ESVOC SPERC 1.1.v1.
Amount of substances in waste resulting from service life of articles	Not applicable	
Type of waste, suitable waste codes	Suitable EWC code(s)	
Type of external treatment aiming at recycling or recovery of substances	None	
Type of external treatment aiming at final disposal of the waste.	None	Waste water will be treated on- site and no emission to the municipal STP is expected.
Fraction of substance released into the environment via air from waste handling	Not applicable	
Fraction of substance released into the environment via waste water from waste handling	Not applicable	
Fraction of substance disposed of as secondary waste	Not applicable	

9.1.2. Exposure estimation

9.1.2.1. Worker exposure

Acetonitrile is manufactured and processed at industrial sites in closed continuous processes with either no likelihood of exposure or with only occasional opportunity for exposure in contolled conditions e.g. during maintenance, sampling or discharge of the material.

The industrial manufacture or use of Acetonitrile is conducted outdoors in closed batch and continuous processes at large scale industrial plants. Some smaller scale batch processing may be performed indoors.

There is potential exposure to acetonitrile during the transfer of the substance. However transfer of the substance is conducted at dedicated facilities using a closed-system with vapour return.

Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. The bulk production of acetonitrile is transported to an external terminal (tankers, barges, ships, large scale bulk storage vessels) for use in industrial processes. Workers involved in Acetonitrile production, handling, sampling and transfer of materials are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure. Systemic dermal exposures to acetonitrile in workers and inhalation exposure concentrations for activities in this scenario have been estimated using the ECETOC TRA Tier 1 model.

Table 64: Exposure concentrations to workers

Routes of exposure	Description of activity	PROC	State of material	Estimated Exposure Concentrations		Measured exposure concentrations	
				Value*	unit	Value	unit
Dermal exposure	Manufacturing including sampling	PROC 1	Liquid	0.343	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 2	Liquid	1.37	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 3	Liquid	0.343	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 4	Liquid	6.86	mg/kg/day	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8a	Liquid	13.71	mg/kg/day	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8b	Liquid	6.86	mg/kg/day	No measured data	
	Transfer of substance	PROC 9	Liquid	0.686**	mg/kg/day	No measured data	
Inhalation exposure	Manufacturing including sampling	PROC 1	Liquid	0.012	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 2	Liquid	12.0	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 3	Liquid	29.9	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 4	Liquid	24.0	mg/m^3	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8a	Liquid	60.0	mg/m^3	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8b	Liquid	60.0	mg/m^3	No measured data	
	Transfer of substance	PROC 9	Liquid	0.855**	mg/m^3	No measured data	

** Minimum exposure as determined by ECETOC based outdoors and without use of respiratory protection as a worst case scenario.*
*** Minimum exposure as determined by ECETOC based on indoors with LEV and without use of respiratory protection.*

Measured dermal exposure data are not available. There is possible exposure during transfer and sampling, however the use closed system with vapour return, and PPE, like eye goggles, protective gloves/gauntlets (for example butyl rubber gloves), boots and protective clothing that covers arms and legs, minimises dermal exposure.

Measured inhalation exposure data are not available. The manufacture of acetonitrile is performed outdoors in closed batch and continuous processes. There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment may be used, for example, cleaning tanks or reactors. The bulk production of acetonitrile is transported to an external terminal (tankers, barges, ships, large scale bulk storage vessels) for filling into vessels. Workers involved in Acetonitrile production, handling, sampling and transfer of materials are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

9.1.2.2. Consumer exposure

Consumers are not directly exposed to the manufacture of acetonitrile.

9.1.2.3. Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore, removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

9.1.2.4. Environmental exposure

First tier conservative exposure estimations were carried out using the EUSES 2.1 tool and the specified defaults. ERC 1 was used to determine the environmental emissions for ES1. Second tier worst case environmental exposure estimations were carried out using EUSES 2.1 to take into account more realistic factors that affect the environmental concentrations. For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acetonitrile and emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment:
Chapter R.16: Environmental Exposure Estimation”. It was determined that ERC 1 covers the manufacturing stage for acetonitrile. It is noted that the use of ERC 1 to estimate emissions to the environment results in an unrealistic assessment for acetonitrile, as default emission fractions for ERC 1 represent a worst case. As such, the assessment was refined using an appropriate SPERC to give a more accurate estimation of releases of acetonitrile to the environment.

9.1.2.4.1. Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES 2.1. Emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 65: EUSES inputs for ES1

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	41.0519	g/mol	
Vapour Pressure at 25°C	13900	Pa	
Water Solubility	1,000,000	g/L	
Octanol/water partition coefficient	-0.54	logKow	
Koc	8.15 (arithmetic mean based on range of values)		
Biodegradability	Readily Biodegradable		
Life Cycle Step	Manufacture		
Tonnage	8500 regional 8500 local	Tonnes per annum	
Environmental Release Category	ERC1		
Specific Environmental Release Category (SPERC)	ESVOC SPERC 1.1.v1		
Fraction of Tonnage for Region	1		1
Fraction of the main local source	1		1
Release to Air	0.5 Specified by ESVOC 1.1.v1	%	5
Release to Water	1 Specified by ESVOC 1.1.v1	%	6
Release to soil (direct)	0.01	%	0.01
STP	Yes – onsite WWTP		Yes
Emission events per year	300 (from ESVOC SPERC 1.1.v1)	Days	100

For the tier 2 assessment of environmental releases, a solvent specific SPERC was used to give a more realistic estimation of releases from manufacture. ESVOC SPERC 1.1.v1 was used as this is considered to cover all processes relating to the industrial manufacture of solvents.

Table 66: Tier 2 Predicted releases to the environment

Compartments	Predicted releases	Measured release	Explanation / source of measured data
Release to air	142 kg/d	-	Based on ESVOC SPERC 1.1.v1 release factors
Wastewater	283 kg/d	-	Based on ESVOC SPERC 1.1.v1 release factors
Soil (direct only) Agricultural soil	0.01%	-	ERC release factor

The predicted releases were estimated using the EUSES 2.1 program.

9.1.2.4.2. Exposure concentration in sewage treatment plants (STP)

As discussed above, facilities manufacturing acetonitrile will have on-site waste water treatment facilities and emission to the municipal STP will not occur. As such, a risk assessment for the STP is not deemed necessary for manufacturing.

9.1.2.4.3. Exposure concentrations in the aquatic pelagic compartment

Tier 2 Predicted Exposure Concentrations (PEC) for the aquatic pelagic compartment

Table 67: Tier 2 Predicted Concentrations (PEC) for the aquatic pelagic compartment

Protection target	Exposure concentration
Freshwater (mg/L)	Local PEC: 1.79
Marine water (mg/L)	Local PEC: 0.179

9.1.2.4.4. Exposure concentration in sediments

Acetonitrile has a low adsorption potential on sediments. Evidence indicates that acetonitrile will not accumulate in sediments based on this and its rapid degradation in the environment. Nevertheless, PECs calculated in EUSES are presented below for completeness.

Table 68: Tier 2 Predicted Concentrations (PEC) for the aquatic sediment compartment

Protection target	Exposure concentration
Freshwater sediment (mg/kg dw)	Local PEC: 7.89
Marine sediment (mg/kg dw)	Local PEC: 0.789

As these predicted environmental concentrations do not take into account the rapid degradation of acetonitrile in the environment they should be regarded as worst case.

9.1.2.4.5. Exposure concentration in soil and groundwater

Table 69: Tier 2 Predicted exposure concentrations (PEC) for soil and groundwater

Protection target	Exposure concentration
Agricultural soil (mg/kg dw)	Local PEC: 3.7 $x10^{-3}$
Groundwater (mg/L)	Local PEC: 0.0141

These values are considered to be conservative as acetonitrile is likely to degrade rapidly in the environment.

9.1.2.4.6. Atmospheric compartment

Table 70: Tier 2 Predicted Exposure Concentrations (PEC) in air

Protection target	Exposure concentration
Annual average PEC in air, total (mg/m^3)	Annual average local PEC: 0.0324

9.1.2.4.7. Exposure concentration relevant for the food chain (Secondary poisoning)

Based on the above results, acetonitrile has been demonstrated to be present in the environment in relatively small quantities. This is also the case for atmospheric, aquatic and soil compartments; furthermore acetonitrile is readily biodegradable and has very low potential for bioaccumulation. Therefore it is considered unlikely that birds or mammals will be exposed indirectly either by way of direct contact with the air, surface waters or soils, or by way of drinking water, or through exposure in the food chain.

9.1.2.4.8. Regional exposure levels and environmental concentrations

Regional exposure for the manufacture of acetonitrile has been modelled using EUSES 2.1. No significant PEC values are indicated for the regional scale even under the conservative assumptions of the Tier 2 EUSES assessment.

Table 71: Regional tier 2 concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
Freshwater	2.22×10^{-4}	mg/l	NA	mg/l	
Marine water	2.06×10^{-5}	mg/l	NA	mg/l	
Freshwater sediments	8.5×10^{-4}	mg/kg dw	NA	mg/kg	
Marine sediments	8.02×10^{-5}	mg/kg dw	NA	mg/kg	
Agricultural soil	4.62×10^{-6}	mg/kg dw	NA	mg/kg	
Grassland	6.99×10^{-6}	mg/kg dw	NA	mg/kg	
Air	2.27×10^{-6}	mg/m3	NA	mg/m^3	

9.2. Exposure scenario 2 – Industrial uses of acetonitrile

9.2.1. Exposure scenario

Acetonitrile is used in industrial processes as an industrial solvent or processing aid as well as in production of other substances..

Sector of Use:
SU3: Industrial manufacturing.
SU8: Manufacture of bulk, large scale chemicals (including petroleum products).
SU9: Manufacture of fine chemicals.

Product Categories:
PC19: Intermediates.
PC20: Products such as pH regulators, flocculants, precipitants, neutralisation (specifically Azeotrope breaking)
PC35: Washing, cleaning products (including solvent based products).
PC40: Extraction agent.

Process Categories:
PROC1: Use in closed process, no likelihood of exposure.
PROC2: Use in closed, continuous process with occasional controlled exposure.
PROC3: Use in closed batch process (synthesis or formulation). Industrial setting.
PROC4: Use in batch and other process (synthesis) where opportunity for exposure arises.
PROC8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at nondedicated facilities. Industrial setting.
PROC8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities. Industrial setting.
PROC9: Transfer of substance or preparation into small containers at dedicated facilities.

Environmental Release Category:
ERC6a: Industrial use of intermediates
ERC6b: Industrial use of reactive processing aids
ERC7: Industrial use of substances in closed systems

9.2.1.1. Description of activities and processes covered in the exposure scenario

Acetonitrile is used in industrial processes which are either closed, continuous processes, or closed batch processes and in batch synthesis where some opportunity for exposure may arise.
There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required outdoors, except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors.

There is also potential exposure to workers during transfer of acetonitrile when filling smaller vessels for further use (e.g. drumming) at dedicated facilities. This is usually conducted outside but under cover from precipitation.

Some transfers may occur at facilities which are industrial or professional but not specifically dedicated to Acetonitrile alone.

Workers involved in industrial uses of Acetonitrile including production, handling, sampling and transfer of materials are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

9.2.1.2. Operational conditions related to frequency, duration and amount of use

Table 72: Duration, frequency and amount (for industrial use)

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	1000 tonnes/y	Worst case tonnage used in industrial processes
Emission days per site	100 d/y	Default

9.2.1.3. Operational conditions and risk management measures related to product characteristics

Table 73: Characteristics of substance

Information type	Data field	Explanation
Physical state	Liquid	See section 1.3
For solids: Categorisation of dust grades	Not applicable	
Concentration of substance in preparation	99.9%	
Concentration after dilution for use (if relevant)	Not applicable	
Risk management measures related to the design of product		Acetonitrile is used in industrial processes which are either a closed, continuous process, or closed batch processes and in batch synthesis where some opportunity for exposure may arise. Exposure to acetonitrile is likely during charging, sampling or discharge of the material. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

9.2.1.4. Operational conditions related to available dilution capacity and characteristics of exposed humans

Table 74: Operational conditions related to respiration and skin contact

Information type	Data field	Explanation
Respiration volume under conditions of use	10 m^3/d	Default for Light work *(Guidance Section R 8.4.2)*
Room size and ventilation rate	m^3 ; exchange per hour	*If room size and general ventilation is employed to control risk, explain the background of the values assumed.*
Area of skin contact with the substance under conditions of use	0 cm^2	Exposure to acetonitrile is only possible during charging, sampling or discharge of the material and filling of tankers/barges/bulk storage vessels.
Body weight	70 kg	Default for workers

9.2.1.5. Other operational conditions of use

Table 75: Technical fate of substance and losses from processes/use to waste, waste water and air

Information type	Data field	Explanation
Fraction of applied amount lost from process/use to waste gas,	ERC 6a: 0.05 ERC6b: 0.001 ERC7: 0.05	ERC default release factors
Fraction of applied amount lost from process/use to waste water	ERC 6a: 0.02 ERC6b: 0.05 ERC7: 0.05	ERC default release factors
Fraction of applied amount lost from process/use to waste	0 kg/kg	Loss of acetonitrile to waste is not foreseen.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

9.2.1.6. Risk management measures

Acetonitrile is used in industrial processes which are either a closed, continuous process, or closed batch processes and in batch synthesis where some opportunity for exposure may arise. Some smaller scale batch processing may be performed indoors with LEV.

There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. For operations with potential inhalation exposure to workers, use of respiratory protection or local exhaust ventilation (LEV) will be required to ensure that risks to workers are adequately controlled with acceptable margins of safety.

Workers involved in industrial uses of Acetonitrile including production,handling, sampling and transfer of materials are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

Table 76: Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) should be required for indoor industrial use.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face- shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves
Other risk management measures related to workers		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the production, handling, sampling and transfer of materials are well-trained.
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	No	As a worst case scenario it is assumed that waste water is directed to a municipal STP without any on-site treatment.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	Varies depending on system.	Worst case estimated production releases are considered below and have been determined to be safe for the environment.
Air emission abatement	No specific air abatement measures	No specific air emission abatement included for the purposes of this risk assessment.
Resulting amount waste gas released to environment	ERC6a: 500 kg/day ERC6b: 10 kg/day ERC7: 500 kg/day	Based on the closed and highly contained systems for industrial use of acetonitrile, these amounts are considered to be vast overestimations.
Onsite waste treatment	No	As a worst case scenario it is assumed that waste water is directed to a municipal STP without any on-site treatment.
Municipal or other type of external waste water treatment	Municipal STP	
Effluent (of the waste water treatment plant) discharge rate	2000 m^3/d	Default: 2000 m^3/d
Recovery of sludge for agriculture or horticulture	Yes	As a worst case scenario it is assumed that sludge from the STP will be spread on land.

9.2.1.7. Waste related measures

Table 77: Fraction of substance in waste and waste management measures.

Information type	Data field	Explanation
Amount of substances in waste water resulting from identified uses covered in the exposure scenario	ERC6a: 200 kg/day ERC6b: 500 kg/day ERC7: 500 kg/day	Based on worst case emission to waste waters from ERC default release factors.
Amount of substances in waste resulting from service life of articles	Not applicable	
Type of waste, suitable waste codes	Suitable EWC code(s)	
Type of external treatment aiming at recycling or recovery of substances	None	
Type of external treatment aiming at final disposal of the waste.	Municipal STP	
Fraction of substance released into the environment via air from waste handling	Not applicable	
Fraction of substance released into the environment via waste water from waste handling	Not applicable	
Fraction of substance disposed of as secondary waste	Not applicable	

9.2.2. Exposure estimation

9.2.2.1. Worker exposure

Acetonitrile is used in industrial processes which are either a closed, continuous process, or closed batch processes and in batch synthesis where some opportunity for exposure may arise.

There is potential exposure to acetonitrile during the transfer of the substance. However transfer of the substance is conducted at dedicated facilities using a closed-system with vapour return. Some bulk transfers may occur at facilities which are industrial or professional but not specifically dedicated to Acetonitrile alone however the use of closed systems with vapour return is a requirement because of the flammability risk. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. For operations with potential inhalation exposure to workers, use of respiratory protection or local exhaust ventilation (LEV) will be required to ensure that risks to workers are adequately controlled with acceptable margins of safety.

Workers involved in industrial uses of Acetonitrile including production, handling, sampling and transfer of materials are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

Systemic dermal exposures to acetonitrile in workers and inhalation exposure concentrations for activities in this scenario have been estimated using the ECETOC TRA Tier 1 model.

Table 78: Exposure concentrations to workers

Routes of exposure	Description of activity	PROC	State of material	Estimated Exposure Concentrations		Measured exposure concentrations	
				Value*	unit	Value	unit
Dermal exposure	Manufacturing including sampling	PROC 1	Liquid	0.343	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 2	Liquid	1.37	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 3	Liquid	0.343	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 4	Liquid	6.86	mg/kg/day	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8a	Liquid	13.71	mg/kg/day	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8b	Liquid	6.86	mg/kg/day	No measured data	
	Transfer of substance	PROC 9	Liquid	0.686**	mg/kg/day	No measured data	
Inhalation exposure	Manufacturing including sampling	PROC 1	Liquid	0.012	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 2	Liquid	12.0	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 3	Liquid	29.9	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 4	Liquid	24.0	mg/m^3	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8a	Liquid	60.0	mg/m^3	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8b	Liquid	60.0	mg/m^3	No measured data	
	Transfer of substance	PROC 9	Liquid	0.855**	mg/m^3	No measured data	

** Minimum exposure as determined by ECETOC based outdoors and without use of respiratory protection as a worst case scenario.*

*** Minimum exposure as determined by ECETOC based on indoors with LEV and without use of respiratory protection.*

Measured dermal exposure data are not available. There is possible exposure during transfer and sampling, however the use closed system with vapour return, and PPE, like eye goggles, protective gloves/gauntlets (for example butyl rubber gloves), boots and protective clothing fully covering the arms and legs of operators, minimises dermal exposure.
Measured inhalation exposure data are not available.. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment may be used, for example, cleaning tanks or reactors. For operations with potential inhalation exposure to workers, use of respiratory protection or local exhaust ventilation (LEV) will be required to ensure that risks to workers are adequately controlled with acceptable margins of safety.

Workers involved in the industrial use of Acetonitrile including production, handling, sampling and transfer of materials are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

9.2.2.2. Consumer exposure

Consumers are not directly exposed to the industrial uses of Acetonitrile in production or processing.

9.2.2.3. Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore, removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

9.2.2.4. Environmental exposure

First tier conservative exposure estimations were carried out using the EUSES 2.1 tool and the specified defaults. ERC6a, ERC6b and ERC7 were used to determine the environmental emissions for ES2. Second tier worst case environmental exposure estimations were not necessary as safe use was demonstrated for all uses in the first tier.

For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acetonitrile and emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. It was determined that ERC6a, ERC6b and ERC7 covered the use of acetonitrile in industrial settings.

It is noted that the use of ERCs to estimate emissions to the environment results in an unrealistic assessment for acetonitrile, as default emission fractions for the ERCs represent a worst case. As such, the assessment was refined using appropriate SPERCs to give a more accurate estimation of releases of acetonitrile to the environment.

9.2.2.4.1. Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES 2.1. Emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 79: EUSES inputs for ES2

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	41.0519	g/mol	
Vapour Pressure at 25°C	13900	Pa	
Water Solubility	1,000,000	g/L	
Octanol/water partition coefficient	-0.54	logKow	
Koc	8.15 (arithmetic mean based on range of values)		
Biodegradability	Readily Biodegradable		
Input parameter:	Value:	Unit:	ERC default (if applicable)
Life Cycle Step	Industrial use		
Tonnage	1000 regional 1000 local	Tonnes per annum	
Environmental Release Category	ERC6a, ERC6b, ERC 7		
Release to Air	ERC6a: 5 ERC6b: 0.1 ERC7: 5	%	ERC6a: 5 ERC6b: 0.1 ERC7: 5
Release to Water	ERC6a: 2 ERC6b: 5 ERC7: 5	%	ERC6a: 2 ERC6b: 5 ERC7: 5
Release to Soil	ERC6a: 0.1 ERC6b: 0.025 ERC7: 5	%	ERC6a: 0.1 ERC6b: 0.025 ERC7: 5
Fraction of Tonnage for Region	1		1
Fraction of the main local source	1		1
STP	Yes		Yes
Emission events per year	100	Days	100

Table 80: Predicted Releases to the Environment

Environmental Release Category (ERC)	Compartments	Predicted releases	Measured release	Explanation / source of measured data
ERC6a	Release to air	500 kg/d	-	ERC release factor
ERC6a	Wastewater	200 kg/d	-	ERC release factor
ERC6a	Soil (direct only) Agricultural soil	0.1%	-	ERC release factor
ERC6b	Release to air (direct only)	10 kg/d	-	ERC release factor
ERC6b	Wastewater	500 kg/d	-	ERC release factor
ERC6b	Soil (direct only) Agricultural soil	0.025%	-	ERC release factor
ERC7	Release to air	500 kg/d	-	ERC release factor
ERC7	Wastewater	500 kg/d	-	ERC release factor
ERC7	Soil (direct only) Agricultural soil	5%	-	ERC release factor

The predicted releases were estimated using the EUSES 2.1 program.

9.2.2.4.2 Exposure concentration in sewage treatment plants (STP)

Table 81: Tier 1 Predicted Exposure Concentrations (PEC) for the STP

Protection target	Exposure concentration
ERC 6a	
Sewage treatment plant (mg/L)	Local PEC: 12.4
ERC 6b	
Sewage treatment plant (mg/L)	Local PEC: 31.1
ERC 7	
Sewage treatment plant (mg/L)	Local PEC: 31.1mg/L

9.2.2.4.3 Exposure concentrations in the aquatic pelagic compartment

Table 82: Tier 1 Predicted Exposure Concentrations (PEC) for the aquatic pelagic environment

Protection target	Exposure concentration
ERC 6a	
Freshwater (mg/L)	Local PEC: 1.24
Marine water (mg/L)	Local PEC: 0.124
ERC 6b	
Freshwater (mg/L)	Local PEC: 3.11
Marine water (mg/L)	Local PEC: 0.311
ERC 7	
Freshwater (mg/L)	Local PEC: 3.11
Marine water (mg/L)	Local PEC: 0.311

9.2.2.4.4 Exposure concentration in sediments

Acetonitrile has a low adsorption potential on sediments. Evidence indicates that acetonitrile will not accumulate in sediments based on this and its rapid degradation in the environment. Nevertheless, PECs calculated in EUSES are presented below for completeness.

Table 83: Tier 1 Predicted Exposure Concentrations (PEC) for the aquatic sediment compartment

Protection target	Exposure concentration
ERC 6a	
Freshwater sediment (mg/kg dw)	Local PEC: 5.48
Marine sediment (mg/kg dw)	Local PEC: 0.548
ERC 6b	
Freshwater sediment (mg/kg dw)	Local PEC: 13.7
Marine sediment (mg/kg dw)	Local PEC: 1.37
ERC 7	
Freshwater sediment (mg/kg dw)	Local PEC: 13.7
Marine sediment (mg/kg dw)	Local PEC: 1.37

As these predicted environmental concentrationsdo not take into account the rapid degradation of acetonitrile in the environment they should be regarded as worst case.

9.2.2.4.5 Exposure concentration in soil and groundwater

Table 84: Tier 1 Predicted Exposure Concentrations (PEC) for soil and groundwater

Protection target	Exposure concentration
ERC 6a	
Agricultural soil (mg/kg dw)	Local PEC: 0.199
Groundwater (mg/L)	Local PEC: 0.177
ERC 6b	
Agricultural soil (mg/kg dw)	Local PEC: 0.485
Groundwater (mg/L)	Local PEC: 0.402
ERC 7	
Protection target	Exposure concentration
Agricultural soil (mg/kg dw)	Local PEC: 0.49
Groundwater (mg/L)	Local PEC: 0.418

These values are considered to be conservative as acetonitrile is likely to degrade rapidly in the environment.

9.2.2.4.6 Atmospheric compartment

Table 85: Tier 1 Predicted Exposure Concentrations (PEC) in air

Protection target	Exposure concentration
ERC 6a	
Annual average PEC in air, total (mg/m^3)	Annual average local PEC: 0.0381
ERC 6b	
Annual average PEC in air, total (mg/m^3)	Annual average local PEC: $7.62x10^{-4}$
ERC 7	
Annual average PEC in air, total (mg/m^3)	Annual average local PEC: 0.0381

9.2.2.4.7 Exposure concentration relevant for the food chain (Secondary poisoning)

Based on the above results, acetonitrile has been demonstrated to be present in the environment in relatively small quantities. This is also the case for atmospheric, aquatic and soil compartments; furthermore acetonitrile is readily biodegradable and has very low potential for bioaccumulation. Therefore it is considered unlikely that birds or mammals will be exposed indirectly either by way of direct contact with the air, surface waters or soils, or by way of drinking water, or through exposure in the food chain.

9.2.2.4.8 Regional exposure levels and environmental concentrations

Regional exposure for the manufacture of acetonitrile has been modelled using EUSES 2.1. No significant PEC values are indicated for the regional scale even under the conservative assumptions of the Tier 2 EUSES assessment.

Table 86: Regional tier 1 concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
ERC6a					
Freshwater	5.83 x 10^{-5}	mg/l	NA	mg/l	
Marine water	5.83 x 10^{-6}	mg/l	NA	mg/l	
Freshwater sediments	2.23 x 10^{-4}	mg/kg dw	NA	mg/kg	
Marine sediments	2.26 x 10^{-5}	mg/kg dw	NA	mg/kg	
Agricultural soil	4.51 x 10^{-6}	mg/kg dw	NA	mg/kg	
Grassland	7.42 x 10^{-6}	mg/kg dw	NA	mg/kg	
Air	2.41 x 10^{-6}	mg/m3	NA	mg/m^3	
ERC6b					
Freshwater	1.27 x 10^{-4}	mg/l	NA	mg/l	
Marine water	1.16 x 10^{-5}	mg/l	NA	mg/l	
Freshwater sediments	4.87 x 10^{-4}	mg/kg dw	NA	mg/kg	
Marine sediments	4.49 x 10^{-5}	mg/kg dw	NA	mg/kg	
Agricultural soil	6.87 x 10^{-7}	mg/kg dw	NA	mg/kg	
Grassland	6.95 x 10^{-7}	mg/kg dw	NA	mg/kg	
Air	2.26 x 10^{-7}	mg/m3	NA	mg/m^3	
ERC7					
Freshwater	2.25 x 10^{-4}	mg/l	NA	mg/l	
Marine water	2.1 x 10^{-5}	mg/l	NA	mg/l	
Freshwater sediments	8.63 x 10^{-4}	mg/kg dw	NA	mg/kg	
Marine sediments	8.13 x 10^{-5}	mg/kg dw	NA	mg/kg	
Agricultural soil	6.51 x 10^{-6}	mg/kg dw	NA	mg/kg	
Grassland	1.05 x 10^{-5}	mg/kg dw	NA	mg/kg	
Air	3.42 x 10^{-6}	mg/m3	NA	mg/m3	

Exposure scenario 3 – Pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile

9.3.1. Exposure scenario

Acetonitrile is as an intermediate and process solvent in the manufacture of pharmaceutical, fine chemicals and active substances used in plant protection, as well as biocidal products. These processes occur at industrial sites in closed continuous processes with either no likelihood of exposure or with only occasional opportunity for exposure in controlled conditions e.g. during bulk delivery, maintenance, sampling or discharge of the material. It is also used in manufacuring processes which are either closed, continuous processes, or closed batch processes and in batch synthesis where some opportunity or exposure may arise. Exposure to workers has been determined using ECETOC TRA.

Sector of Use:
SU9: Manufacture of fine chemicals.

Product Categories:
PC19: Intermediates.
PC21: Laboratory chemicals.
PC29: Pharmaceuticals.

Process Categories:
PROC1: Use in closed process, no likelihood of exposure.
PROC2: Use in closed, continuous process with occasional controlled exposure.
PROC3: Use in closed batch process (synthesis or formulation). Industrial setting.
PROC4: Use in batch and other process (synthesis) where opportunity for exposure arises.
PROC8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at nondedicated facilities. Industrial setting.
PROC8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities. Industrial setting.
PROC15: Use as a laboratory agent.

Environmental Release Category:
ERC4: Industrial use of processing aids in processes and products, not becoming part of articles.
ERC6a: Industrial use resulting in manufacture of another substance (use of intermediates).

9.3.1.1. Description of activities and processes covered in the exposure scenario

Acetonitrile is used as an intermediate and process solvent in the manufacture of pharmaceutical, fine chemicals and active substances used in plant protection as well as solid baits used as biocidal products. These processes occur at industrial sites in closed continuous processes with either no likelihood of exposure or with only occasional opportunity for exposure in controlled conditions e.g. during maintenance, sampling or discharge of the material. It is also used in manufacturing processes which are either closed, continuous processes, or closed batch processes and in batch synthesis where some opportunity for exposure may arise.

These processes using Acetonitrile are conducted outdoors in closed batch and continuous processes. Some smaller scale batch processing and synthesis may be performed indoors under highly controlled conditions and LEV. Similarly it will be used on a small scale as a laboratory agent in pharmaceutical laboratories in assessment and quality control processes. These are likely to be highly controlled environments in high tech laboratories in instruments in laboratory closed system batch processes.

There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required outdoors, except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. For operations with potential inhalation exposure to workers, use of respiratory protection or local exhaust ventilation (LEV) will be required to ensure that risks to workers are adequately controlled with acceptable margins of safety.

The bulk transfer of Acetonitrile following delivery is conducted outside at dedicated facilities using a closed system processes with a vapour return from road or rail tankers, barges or ships to large scale bulk storage vessels.

Some transfers may occur at facilities which are industrial or professional but not specifically dedicated to Acetonitrile alone.

Workers involved in pharmaceutical, fine chemical and active substance production as well as plant protection and biocidal products,manufacture are well tranined in procedures for handling, sampling and transfer of intermediate and process materials and in good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

It should be noted that acetonitrile is only used in the production of the a.i. (active ingredient) of biocidal products, and is not present in the finished formulation or product.

9.3.1.2. Operational conditions related to frequency, duration and amount of use

Table 87: Duration, frequency and amount (for industrial use)

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	500 tonnes/y	The worst case tonnage for a single site is assumed to be 500 tonnes/year (based on a main source fraction of 0.1) as the substance is used at many different sites for manufacture of pharmaceuticals, fine chemicals and active substances.
Emission days per site	200 d/y	Considered to be worst case number of emission days for sites using acetonitrile in pharmaceutical, fine chemical and active substance manufacture

9.3.1.3. Operational conditions and risk management measures related to product characteristics

Table 88: Characteristics of the substance

Information type	Data field	Explanation
Physical state	Liquid	See section 1.3
For solids: Categorisation of dust grades	Not applicable	
Concentration of substance in preparation	99.9%	
Concentration after dilution for use (if relevant)	Not applicable	
Risk management measures related to the design of product		The pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile are conducted outdoors in industrial scale processing plants. There is some use indoors in highly controlled conditions with LEV. There is potential exposure to acetonitrile during the transfer of the substance. Exposure to acetonitrile is possible during charging, sampling or discharge of the material. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

9.3.1.4. Operational conditions related to available dilution capacity and characteristics of exposed humans

Table 89: Operational conditions related to respiration and skin contact

Information type	Data field	Explanation
Respiration volume under conditions of use	10 m^3/d	Default for Light work *(Guidance Section R 8.4.2)*
Room size and ventilation rate	m^3 ; exchange per hour	*If room size and general ventilation is employed to control risk, explain the background of the values assumed.*
Area of skin contact with the substance under conditions of use	0 cm^2	Exposure to acetonitrile is only possible during charging, sampling or discharge of the material and filling of vessels.
Body weight	70 kg	Default for workers

9.3.1.5. Other operational conditions of use

Table 90: Technical fate of substance and losses from process/use to waste, waste water and air

Information type	Data field	Explanation
Fraction of applied amount lost from process/use to waste gas,	ERC4: 1 ERC6a: 0.05	ERC default releases
Fraction of applied amount lost from process/use to waste water	ERC4: 1 ERC6a: 0.02	ERC default releases
Fraction of applied amount lost from process/use to waste	0	Loss of acetonitrile to waste is not likely as acetonitrile will be transferred to a closed vessel.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

9.3.1.6. Risk management measures

The pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile are conducted outdoors in industrial scale processing plants in closed and continuous processes. There is some use in batch processing and synthesis indoors, in highly contolled conditions with LEV. Modern laboratories have local exhaust ventilation (LEV) systems and therefore, the potential for worker exposure to acetonitrile is limited Workers involved in these tasks are professional, well-trained in these procedures and occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure. Pumps, dispensers and pipettes are also used to limit volatilisation. If only general ventilation is employed for indoors activities (*i.e.* weighing acetonitrile in scales outside fumehood), use of respiratory protection may be required.

Table 91: Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) should be required for activities where exposure arises.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face- shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves Respiratory protection
Other risk management measures related to workers		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the production, handling, sampling and transfer of materials are well-trained.
Risk management measures related to environmental emissions from industrial sites		

Information type	Data field	Explanation
Onsite pre-treatment of waste water	No	As a worst case scenario it is assumed that waste water is directed to a municipal STP without any on-site treatment. However, in reality it is likely that the majority of sites manufacturing pharmaceuticals, fine chemicals and active substances will have on-site waste water treatment. It is also likely that the microbial populations in such a facility will be adapted to acetonitrile due to frequent exposure, and hence efficient removal of the substance from the waste stream can be expected. Consequently, it is considered that the assumption that there will be no on-site treatment of waste water is a very worst case scenario.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	Varies depending on system.	Worst case estimated production releases are considered below and have been determined to be safe for the environment.
Air emission abatement	No specific air abatement measures	No specific air emission abatement included for the purposes of this risk assessment.
Resulting amount waste gas released to environment	ERC4: 2500 kg/day ERC6a: 125 kg/day	Based on the closed and highly contained systems for industrial use of acetonitrile, these amounts are considered to be vast overestimations.
Onsite waste treatment	No	As a worst case scenario it is assumed that waste water is directed to a municipal STP without any on-site treatment.
Municipal or other type of external waste water treatment	No	Waste water from acetonitrile production will be emitted to surface water following on-site waste water treatment.
Effluent (of the waste water treatment plant) discharge rate	2000 m^3/d	Default: 2000 m^3/d
Recovery of sludge for agriculture or horticulture	Yes	As a worst case acenario it is assumed that sludge from the STP will be spread on land.
Maximum permissible concentration in effluent from STP	32 mg/L	To demonstrate safe use a maximum permissible concentration in STP effluent has been set.

9.3.1.7. Waste related measures

Table 92: Fraction of substance in waste and waste management measures.

Information type	Data field	Explanation
Amount of substances in waste water resulting from identified uses covered in the exposure scenario	ERC4: 2500 kg/day ERC6a: 50 kg/day	Based on worst case emission to waste waters from ERC default release factors.
Amount of substances in waste resulting from service life of articles	Not applicable	
Type of waste, suitable waste codes	Suitable EWC code(s)	
Type of external treatment aiming at recycling or recovery of substances	None	
Type of external treatment aiming at final disposal of the waste.	Municipal STP	
Fraction of substance released into the environment via air from waste handling	Not applicable	
Fraction of substance released into the environment via waste water from waste handling	Not applicable	
Fraction of substance disposed of as secondary waste	Not applicable	

9.3.2. Exposure estimation

9.3.2.1. Worker exposure

The pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile are performed outdoors in closed batch and continuous processes. Most modern laboratories have local exhaust ventilation (LEV) systems and therefore, the potential for worker exposure to acetonitrile is limited. Workers involved in these tasks are professional, well-trained in these procedures and occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.
If only general ventilation is employed (*i.e.* weighing acetonitrile in scales outside fumehood), use of respiratory protection may be required to ensure that risks to workers are adequately controlled with acceptable margins of safety.

Table 93: Exposure concentrations to workers

Routes of exposure	Description of activity	PROC	State of material	Estimated Exposure Concentrations		Measured exposure concentrations	
				Value*	unit	Value	unit
Dermal exposure	Manufacturing including sampling	PROC 1	Liquid	0.343	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 2	Liquid	1.37	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 3	Liquid	0.343	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 4	Liquid	6.86	mg/kg/day	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8a	Liquid	13.71	mg/kg/day	No measured data	

Routes of exposure	Description of activity	PROC	State of material	Estimated Exposure Concentrations		Measured exposure concentrations	
				Value*	unit	Value	unit
	Transfer of substance, filling, cleaning of equipment	PROC 8b	Liquid	6.86	mg/kg/day	No measured data	
	Use as laboratory reagent	PROC 15	Liquid	0.0343**	mg/kg/day	No measured data	
Inhalation exposure	Manufacturing including sampling	PROC 1	Liquid	0.012	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 2	Liquid	12.0	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 3	Liquid	29.9	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 4	Liquid	24.0	mg/m^3	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8a	Liquid	60.0	mg/m^3	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8b	Liquid	60.0	mg/m^3	No measured data	
	Use as laboratory reagent	PROC 15	Liquid	1.71**	mg/m^3	No measured data	

** Minimum exposure as determined by ECETOC based outdoors and without use of respiratory protection as a worst case scenario.*
*** Minimum exposure as determined by ECETOC based on indoors with LEV and without use of respiratory protection.*

Measured dermal exposure data are not available. There is possible exposure during transfer and sampling, however the use of eye goggles, protective gloves (for example butyl rubber gloves), boots and protective clothing fully covering arms and legs, minimises dermal exposure.

Measured inhalation exposure data are not available. The pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile are performed outdoors in closed batch and continuous processes. There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. For operations with potential inhalation exposure to workers, use of respiratory protection or local exhaust ventilation (LEV) will be required to ensure that risks to workers are adequately controlled with acceptable margins of safety.

The bulk delivery of acetonitrile is via barges, ships, road or rail tankers to bulk storage vessels outdoors. Workers involved in these tasks are professional, well-trained in these procedures and occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to

minimise skin exposure.

9.3.2.2. Consumer exposure

Consumers are not directly exposed to the pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile.

9.3.2.3. Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore, removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

9.3.2.4. Environmental exposure

First tier conservative exposure estimations were carried out using the EUSES 2.1 tool and the specified defaults. ERC 4 and ERC6a were used to determine the environmental emissions for ES3. Second tier worst case environmental exposure estimations were carried out using EUSES 2.1 to take into account more realistic factors that affect the environmental concentrations. For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acetonitrile and emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. It was determined that ERC 4 and ERC6a covered the use of acetonitrile in the manufacture of pharmaceutical, fine cemical and active substance products.

The use of ERC 4 and ERC6a to estimate emissions to the environment results in an unrealistic assessment for acetonitrile, as default emission fractions for the ERCs represent a worst case. As such, the assessment was refined using more realistic conditions of use for manufacture of pharmaceuticals, fine chemicals and active substances. The main source fraction was set to 0.1 and the number of emission days was set to 200 per year to give a more accurate representation of the use of acetonitrile in this sector.

A maximum concentration in STP effluent was included to demonstrate safe use for the environment

It should be noted that the PECs presented in the tier 2 assessment are still considered to be conservative due to a number of worst-case assumptions which were considered during derivation. For instance, it has been assumed that there is no on-site waste water treatment before release to the municipal STP. However, in most cases facilities manufacturing pharmaceuticals, fine chemicals and active substances using acetonitrile will have onsite waste treatment facilities which will have adapted microbial populations, leading to the efficient degradation of acetonitrile and limiting the releases to the municipal STP.

In addition to this such manufacturing facilities are expected to have a high degree of recycling and recapture of volatile solvents, which would also limit the amount of acetonitrile being lost to the environment. Thus, the releases to the environment used in this scenario, especially those used for ERC 4, are considered to be overestimates and lead to a conservative risk assessment.

9.3.2.4.1. Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES 2.1. Emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 94: EUSES inputs for ES3

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	41.0519	g/mol	
Vapour Pressure at 25°C	13900	Pa	
Water Solubility	1,000,000	g/L	
Octanol/water partition coefficient	-0.54	logKow	
Koc	8.15 (arithmetic mean based on range of values)		
Biodegradability	Readily Biodegradable		
Life Cycle Step	Industrial use		
Tonnage	5000 regional 5000 local	Tonnes per annum	
Environmental Release Category	ERC4, ERC6a		
Release to Air	ERC4: 100 ERC6a: 5	%	ERC4: 100 ERC6a: 5
Release to Water	ERC4: 100 ERC6a: 2	%	ERC4: 100 ERC6a: 2
Release to Soil	ERC4: 5 ERC6a: 0.1	%	ERC4: 5 ERC6a: 0.1
Fraction of Tonnage for Region	1		1
Fraction of the main local source	0.1		1
STP	Yes		Yes
Emission events per year	200	Days	100
Concentration of chemical in STP-effluent (set as a maximum permissible value for ERC 4 only)	32	mg/L	

Table 95: Predicted Releases to the Environment

Environmental Release Category (ERC)	Compartments	Predicted releases	Measured release	Explanation / source of measured data
ERC 4	Release to air	2500 kg/d	-	ERC release factor
ERC 4	Wastewater	2500 kg/d	-	ERC release factor
ERC 4	Soil (direct only) Agricultural soil	5%	-	ERC release factor
ERC 6a	Release to air	125 kg/d	-	ERC release factor
ERC 6a	Wastewater	50 kg/d	-	ERC release factor
ERC 6a	Soil (direct only) Agricultural soil	0.1%	-	ERC release factor

9.3.2.4.2. Exposure concentration in sewage treatment plants (STP)

Table 96: Tier 1 Predicted Exposure Concentrations (PEC) for the STP

Protection target	Exposure concentration
ERC 4*	
Sewage treatment plant (mg/L)	Local PEC: 32
ERC 6a	
Sewage treatment plant (mg/L)	Local PEC: 3.11

*the PEC detailed for ERC4 is a maximum permissible value to demonstrate safe use of acetonitrile

9.3.2.4.3. Exposure concentrations in the aquatic pelagic compartment

Table 97: Tier 2 Predicted Exposure Concentrations (PEC) for the aquatic pelagic compartment

Protection target	Exposure concentration
ERC 4*	
Freshwater (mg/L)	Local PEC: 3.21
Marine water (mg/L)	Local PEC: 0.321
Protection target	Exposure concentration
ERC 6a	
Freshwater (mg/L)	Local PEC: 0.311
Marine water (mg/L)	Local PEC: 0.0311

*Local PECs presented for ERC 4 are based on a maximum permissible concentration in STP-effluent of 32 mg/L.

9.3.2.4.4 Exposure concentration in sediments

Acetonitrile has a low adsorption potential on sediments. Evidence indicates that acetonitrile will not accumulate in sediments based on this and its rapid degradation in the environment. Nevertheless, PECs calculated in EUSES are presented below for completeness.

Table 98: Tier 2 Predicted Exposure Concentrations (PEC) for the aquatic sediment compartment

Protection target	Exposure concentration
ERC 4*	
Freshwater sediment (mg/kg dw)	Local PEC: 14.2
Marine sediment (mg/kg dw)	Local PEC: 1.42
ERC 6a	
Freshwater sediment (mg/kg dw)	Local PEC: 1.37
Marine sediment (mg/kg dw)	Local PEC: 0.137

*Local PECs presented for ERC 4 are based on a maximum permissible concentration in STP-effluent of 32 mg/L.

As these predicted environmental concentrations do not take into account the rapid degradation of acetonitrile in the environment they should be regarded as worst case.

9.3.2.4.5 Exposure concentration in soil and groundwater

Table 99: Tier 2 Predicted Exposure Concentrations (PEC) for soil and groundwater

Protection target	Exposure concentration
ERC 4	
Agricultural soil (mg/kg dw)	Local PEC: 2.47
Groundwater (mg/L)	Local PEC: 2.17
ERC 6a	
Agricultural soil (mg/kg dw)	Local PEC: 0.0509
Groundwater (mg/L)	Local PEC: 0.0484

These values are considered to be conservative as acetonitrile is likely to degrade rapidly in the environment.

9.3.2.4.6. Atmospheric compartment

Table 100: Tier 2 Predicted Exposure Concentrations (PEC) in air

Protection target	Exposure concentration
ERC 4	
Annual average PEC in air, total (mg/m^3)	Annual average local PEC: 0.381
ERC 6a	
Annual average PEC in air, total (mg/m^3)	Annual average local PEC: 0.0191

9.3.2.4.7. Exposure concentration relevant for the food chain (Secondary poisoning)

Based on the above results, acetonitrile has been demonstrated to be present in the environment in relatively small quantities. This is also the case for atmospheric, aquatic and soil compartments; furthermore acetonitrile is readily biodegradable and has very low potential for bioaccumulation. Therefore it is considered unlikely that birds or mammals will be exposed indirectly either by way of direct contact with the air, surface waters or soils, or by way of drinking water, or through exposure in the food chain.

9.3.2.4.8 Regional exposure levels and environmental concentrations

Regional exposure for the manufacture of acetonitrile has been modelled using EUSES 2.1. No significant PEC values are indicated for the regional scale even under the conservative assumptions of the Tier 2 EUSES assessment.

Table 101: Regional tier 1 concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
ERC4*					
Freshwater	0.0137	mg/l	NA	mg/l	
Marine water	1.3×10^{-3}	mg/l	NA	mg/l	
Freshwater sediments	0.0525	mg/kg dw	NA	mg/kg	
Marine sediments	5.04×10^{-3}	mg/kg dw	NA	mg/kg	
Agricultural soil	4.92×10^{-4}	mg/kg dw	NA	mg/kg	
Grassland	6.91×10^{-4}	mg/kg dw	NA	mg/kg	
Air	2.55×10^{-4}	mg/m3	NA	mg/m^3	
ERC6a					
Freshwater	2.91×10^{-4}	mg/l	NA	mg/l	
Marine water	2.92×10^{-5}	mg/l	NA	mg/l	
Freshwater sediments	1.12×10^{-3}	mg/kg dw	NA	mg/kg	
Marine sediments	1.13×10^{-4}	mg/kg dw	NA	mg/kg	
Agricultural soil	2.26×10^{-5}	mg/kg dw	NA	mg/kg	
Grassland	3.71×10^{-5}	mg/kg dw	NA	mg/kg	
Air	1.21×10^{-5}	mg/m3	NA	mg/m^3	

*Local PECs presented for ERC 4 are based on a maximum permissible concentration in STP-effluent of 32 mg/L.

9.4. Exposure scenario 4 – Laboratory use of acetonitrile

9.4.1. Exposure scenario

Acetonitrile is used as a laboratory reagent.

Sector of Use:
SU02: NACE M72 Scientific Research and Development.

Product Categories:
PC21: Laboratory chemicals.
PC40: Extraction chemicals.

Process Categories:
PROC3: Use in closed batch process (synthesis or formulation). Industrial setting.
PROC15: Use as a laboratory agent.

Environmental Release Category:
ERC8a: Wide dispersive indoor use of reactive substances in open systems

9.4.1.1. Description of activities and processes covered in the exposure scenario
Acetonitrile is used as a laboratory reagent and solvent where opportunity for exposure arises during transfer of the substance from small containers to reaction vessels or vice versa and in sample processing and sampling. Modern laboratories have local exhaust ventilation (LEV) systems in order to meet occupational exposure legislation and therefore, the potential for worker exposure to acetonitrile is limited. Workers involved in the handling, sampling and transfer of the substance are well-trained in these procedures and they use personal protection equipment (eg protective eye goggles, butyl rubber gloves and laboratory coats) in order to minimise exposure. If only general ventilation is employed (*i.e.* weighing acetonitrile in scales outside fumehood), use of respiratory protection may be advisable, especially when handling large volumes or working for prolonged periods.

9.4.1.2. Operational conditions related to frequency, duration and amount of use

Table 102: Duration, frequency and amount (for professional use)

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	2000 tonnes/y	Worst case tonnage used per year
Emission days per site	100 d/y	Default

9.4.1.3. Operational conditions and risk management measures related to product characteristics

Table 103: Characteristics of the substance

Information type	Data field	Explanation
Physical state	Liquid	See section 1.3
For solids: Categorisation of dust grades	Not applicable	
Concentration of substance in	99.9%	
Information type	**Data field**	**Explanation**
preparation		
Concentration after dilution for use (if relevant)	Not applicable	
Risk management measures related to the design of product		Acetonitrile is used as a laboratory reagent where opportunity for exposure arises during transfer of the substance from small containers to reaction vessels or vice versa and during sampling. Modern laboratories generally have local exhaust ventilation (LEV) systems and therefore, the potential for worker exposure to acetonitrile is limited. Workers involved in the handling, sampling and transfer of the substance are well-trained in these procedures and they use personal protection equipment (protective eye goggles, gloves, and laboratory coats) in order to minimise exposure. If only general ventilation is employed (*i.e.* weighing acetonitrile in scales outside fumehood), use of respiratory protection may be advisable.

9.4.1.4. Operational conditions related to available dilution capacity and characteristics of exposed humans

Table 104: Operational conditions related to respiration and skin contact

Information type	Data field	Explanation
Respiration volume under conditions of use	10 m^3/d	Default for Light work *(Guidance Section R 8.4.2)*
Room size and ventilation rate	m^3 ; exchange per hour	*If room size and general ventilation is employed to control risk, explain the background of the values assumed.*
Area of skin contact with the substance under conditions of use	0 cm^2	As the use of acetonitrile takes place in a contained environment with little or no potential for exposure to operators, it is highly unlikely to come into contact with the skin. The only possible route of exposure is through accidental skincontact.
Body weight	70 kg	Default for workers

9.4.1.5. Other operational conditions of use

Table 105: Technical fate of substance and losses from process/use to waste, waste water and air

Information type	Data field	Explanation
Respiration volume under conditions of use	10 m^3/d	Default for Light work *(Guidance Section R 8.4.2)*
Room size and ventilation rate	m^3 ; exchange per hour	*If room size and general ventilation is employed to control risk, explain the background of the values assumed.*
Area of skin contact with the substance under conditions of use	0 cm^2	As the use of acetonitrile takes place in a contained environment with little or no potential for exposure to operators, it is highly unlikely to come into contact with the skin. The only possible route of exposure is through accidental skin contact.
Body weight	70 kg	Default for workers

9.4.1.6. Risk management measures

Acetonitrile is used as a laboratory reagent and solvent where opportunity for exposure arises during transfer of the substance from small containers to reaction vessels or vice versa and in sample processing and sampling. Modern laboratories have local exhaust ventilation (LEV) systems in oder to comply with occupational exposure legislation and therefore, the potential for worker exposure to acetonitrile is limited. Workers involved in laboratory handling, sampling and transfer of Acetonitrile are well-trained in these procedures and they use personal protection equipment (eg protective eye goggles, butyl rubber gloves and laboratory coats) in order to minimise exposure. Pumps, dispensers and pipettes are also used to limit volatilisation. If only general ventilation is employed (*i.e.* weighing acetonitrile in scales outside fumehood), use of respiratory protection may be advisable.

Table 106: Risk management measures for professional use

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) should be required for activities where exposure arises.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves
Risk management measures related to environmental emissions from wide dispersive professional use		
Municipal or other type of waste water treatment	Municipal	Default
Effluent (of the waste water treatment plant) discharge rate	2,000 m^3/d	Default
Other risk management measures		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the handling, sampling and transfer of materials are well-trained.

9.4.1.7. Waste related measures

Table 107: Fraction of substance in waste and waste management measures.

Information type	Data field	Explanation
Amount of substances in waste water resulting from identified uses covered in the exposure scenario	ERC8a: 1.37 kg/day	Based on emission to waste waters estimated using release factors from appropriate SPERCs
Amount of substances in waste resulting from service life of articles	Not applicable	
Type of waste, suitable waste codes	Suitable EWC code(s)	
Type of external treatment aiming at recycling or recovery of substances	None	
Type of external treatment aiming at final disposal of the waste.	Municipal STP	
Fraction of substance released into the environment viaair from waste handling	Not applicable	
Fraction of substance released into the environment via waste water from waste handling	Not applicable	
Fraction of substance disposed of as secondary waste	Not applicable	

9.4.2. Exposure estimation

9.4.2.1. Worker exposure

Acetonitrile is used as a laboratory reagent where opportunity for exposure arises during transfer of the substance from small containers to reaction vessels or vice versa and sampling. Modern laboratories have local exhaust ventilation (LEV) systems in order to comply with occupational exposure legislation and therefore, the potential for worker exposure to acetonitrile is limited. Workers involved in laboratory handling, sampling and transfer of Acetonitrile are well-trained in these procedures and they use personal protection equipment (eg protective eye goggles, butyl rubber gloves and laboratory coats) in order to minimise exposure.. If only general ventilation is employed (*i.e.* weighing acetonitrile in scales outside fumehood), use of respiratory protection may be advisable.

Systemic dermal exposures to acetonitrile in workers and inhalation exposure concentrations for activities in this scenario have been estimated using the ECETOC TRA Tier 1 model.

Table 108: Exposure concentrations to workers

Routes of exposure	**Description of activity**	**PROC**	**State of material**	**Estimated Exposure Concentrations**			**Measured exposure concentrations**	
				Value [1]	**Value** [2]	**unit**	**Value**	**unit**
Dermal exposure	Manufacturing including sampling	PROC 3	Liquid	0.343	0.034	mg/kg/day	No measured data	
	Use as laboratory reagent	PROC 15	Liquid	0.343	0.034	mg/kg/day	No measured data	
Inhalation exposure	Manufacturing including sampling	PROC 3	Liquid	42.8	8.55	mg/m^3	No measured data	
Routes of exposure	**Description of activity**	**PROC**	**State of material**	**Estimated Exposure Concentrations**			**Measured exposure concentrations**	
				Value [1]	**Value** [2]	**unit**	**Value**	**unit**
Inhalation exposure	Use as laboratory reagent	PROC 15	Liquid	17.1	3.42	mg/m^3	No measured data	

1 *Minimum exposure as determined by ECETOC based indoors, without LEV and without the use of respiratory protection as a worst case scenario.*
2 *Minimum exposure as determined by ECETOC based indoors, with LEV and without the use of respiratory protection.*

Measured dermal exposure data are not available. There is possible exposure during transfer and sampling, however the widespread use of protective personal equipment (gloves) minimises dermal exposure of this substance.

Measured inhalation exposure data are not available. No respiratory protection is generally required. Professional workers involved in laboratory handling, sampling and transfer of Acetonitrile are well-trained in these procedures and use personal protection equipment (eg protective eye goggles, butyl rubber gloves and laboratory coats) in order to minimise exposure.

9.4.2.2. Consumer exposure

Consumers are not directly exposed to the use of acetonitrile as a laboratory reagent.

9.4.2.3. Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the use of acetonitrile as a laboratory reagent does not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

9.4.2.4. Environmental exposure

First tier conservative exposure estimations were carried out using the EUSES 2.1 tool and the specified defaults. ERC 8awas used to determine the environmental emissions for ES4. Second tier worst case environmental exposure estimations were carried out using EUSES 2.1 to take into account more realistic factors that affect the environmental concentrations. For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acetonitrile and emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. It was determined that ERC8a covered the use of acetonitrile in laboratories.

It is noted that the use of these ERCs to estimate emissions to the environment results in an unrealistic assessment for acetonitrile, as default emission fractions for ERC 8a represent a worst case. As such, the assessment was refined using appropriate SPERCs to give a more accurate estimation of releases of acetonitrile to the environment.

9.4.2.4.1 Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES 2.1. Emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. Regional data and emission fractions were calculated using EUSES and are shown below.

Table 109: EUSES inputs for ES4

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	41.0519	g/mol	
Vapour Pressure at 25°C	13900	Pa	
Water Solubility	1,000,000	g/L	
Octanol/water partition coefficient	-0.54	logKow	
Koc	8.15 (arithmetic mean based on range of alues)		
Biodegradability	Readily Biodegradable		
Life Cycle Step	Manufacture		
Tonnage	2000 regional 2000 local	Tonnes per annum	
Environmental Release Category	ERC 8a		
Release to Air	ERC8a: 50 (from ESVOC SPERC 8.17.v1)	%	ERC8a: 100
Release to Water	ERC8a: 50 (from ESVOC SPERC 8.17.v1)	%	ERC8a: 100
Release to Soil	ERC8a: 0.00 (from ESVOC SPERC 8.17.v1)	%	ERC8a: n.a.
Fraction of Tonnage for Region	1		1
Fraction of the main local source	0.0005 (from ESVOC SPERC 8.17.v1)		0.1
STP	Yes		Yes
Emission events per year	365 (from ESVOC SPERC 8.17.v1)	Days	100

The releases and PECs presented below are based on release factors from ESVOC SPERC 8.17.v1. As the default release factors were deemed to be overly conservative and not represent realistic releases of acetonitrile from laboratory uses, information from the SPERC which relates to acetonitrile use in laboratories was used. The ERC 8a releases were refined with release factors from ESVOC SPERC 8.17.v1 (Use of small quantities within laboratory settings).

Table 110: Predicted Releases to the Environment

Environmental Release Category (ERC)	Compartments	Predicted releases	Measured release	Explanation / source of measured data
ERC 8a	Release to air	1.37 kg/d	-	ERC release factor
ERC 8a	Wastewater	1.37 kg/d	-	ERC release factor
ERC 8a	Soil (direct only) Agricultural soil	0.00 kg/d	-	ERC release factor

The predicted releases were estimated using the EUSES 2.1 program.

9.4.2.4.2 Exposure concentration in sewage treatment plants (STP)

Table 111: Tier 1 Predicted Exposure Concentrations (PEC) for the STP

Protection target	Exposure concentration
ERC 8a	
Sewage treatment plant (mg/L)	**Local PEC:** 0.0851

9.4.2.4.3 Exposure concentrations in the aquatic pelagic compartment

Table 112: Tier 1 Predicted Exposure Concentrations (PEC) for the aquatic pelagic compartment

Protection target	Exposure concentration
ERC 8a	
Freshwater (mg/L)	**Local PEC:** 0.0112
Marine water (mg/L)	**Local PEC:** 1.1 $x10^{-3}$

9.4.2.4.4 Exposure concentration in sediments

Acetonitrile has a low adsorption potential on sediments. Evidence indicates that acetonitrile will not accumulate in sediments based on this and its rapid degradation in the environment. Nevertheless, PECs calculated in EUSES are presented below for completeness.

Table 113: Tier 1 Predicted Exposure Concentrations (PEC) for the aquatic sediment compartment

Protection target	Exposure concentration
ERC 8a	
Freshwater sediment (mg/kg dw)	**Local PEC:** 0.0107
Marine sediment (mg/kg dw)	**Local PEC:** 1.06 $x10^{-3}$

As these predicted environmental concentrations do not take into account the rapid degradation of acetonitrile in the environment they should be regarded as worst case.

9.4.2.4.5 Exposure concentration in soil and groundwater

Table 114: Tier 1 Predicted Exposure Concentrations (PEC) for soil and groundwater

Protection target	Exposure concentration
ERC 8a	
Agricultural soil (mg/kg dw)	**Local PEC:** 1.35 $x10^{-3}$
Groundwater (mg/L)	**Local PEC:** 1.78 $x10^{-3}$

These values are considered to be conservative as acetonitrile is likely to degrade rapidly in the environment.

9.4.2.4.6 Atmospheric compartment

Table 115: Tier 1 Predicted Exposure Concentrations (PEC) in air

Protection target	Exposure concentration
ERC 8a	
Annual average PEC in air, total (mg/m^3)	**Annual average local PEC:** 0.0381

9.4.2.4.7 Exposure concentration relevant for the food chain (Secondary poisoning)

Based on the above results, acetonitrile has been demonstrated to be present in the environment in relatively small quantities. This is also the case for atmospheric, aquatic and soil compartments; furthermore acetonitrile is readily biodegradable and has very low potential for bioaccumulation. Therefore it is considered unlikely that birds or mammals will be exposed indirectly either by way of direct contact with the air, surface waters or soils, or by way of drinking water, or through exposure in the food chain.

9.4.2.4.8 Regional exposure levels and environmental concentrations

Regional exposure for the manufacture of acetonitrile has been modelled using EUSES 2.1. No significant PEC values are indicated for the regional scale even under the conservative assumptions of the Tier 2 EUSES assessment.

Table 116: Regional tier 1 concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
ERC8a					
Freshwater	2.65×10^{-3}	mg/l	NA	mg/l	
Marine water	2.51×10^{-4}	mg/l	NA	mg/l	
Freshwater sediments	0.0101	mg/kg dw	NA	mg/kg	
Marine sediments	9.75×10^{-4}	mg/kg dw	NA	mg/kg	
Agricultural soil	9.67×10^{-5}	mg/kg dw	NA	mg/kg	
Grassland	1.54×10^{-4}	mg/kg dw	NA	mg/kg	
Air	5×10^{-5}	mg/m^3	NA	mg/m^3	

9.5. Exposure scenario 5 – Photographic/printing uses of acetonitrile

9.5.1. Exposure scenario

Acetonitrile is used in photographic/printing applications.

Sector of Use:
SU02: NACE C18 Printing.
SU02: NACE M74.2 Photographic activities.

Product Categories:
PC30: Photochemicals.

Process Categories:
PROC3: Use in closed batch process (synthesis or formulation). Industrial setting.
PROC15: Use as a laboratory agent.

Environmental Release Category:
ERC8a: Wide dispersive indoor use of processing aids, open

Article Category:
AC01: Photographic and reprographic articles.

9.5.1.1. Description of activities and processes covered in the exposure scenario

The photographic/printing use of acetonitrile allows the opportunity for exposure to arise during transfer of the substance from small containers to reaction vessels or vice versa and sampling. Most modern professional photographic processing is conducted in closed systems with recycling of processing agents and solvents. Given the flammability risk with Acetonitrile, its use in such processes will be highly controlled. Limited opportunity for exposure will occur in these situations.

The photographic/printing use of acetonitrile is performed indoors with general ventilation. Generally, no respiratory protection is required. Professional workers involved in photographic uses of Acetonitrile handling, sampling and transfer are well-trained in these procedures, as well as good occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective clothing to minimise skin exposure.

9.5.1.2. Operational conditions related to frequency, duration and amount of use

Table 117: Duration, frequency and amount (for professional use)

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	5 tonnes/y	Tonnage produced per year
Emission days per site	365 d/y	Default

9.5.1.3. Operational conditions and risk management measures related to product characteristics

Table 118: Characteristics of the substance

Information type	Data field	Explanation
Physical state	Liquid	See section 1.3
For solids: Categorisation of dust grades	Not applicable	
Concentration of substance in preparation	99.9%	
Concentration after dilution for use (if relevant)	Not applicable	
Risk management measures related to the design of product		The photographic/printing use of acetonitrile is performed indoors with general ventilation. Most modern professional photographic processing is conducted in closed systems with recycling of processing agents and solvents. Given the flammability risk of Acetonitrile, its use in such processes will be highly controlled. Limited opportunity for exposure will occur in these situations. Exposure to acetonitrile is likely during handling, sampling and transfer of the material. Professional workers involved in photographic uses of Acetonitrile handling, sampling and transfer are well-trained in these procedures, as well as good occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective clothing to minimise skin exposure.

9.5.1.4. Operational conditions related to available dilution capacity and characteristics of exposed humans

Table 119: Operational conditions related to respiration and skin contact

Information type	Data field	Explanation
Respiration volume under conditions of use	10 m^3/d	Default for Light work *(Guidance Section R 8.4.2)*
Room size and ventilation rate	m^3 ; exchange per hour	*If room size and general ventilation is employed to control risk, explain the background of the values assumed.*
Area of skin contact with the substance under conditions of use	0 cm^2	As the use of acetonitrile takes place in a contained environment with little or no potential for exposure to operators ,it is highly unlikely to come into contact with the skin. The only possible route of exposure is through accidental skin contact.
Body weight	70 kg	Default for workers

9.5.1.5. Other operational conditions of use

Table 120: Technical fate of substance and losses from process/use to waste, waste water and air

Information type	Data field	Explanation
Fraction of applied amount lost from process/use to waste gas,	1	ERC default
Fraction of applied amount lost from process/use to waste water	1	ERC default
Fraction of applied amount lost from process/use to waste	0 kg/kg	Loss of acetonitrile to waste is not likely as acetonitrile will be transferred to a closed vessel.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

9.5.1.6. Risk management measures

The photographic/printing use of acetonitrile is performed indoors with general ventilation. Most modern professional photographic processing is conducted in closed systems with recycling of processing agents and solvents. Given the flammability risk of Acetonitrile, its use and release in such processes will be highly controlled. Limited opportunity for exposure will occur in these situations.Normally no LEV ventilation is required. Only general ventilation is used. Respiratory protection is generally not required.

Professional workers involved in photographic uses of Acetonitrile handling, sampling and transfer are welltrainedin these procedures, as well as good occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective clothing to minimise skin exposure.

Table 121: Risk management measures for professional use

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	No local exhaust ventilation (LEV) is used, only general ventilation used.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves
Risk management measures related to environmental emissions from wide dispersive professional use		
Municipal or other type of waste water treatment	Municipal STP	Default
Effluent (of the waste water treatment plant) discharge rate	2,000m^3/d	Default
Other risk management measures		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the handling, sampling and transfer of materials are well-trained.

9.5.1.7. Waste related measures

Table 122: Fraction of substance in waste and waste management measures.

Information type	Data field	Explanation
Amount of substances in waste water resulting from identified uses covered in the exposure scenario	ERC8a: 1.37 kg/day	Based on worst case emission to waste waters from ERC default release factors.
Amount of substances in waste resulting from service life of articles	Not applicable	
Type of waste, suitable waste codes	Suitable EWC code(s)	
Type of external treatment aiming at recycling or recovery of substances	None	
Type of external treatment aiming at final disposal of the waste.	Municipal STP	
Fraction of substance released into the environment via air from waste handling	Not applicable	
Fraction of substance released into the environment via waste water from waste handling	Not applicable	
Fraction of substance disposed of as secondary waste	Not applicable	

9.5.2. Exposure estimation

9.5.2.1. Worker exposure

The photographic/printing use of acetonitrile is performed indoors with general ventilation. Most modern professional photographic processing is conducted in closed systems with recycling of processing agents and solvents. Given the flammability risk of Acetonitrile its use in such processes will be highly controlled. Limited opportunity for exposure will occur in these situations. Generally, no respiratory protection is required.

Professional workers involved in photographic uses of Acetonitrile handling, sampling and transfer are welltrained in these procedures, as well as good occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective clothing to minimise skin exposure. Dermal contact is therefore minimised.

Systemic dermal exposures to acetonitrile in workers and inhalation exposure concentrations for activities in this scenario have been estimated using the ECETOC TRA Tier 1 model.

Table 123: Exposure concentrations to workers

Routes of exposure	Description of activity	PROC	State of material	Estimated Exposure Concentrations		Measured exposure concentrations	
				Value*	unit	Value	unit
Dermal exposure	Manufacturing including ampling	PROC 3	Liquid	0.343	mg/kg/day	No measured data	
	Use as laboratory reagent	PROC 15	Liquid	0.343	mg/kg/day	No measured data	
Inhalation exposure	Manufacturing including Sampling	PROC 3	Liquid	42.8	mg/m^3	No measured data	
	Use as laboratory reagent	PROC 15	Liquid	17.1	mg/m^3	No measured data	

** Minimum exposure as determined by ECETOC based on indoors without LEV and without use of respiratory protection as a worst case scenario.*

Measured dermal exposure data are not available. There is possible exposure during transfer and sampling, however the widespread use of protective personal equipment (gloves) minimises dermal exposure of this substance.

Measured inhalation exposure data are not available. The photographic/printing use of acetonitrile is performed indoors with general ventilation. No respiratory protection is required.

Professional workers involved in photographic uses of Acetonitrile handling, sampling and transfer are welltrained in these procedures, as well as good occupational hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective clothing to minimise skin exposure.

9.5.2.2. Consumer exposure

Consumers are not directly exposed to the photographic/printing use of acetonitrile.

9.5.2.3. Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the photographic/printing use of acetonitrile does not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

9.5.2.4. Environmental exposure

First tier conservative exposure estimations were carried out using the EUSES 2.1 tool and the specified defaults. ERC 8a was used to determine the environmental emissions for ES5. For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acetonitrile and emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. It was determined that ERC8a covered the use of acetonitrile in laboratories.

It is noted that the use of these ERCs to estimate emissions to the environment results in an unrealistic assessment for acetonitrile, as default emission fractions for ERC 8a represent a worst case.

9.5.2.4.1 Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES 2.1. Emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 124: EUSES inputs for ES5

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	41.0519	g/mol	
Vapour Pressure at 25°C	13900	Pa	
Water Solubility	1,000,000	g/L	
Octanol/water partition coefficient	-0.54	logKow	
Koc	8.15 (arithmetic mean based on range of values)		
Biodegradability	Readily Biodegradable		
Life Cycle Step	Manufacture		
Tonnage	5 regional 5 local	Tonnes per annum	
Environmental Release Category	ERC8a		
Release to Air	100	%	100
Release to Water	100	%	100
Release to Soil	n.a	%	n.a
Fraction of Tonnage for Region	1		1
Fraction of the main local source	0.1		0.1
STP	Yes		Yes
Emission events per year	365	Days	365

Table 125: Predicted Releases to the Environment

Environmental Release Category (ERC)	Compartments	Predicted releases	Measured release	Explanation / source of measured data
ERC 8a	Release to air	1.37 kg/d	-	ERC release factor
ERC 8a	Wastewater	1.37 kg/d	-	ERC release factor
ERC 8a	Soil (direct only) Agricultural soil	0 kg/d	-	ERC release factor

The predicted releases were estimated using the EUSES 2.1 program.

9.5.2.4.2. Exposure concentration in sewage treatment plants (STP)

Table 126: Tier 1 Predicted Exposure Concentrations (PEC) for the STP

Protection target	Exposure concentration
Sewage treatment plant (mg/L)	**Local PEC:** 0.0851

9.5.2.4.3. Exposure concentrations in the aquatic pelagic compartment

Table 127: Tier 1 Predicted Exposure Concentrations (PEC) for the aquatic pelagic compartment

Protection target	Exposure concentration
Freshwater (mg/L)	**Local PEC:** 8.52 $x10^{-3}$
Marine water (mg/L)	**Local PEC:** 8.52 $x10^{-4}$

Table 128: Tier 1 Predicted Exposure Concentrations (PEC) for the aquatic sediment compartment

Protection target	Exposure concentration
Freshwater sediment (mg/kg dw)	**Local PEC:** 0.0376
Marine sediment (mg/kg dw)	**Local PEC:** 3.76 $x10^{-3}$

As these predicted environmental concentrations do not take into account the rapid degradation of acetonitrile in the environment they should be regarded as worst case.

9.5.2.4.5. Exposure concentration in soil and groundwater

Table 129: Tier 1 Predicted Exposure Concentrations (PEC) for soil and groundwater

Protection target	Exposure concentration
Agricultural soil (mg/kg dw)	**Local PEC:** 1.38 $x10^{-3}$
Groundwater (mg/L)	**Local PEC:** 1.27 $x10^{-3}$

These values are considered to be conservative as acetonitrile is likely to degrade rapidly in the environment.

9.5.2.4.6. Atmospheric compartment

Table 130: Tier 1 Predicted Exposure Concentrations (PEC) for air

Protection target	Exposure concentration
Annual average PEC in air, total (mg/m^3)	**Annual average local PEC:** $3.81x10^{-4}$

9.5.2.4.7. Exposure concentration relevant for the food chain (Secondary poisoning)

Based on the above results, acetonitrile has been demonstrated to be present in the environment in relatively small quantities. This is also the case for atmospheric, aquatic and soil compartments; furthermore acetonitrile is readily biodegradable and has very low potential for bioaccumulation. Therefore it is considered unlikely that birds or mammals will be exposed indirectly either by way of direct contact with the air, surface waters or soils, or by way of drinking water, or through exposure in the food chain.

9.4.2.4.8 Regional exposure levels and environmental concentrations

Regional exposure for the manufacture of acetonitrile has been modelled using EUSES 2.1. No significant PEC values are indicated for the regional scale even under the conservative assumptions of the Tier 2 EUSES assessment.

Table 131: Regional tier 1 concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
Freshwater	$1.32\ x10^{-5}$	mg/l	NA	mg/l	
Marine water	$1.26\ x\ 10^{-6}$	mg/l	NA	mg/l	
Freshwater sediments	$5.07\ x10^{-5}$	mg/kg dw	NA	mg/kg	
Marine sediments	$4.87\ x10^{-6}$	mg/kg dw	NA	mg/kg	
Agricultural soil	$4.84x\ 10^{-7}$	mg/kg dw	NA	mg/kg	
Grassland	$6.78\ x\ 10^{-7}$	mg/kg dw	NA	mg/kg	
Air	$2.5\ x\ 10^{-7}$	mg/m3	NA	mg/m^3	

9.6. Exposure scenario 6 – Repackaging/dilution (Azeotrope creation) of acetonitrile

9.6.1. Exposure scenario

Acetonitrile can be mixed with various solvents including water (azeotropes) and repackaged for sale for professional uses (e.g. laboratory uses). The dilution/mixing applications take place at dedicated facilities in a closed batch reactor where opportunity for exposure can arise (*i.e.* taking samples at different points of the process, when transferring or loading the substance to/from reactor, when mixing or blending). Transfer or drumming to smaller vessels is conducted in a closed system with a vapour return at dedicated facilites. For tasks where opportunity for exposure arises, use of personal protection equipment is required. These processes are largely conducted outside under cover from precipitation. If conducted indoors the use of local exhaust ventilation (LEV) should also be employed during these activities.

Sector of Use:
SU10: Formulation of preparations and/or repackaging.

Product Categories:
PC21: Laboratory chemicals.
PC40: Extraction chemicals.

Process Categories:
PROC3: Use in closed batch process (synthesis or formulation). Industrial setting.
PROC5: Mixing or blending on batch processes for formulation of preparations and articles (multistage and/or significant contact).
PROC9: Transfer of substance or preparation into small containers at dedicated facilities.

Environmental Release Category:
ERC2: Formulation of preparations.

9.6.1.1. Description of activities and processes covered in the exposure scenario

The use of acetonitrile in repacking/dilution applications take place in a closed batch reactor where opportunity for exposure can arise (*i.e.* taking samples at different points of the process, when transferring or loading the substance to/from reactor, when mixing or blending). For tasks where opportunity for exposure arises, use of personal protection equipment is required; protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure . Use of local exhaust ventilation (LEV) should also be employed during these activities if conducted indoors, given the flammability of Acetonitrile and the potential for significant inhalation exposure.

9.6.1.2. Operational conditions related to frequency, duration and amount of use

Table 132: Duration, frequency and amount (for professional use)

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	5 tonnes/y	Worst case on-site tonnage
Emission days per site	20 d/y	Default

9.6.1.3. Operational conditions and risk management measures related to product characteristics

Table 133: Characteristics of the substance

Information type	Data field	Explanation
Physical state	Liquid	See section 1.3
For solids: Categorisation of dust grades	Not applicable	
Concentration of substance in preparation	99.9%	
Concentration after dilution for use (if relevant)	Not applicable	
Risk management measures related to the design of product		The use of acetonitrile for repackaging/dilution applications takes place in closed batch or continuous processes where potential exposure to workers arises for some specific tasks (*i.e.* taking samples, transfer of the substance, mixing or blending). For tasks where opportunity for exposure arises, use of personal protection equipment is required; use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure . Use of local exhaust ventilation (LEV) should also be employed during these activities if indoors.

9.6.1.4. Operational conditions related to available dilution capacity and characteristics of exposed humans

Table 134: Operational conditions related to respiration and skin contact

Information type	Data field	Explanation
Respiration volume under conditions of use	10 m^3/d	Default for Light work *(Guidance Section R 8.4.2)*
Room size and ventilation rate	m^3 ; exchange per hour	*If room size and general ventilation is employed to control risk, explain the background of the values assumed.*
Area of skin contact with the substance under conditions of use	0 cm^2	Exposure to acetonitrile is only possible during charging, sampling or discharge of the material and filling of trucks.
Body weight	70 kg	Default for workers

9.6.1.5. Other operational conditions of use

Table 135: Technical fate of substance and losses from process/use to waste, waste water and air

Information type	Data field	Explanation
Fraction of applied amount lost from process/use to waste gas,	0.025	ERC default.
Fraction of applied amount lost from process/use to waste water	0.02	ERC default.
Fraction of applied amount lost from process/use to waste	0 kg/kg	Loss of acetonitrile to waste is not likely as acetonitrile will be transferred to a closed vessel.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

9.6.1.6. Risk management measures

Acetonitrile can be mixed with various solvents including water (azeotropes) and repackaged for sale for professional uses (e.g. laboratory uses). The dilution/mixing applications take place at dedicated faciities in a closed batch reactor where opportunity for exposure can arise (*i.e.* taking samples at different points of the process, when transferring or loading the substance to/from reactor, when mixing or blending). Transfer or drumming to smaller vessels is conducted in a closed system with a vapour return at dedicated facilites. For tasks where opportunity for exposure arises, use of personal protection equipment is required; use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure. These processes are largely conducted outside under cover from precipitation. If conducted indoors the use of local exhaust ventilation (LEV) should also be employed during these activities.

Table 136: Risk management measures for professional site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) maybe required for specific activities where potential for exposure could arise.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face- shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves Respiratory protection
Other risk management measures related to workers		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the production, handling, sampling and transfer of materials are well-trained.
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	No	As a worst case scenario it is assumed that waste water is directed to a municipal STP without any on-site treatment.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	0	As a worst case scenario it is assumed that waste water is directed to a municipal STP without any on-site treatment.
Air emission abatement	No specific air abatement measures	No specific air emission abatement included for the purposes of this risk assessment.
Resulting amount waste gas released to environment	6.25kg/day	Based on ERC 2 default release factors
Onsite waste treatment	No	As a worst case scenario it is assumed that waste water is directed to a municipal STP without any on-site treatment.
Municipal or other type of external waste water treatment	Municipal STP	
Effluent (of the waste water treatment plant) discharge rate	2000 m^3/d	Default: 2000 m^3/d
Recovery of sludge for agriculture or horticulture	Yes	As a worst case acenario it is assumed that sludge from the STP will be spread on land.

9.6.1.7. Waste related measures

Table 137: Fraction of substance in waste and waste management measures.

Information type	Data field	Explanation
Amount of substances in waste water resulting from identified uses covered in the exposure scenario	ERC2: 5 kg/day	Based on worst case emission to waste waters from ERC default release factors.
Amount of substances in waste resulting from service life of articles	Not applicable	
Type of waste, suitable waste codes	Suitable EWC code(s)	
Type of external treatment aiming at recycling or recovery of substances	None	
Type of external treatment aiming at final disposal of the waste.	Municipal STP	
Fraction of substance released into the environment via air from waste handling	Not applicable	
Fraction of substance released into the environment via waste water from waste handling	Not applicable	
Fraction of substance disposed of as secondary waste	Not applicable	

9.6.2. Exposure estimation

9.6.2.1. Worker exposure

Acetonitrile can be mixed with various solvents including water (azeotropes) and repackaged for sale for professional uses (e.g. laboratory uses). The dilution/mixing applications take place at dedicated facilities in a closed batch reactor where opportunity for exposure can arise (*i.e.* taking samples at different points of the process, when transferring or loading the substance to/from reactor, when mixing or blending). Transfer or drumming to smaller vessels is conducted in a closed system with a vapour return at dedicated facilities. For tasks where opportunity for exposure arises, use of personal protection equipment is required; use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure. These processes are largely conducted outside under cover from precipitation. If conducted indoors the use of local exhaust ventilation (LEV) should also be employed during these activities.

Workers involved in the handling, sampling and transfer of materials are well-trained in these procedures and they use personal protection equipment to minimise exposure. For most of the activities, general ventilation is used, however it may be advisable or required to use Local exhaust ventilation (LEV) for specific tasks. During prolonged operations where LEV is not used, use of respiratory protection may be required.

Systemic dermal exposures to acetonitrile in workers and inhalation exposure concentrations for activities in this scenario have been estimated using the ECETOC TRA Tier 1 model.

Table 138: Exposure concentrations to workers

Routes of exposure	Description of activity	PROC	State of material	Estimated Exposure Concentrations				Measured exposure concentrations	
				Value [1]	Value [2]	Value[3]	unit	Value	unit
Dermal exposure	Manufacturing including sampling	PROC 3	Liquid	0.343	0.343	0.034	mg/kg/ day	No measured data	
	Mixing or blending in batch processes	PROC 5	Liquid	13.7	13.7	0.069	mg/kg/ day	No measured data	
	Transfer of substance	PROC 9	Liquid	6.86	6.86	0.686	mg/kg/ day	No measured data	
Inhalation exposure	Manufacturing including sampling	PROC 3	Liquid	42.8	4.28	8.55	mg/m^3	No measured data	
	Mixing or blending in batch processes	PROC 5	Liquid	171	17.1	34.2	mg/m^3	No measured data	
	Transfer of substance	PROC 9	Liquid	171	17.1	34.2	mg/m^3	No measured data	

1 *Minimum exposure as determined by ECETOC based indoors, without LEV and without the use of respiratory protection as a worst case scenario.*
2 *Minimum exposure as determined by ECETOC based indoors, without LEV and with the use of respiratory protection.*
3 *Minimum exposure as determined by ECETOC based indoors, with LEV and without the use of respiratory protection.*

Measured dermal exposure data are not available. There is possible exposure during transfer and sampling, however use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure is routine, to minimise dermal exposure.

Measured inhalation exposure data are not available. The dilution/mixing applications take place at dedicated facilities in a closed batch reactor where opportunity for exposure can arise (*i.e.* taking samples at different points of the process, when transferring or loading the substance to/from reactor, when mixing or blending). Transfer or drumming to smaller vessels is conducted in a closed system with a vapour return at dedicated facilites. For tasks where opportunity for exposure arises, use of personal protection equipment is required. These processes are largely conducted outside under cover from precipitation. If conducted indoors, given the flammability of Acetonitrile and the potential for significant inhalation exposure, the use of local exhaust ventilation (LEV) should also be employed during these activities.

9.6.2.2. Consumer exposure

Consumers are not directly exposed to the repackaging/dilution of acetonitrile.

9.6.2.3. Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment.
Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the repackaging/dilution of acetonitrile do not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receivingV compartments is expected to be minimal. Similarly contamination of food crops or animals used as human

food sources is not envisaged.

9.6.2.4. Environmental exposure

First tier conservative exposure estimations were carried out using the EUSES 2.1 tool and the specified defaults. ERC 2 was used to determine the environmental emissions for ES6. Second tier environmental exposure estimations were not necessary as safe use could be demonstrated in the frst tier. For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acetonitrile and emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. It was determined that ERC2 covered the repackaging/dilution of acetonitrile.

It is noted that the use of these ERCs to estimate emissions to the environment results in an unrealistic assessment for acetonitrile, as default emission fractions for ERC 2 represent a worst case.

9.6.2.4.1. Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES 2.1. Emission defaults are those specified by the ECHA “Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation”. Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 139: EUSES inputs for ES6

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	41.0519	g/mol	
Vapour Pressure at 25°C	13900	Pa	
Water Solubility	1,000,000	g/L	
Octanol/water partition coefficient	-0.54	logKow	
Koc	8.15 (arithmetic mean based on range of values)		
Biodegradability	Readily Biodegradable		
Life Cycle Step	Manufacture		
Tonnage	5 regional 5 local	Tonnes per annum	
Environmental Release Category	ERC2		
Release to Air	2.5	%	2.5
Release to Water	2	%	2
Release to Soil	0.01	%	0.01
Fraction of Tonnage for Region	1		1
Fraction of the main local source	1		1
STP	Yes		Yes
Emission events per year	20	Days	20

Table 140: Predicted Releases to the Environment

Environmental Release Category (ERC)	Compartments	Predicted releases	Measured release	Explanation / source of measured data
ERC 2	Release to air	6.25 kg/d	-	ERC release factor
ERC 2	Wastewater	5 kg/d	-	ERC release factor
ERC 2	Soil (direct only) Agricultural soil	0.01%	-	ERC release factor

The predicted releases were estimated using the EUSES 2.1 program.

9.6.2.4.2 Exposure concentration in sewage treatment plants (STP)

Table 141: Tier 1 Predicted Exposure Concentrations (PEC) for the STP

Protection target	Exposure concentration
Sewage treatment plant (mg/L)	**Local PEC:** 0.311

9.6.2.4.3. Exposure concentrations in the aquatic pelagic compartment

Table 142: Tier 1 Predicted Exposure Concentrations (PEC) for the aquatic pelagic compartment

Protection target	Exposure concentration
Freshwater (mg/L)	**Local PEC:** 0.0311
Marine water (mg/L)	**Local PEC:** 3.11 $x10^{-3}$

9.6.2.4.4. Exposure concentration in sediments

Acetonitrile has a low adsorption potential on sediments. Evidence indicates that acetonitrile will not accumulate in sediments based on this and its rapid degradation in the environment. Nevertheless, PECs calculated in EUSES are presented below for completeness.

Table 143: Tier 1 Predicted Exposure Concentrations (PEC) for the aquatic sediment compartment

Protection target	Exposure concentration
Freshwater sediment (mg/kg dw)	**Local PEC:** 0.137
Marine sediment (mg/kg dw)	**Local PEC:** 0.0137

As these predicted environmental concentrations do not take into account the rapid degradation of acetonitrile in the environment they should be regarded as worst case.

9.6.2.4.5. Exposure concentration in soil and groundwater

Table 144: Tier 1 Predicted Exposure Concentrations (PEC) for soil and groundwater

Protection target	Exposure concentration
Agricultural soil (mg/kg dw)	**Local PEC:** 4.29 $x10^{-3}$
Groundwater (mg/L)	**Local PEC:** 4.06 $x10^{-3}$

These values are considered to be conservative as acetonitrile is likely to degrade rapidly in the environment.

9.6.2.4.6. Atmospheric compartment

Table 145: Tier 1 Predicted Exposure Concentrations (PEC) in air

Protection target	Exposure concentration
Annual average PEC in air, total (mg/m^3)	**Annual average local PEC:** 1.9 $x10^{-4}$

9.6.2.4.7. Exposure concentration relevant for the food chain (Secondary poisoning)

Based on the above results, acetonitrile has been demonstrated to be present in the environment in relatively small quantities. This is also the case for atmospheric, aquatic and soil compartments; furthermore acetonitrile is readily biodegradable and has very low potential for bioaccumulation. Therefore it is considered unlikely that birds or mammals will be exposed indirectly either by way of direct contact with the air, surface waters or soils, or by way of drinking water, or through exposure in the food chain.

9.6.2.4.8. Regional exposure levels and environmental concentrations

Regional exposure for the manufacture of acetonitrile has been modelled using EUSES 2.1. No significant PEC values are indicated for the regional scale even under the conservative assumptions of the Tier 2 EUSES assessment.

Table 146: Regional tier 1 concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
Freshwater	2.69 $x10^{-7}$	mg/l	NA	mg/l	
Marine water	2.57 x 10^{-8}	mg/l	NA	mg/l	
Freshwater sediments	4.74 $x10^{-5}$	mg/kg dw	NA	mg/kg	
Marine sediments	4.56 $x10^{-6}$	mg/kg dw	NA	mg/kg	
Agricultural soil	1.18 x 10^{-8}	mg/kg dw	NA	mg/kg	
Grassland	1.9x 10^{-8}	mg/kg dw	NA	mg/kg	
Air	6.17 x 10^{-9}	mg/m3	NA	mg/m^3	

10. RISK CHARACTERISATION

10.1. Exposure scenario 1 – Manufacture of acetonitrile

10.1.1. Human health

10.1.1.1. Workers

The estimated concentrations for dermal exposures to acetonitrile in workers predicted by the ECETOC TRA Tier 1 model were all below the DNEL value for long-term systemic effects. A risk characterisation for acute systemic and local effects associated with dermal exposures were not carried out as an appropriate DNEL for this endpoint could not be quantified.

No measured dermal data are available. The manufacture of acetonitrile is performed outdoors in an industrial scale closed batch and continuous process. There is potential exposure to acetonitrile during the transfer of the substance. The bulk production of acetonitrile is piped or transported (tankers, barges, ships, large scale bulk storage vessels) to an external terminal prior to distribution to use sites by road-tankers, barges or ships. Workers involved in the production, handling, sampling and transfer of Acetonitrile are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

Systemic inhalation exposures to acetonitrile in workers estimated by the ECETOC TRA Tier 1 model were all below the DNELs for acute and long-term systemic effects and for acute and long-term local effects. These estimates, apart from activity PROC 9, were based on the worst-case assumption that the activities are carried out outdoors, without the use of LEV. The estimate inhalation exposure concentration for activity PROC 9 was based on the assumption that the activity is carried out indoors, with the use of LEV and without appropriate personal protective equipment (PPE), as modern laboratories have local exhaust ventrilation facilities in place to be in compliance with occupational exposure requirements. Although use of respiratory protective equipment is not required for any manufacturing activities, it may be advisable to use respiratory protection for certain critical tasks e.g. cleaning tanks or reactors. Workers involved in the production, handling, sampling and transfer of Acetonitrile are well-trained in the procedures and use of appropriate protective equipment in order to minimise exposure and risks.

It can be concluded that the risks to workers are adequately controlled with acceptable margins of safety when performing activities PROC 1, 2, 3, 4, 8a and 8b outdoors without LEV and without respiratory protection or when performing activity PROC 9 indoors with LEV.

Table 147 : (Semi) Quantitative risk characterisation for workers

	Route	PROC code	ES 1-exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute - systemic effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose	68 mg/m³	0.894

	Route	PROC code	ES 1- exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
				toxicity		
		PROC 9	0.855 mg/m^3	Repeated dose toxicity	68 mg/m³	0.013
Acute - local effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 9	0.855** mg/m^3	Repeated dose toxicity	68 mg/m³	0.013**
Long-term - systemic effects	Dermal	PROC 1	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 2	1.37 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.043
		PROC 3	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 4	6.86 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.214
		PROC 8a	12 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.429
		PROC 9	0.855 mg/m^3	Repeated dose toxicity	68 mg/m³	0.013

	Route	PROC code	ES 1- exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute - local effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 9	0.855** mg/m^3	Repeated dose toxicity	68 mg/m³	0.013**
Long-term - systemic effects	Dermal	PROC 1	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 2	1.37 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.043
		PROC 3	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 4	6.86 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.214
		PROC 8a	12 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.429

**Based on estimations determined by ECETOC for worst case: >4 hours worker exposure, outdoors, no respiratory protection.*
*** Based on estimations determined by ECETOC for: >4 hours worker exposure, indoors with LEV, no respiratory protection.*

10.1.1.2. Consumers

Consumers are not directly exposed to the manufacture of acetonitrile.

10.1.1.3. Indirect exposure of humans via the environment

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the manufacture of acetonitrile does not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

10.1.2. Environment

10.1.2.1 Aquatic compartment (including sediment and secondary poisoning)

The PECs outlined in section 9 are compared to the derived PNECs below.

Table 148: Risk characterisation for the aquatic compartment

Compartments	PEC mg/l	PNEC mg/l or mg/kg dw	PEC/PNEC	Comments/Discussion
Tier 2 Freshwater	1.79	10.2	0.175	Safe use demonstrated for all compartments in tier 2.
Tier 2 Marine	0.179	1.02	0.175	
Tier 2 Freshwater sediment	7.89	45	0.175	
Tier 2 Marine sediment	0.789	4.5	0.175	

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.1.2.2 Terrestrial compartment (including secondary poisoning)

During manufacture of acetonitrile there is no direct exposure of the terrestrial compartment. Concentrations of acetonitrile in the terrestrial compartment are expected to be minimal and the PECs presented here are expected to be vast overestimations of the concentrations that will actually exist in the terrestrial compartment due to the fact that acetonitrile is likely to degrade rapidly in the environment.

Table 149: Risk characterisation for the terrestrial compartment

Compartments	PEC mg/kg dw	PNEC mg/kg dw	PEC/PNEC	Comments/discussion
Tier 2 soil	3.77×10^{-3}	3.02	1.39×10^{-3}	Safe use demonstrated tier 2.

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.1.2.3 Atmospheric compartment

Atmospheric contamination due to production of acetonitrile is minimal, and as there is no indicated effects on plants or animals from atmospheric acetonitrile no PNEC and no RCR is derived.

10.1.2.4 Microbiological activity in sewage treatment systems

A worst case PEC for the STP is presented below. As all RCRs are less than 1 it is considered that safe use has been demonstrated.

Table 150: Risk characterisation for the sewage treatment microorganisms (STP)

Compartments	PEC mg/L	PNEC mg/L	PEC/PNEC	Comments/discussion
Tier 2 Sewage treatment plant (STP)	17.6	32	1.38×10^{-3}	Safe use demonstrated tier 2.

10.2. Exposure scenario 2 – Industrial use of acetonitrile

10.2.1. Human health

10.2.1.1. Workers

The estimated concentrations for dermal exposures to acetonitrile in workers predicted by the ECETOC TRA Tier 1 model were all below the DNEL value for long-term systemic effects. A risk characterisation for acute systemic and local effects associated with dermal exposures were not carried out as an appropriate DNEL for this endpoint could not be quantified.
No measured dermal data are available. There is potential exposure to acetonitrile during the transfer of the substance. Workers involved in the industrial uses of Acetonitrile including production, handling, sampling and transfer of materials are well-trained in these procedures as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

Systemic inhalation exposures to acetonitrile in workers estimated by the ECETOC TRA Tier 1 model were all below the DNELs for acute and long-term systemic effects and for acute and long-term local effects. These estimates, apart from activity PROC 9, were based on the worst-case assumption that the activities are outdoors, without the use of LEV. The estimate inhalation exposure concentration for activity PROC 9 was based on the assumption that the activity is carried out indoors, with the use of LEV and without appropriate personal protective equipment (PPE), as modern laboratories have local exhaust ventrilation facilities in place to be in compliance with occupational exposure requirements. Although use of respiratory protective equipment is not required for any manufacturing activities, it may be advisable to use respiratory protection for certain critical tasks e.g. cleaning tanks or reactors. Workers involved in the production, handling, sampling and transfer of materials are well-trained in the procedures and use of appropriate protective respiratory equipment in order to minimise exposure and risks.

It can be concluded that the risks to workers are adequately controlled with acceptable margins of safety when performing activities PROC 1, 2, 3, 4, 8a and 8b outdoors without LEV and without respiratory protection or when performing activity PROC 9 indoors with LEV.

Table 151: (Semi) Quantitative risk characterisation for workers

	Route	PROC code	ES 1-exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute - systemic effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 9	0.855 mg/m^3	Repeated dose toxicity	68 mg/m³	0.013

	Route	PROC code	ES 1- exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute - local effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 9	0.855** mg/m^3	Repeated dose toxicity	68 mg/m³	0.013**
Long-term - systemic effects	Dermal	PROC 1	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 2	1.37 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.043
		PROC 3	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 4	6.86 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.214
		PROC 8a	12 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.429
		PROC 8b	6.86 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.214
		PROC 9	6.86 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.021

	Route	PROC code	ES 1-exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
		PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 9	0.855** mg/m^3	Repeated dose toxicity	68 mg/m³	0.013**
	Combined routes					RCR Inhalation-systemic + RCR Dermal-systemic
Long-term – local effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 9	0.855** mg/m^3	Repeated dose toxicity	68 mg/m³	0.013**
	Combined routes					RCR Inhalation-systemic + RCR Dermal-systemic

**Based on estimations determined by ECETOC for worst case: >4 hours worker exposure, outdoors, no respiratory protection.*
*** Based on estimations determined by ECETOC for: >4 hours worker exposure, indoors with LEV, no respiratory protection.*

10.2.1.2. Consumers

Consumers are not directly exposed to the manufacture of acetonitrile.

10.2.1.3. Indirect exposure of humans via the environment

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the manufacture of acetonitrile does not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

10.2.2. Environment

10.2.2.1 Aquatic compartment (including sediment and secondary poisoning)

The PECs outlined in section 9 are compared to the derived PNECs below.

Table 152: Risk characterisation for the aquatic compartment

Compartments	PEC mg/l or mg/kg dw	PNEC mg/l or mg/kg dw	PEC/PNEC	Comments/Discussion
ERC 6a				
Tier 1 Freshwater	1.24	10.2	0.122	Safe use demonstrated for all compartments in tier 1.
Tier 1 Marine	0.124	1.02	0.122	
Tier 1 Freshwater sediment	5.48	45	0.122	
Tier 1 Marine sediment	0.548	4.5	0.122	
ERC 6b				
Tier 1 Freshwater	3.11	10.2	0.304	Safe use demonstrated for all compartments in tier 1.
Tier 1 Marine	0.311	1.02	0.304	
Tier 1 Freshwater sediment	13.7	45	0.304	
Tier 1 Marine sediment	1.37	4.5	0.304	
ERC 7				
Tier 1 Freshwater	3.11	10.2	0.304	Safe use demonstrated for all compartments in tier 1.
Tier 1 Marine	0.311	1.02	0.304	
Tier 1 Freshwater sediment	13.7	45	0.304	
Tier 1 Marine sediment	1.37	4.5	0.304	

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.2.2.2 Terrestrial compartment (including secondary poisoning)

There is no direct exposure of the terrestrial compartment from industrial uses of acetonitrile. Concentrations of acetonitrile in the terrestrial compartment are expected to be minimal and the PECs presented here are expected to be vast overestimations of the concentrations that will actually exist in the terrestrial compartment due to the fact that acetonitrile is likely to degrade rapidly in the environment.

Table 153: Risk characterisation for the terrestrial compartment

Compartments	PEC mg/kg dw	PNEC mg/kg dw	PEC/PNEC	Comments/discussion
ERC 6a				
Tier 1 soil	0.199	3.02	0.657	Safe use demonstrated tier 1.
ERC 6b				
Tier 1 soil	0.485	3.02	0.16	Safe use demonstrated tier 1.
ERC 7				
Tier 1 soil	0.49	3.02	0.162	Safe use demonstrated tier 1.

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.2.2.3 Atmospheric compartment

Atmospheric contamination due to industrial uses of acetonitrile is minimal, and as there is no indicated effects on plants or animals from atmospheric acetonitrile no PNEC and no RCR is derived.

10.2.2.4 Microbiological activity in sewage treatment systems

A worst case PEC for the STP is presented below. As all RCRs are less than 1 it is considered that safe use has been demonstrated.

Table 154: Risk characterisation for the sewage treatment microorganisms (STP)

Compartments	PEC mg/L	PNEC mg/L	PEC/PNEC	Comments/discussion
ERC 6a				
Tier 1 Sewage treatment plant (STP)	12.4	32	0.388	Safe use demonstrated tier 1.
ERC 6b				
Tier 1 Sewage treatment plant (STP)	31.1	32	0.97	Safe use demonstrated tier 1.
ERC 7				
Tier 1 Sewage treatment plant (STP)	31.1	32	0.97	Safe use demonstrated tier 1.

10.3. Exposure scenario 3 – Pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile

10.3.1. Human health

10.3.1.1. Workers

The estimated concentrations for dermal exposures to acetonitrile in workers predicted by the ECETOC TRA Tier 1 model were all below the DNEL value for long-term systemic effects. Risk characterisations for acute systemic and local effects associated with dermal exposures were not carried out as an appropriate DNEL for this endpoint could not be quantified.

No measured dermal data are available for the use of Acetonitrile in pharmaceutical, fine chemical and active substance manufacture. These processes occur at industrial sites in closed continuous processes, with either no likelihood of exposure or with only occasional opportunity for exposure in controlled conditions e.g. during bulk delivery, maintenance, sampling or discharge of the material. It is also used in manufacuring processes which are either closed, continuous processes, or closed batch processes and in batch synthesis where some opportunity for exposure may arise. Modern laboratories have local exhaust ventilation (LEV) systems in order to comply with occupational exposure requirements and therefore, the potential for worker exposure to acetonitrile is limited. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors.

The bulk delivery of acetonitrile is via barges, ships, road or rail tankers to bulk storage vessels. Workers involved in industrial uses of Acetonitrile in the production of pharmaceutical, fine chemicals, plant protection and biocidal active substances are well trained in handling, sampling and transfer procedures, as well as good industrial hygiene practices. They use protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure.

Systemic inhalation exposures to acetonitrile in workers estimated by the ECETOC TRA Tier 1 model were all below the DNELs for acute and long-term systemic effects and for acute and long-term local effects. These estimates, apart from activity PROC 15, were based on the worst-case assumption that the activities are carried out outdoors, without the use of LEV. The estimate inhalation exposure concentration for activity PROC 15 was based on the assumption that the activity is carried out indoors, with the use of LEV and without appropriate personal protective equipment (PPE), as modern laboratories have local exhaust ventrilation facilities in place to be in compliance with occupational exposure requirements. Workers involved in the production, handling, sampling and transfer of materials are well-trained in the procedures and use of appropriate protective equipment in order to minimise exposure and risks.

It can be concluded that the risks to workers are adequately controlled with acceptable margins of safety when performing activities PROC 1, 2, 3, 4, 8a and 8b outdoors without LEV and without respiratory protection or when performing activity PROC 15 indoors with LEV.

Table 155: (Semi) Quantitative risk characterisation for workers

	Route	PROC code	ES 1-exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute - systemic effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose	68 mg/m³	0.357

	Route	PROC code	ES 1- exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
				toxicity		
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 15**	1.71 mg/m^3	Repeated dose toxicity	68 mg/m³	0.026
Acute - local effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 15**	1.71 mg/m^3	Repeated dose toxicity	68 mg/m³	0.026
Long-term - systemic effects	Dermal	PROC 1	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 2	1.37 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.043
		PROC 3	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 4	6.86 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.214
		PROC 8a	12 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.429
		PROC 8b	6.86 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.214
		PROC 15**	0.0343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.001

	Route	PROC code	ES 1-exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
		PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 15**	1.71 mg/m^3	Repeated dose toxicity	68 mg/m³	0.026
	Combined routes					RCR Inhalation-systemic + RCR Dermal-systemic
Long-term – local effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 1	0.012 mg/m^3	Repeated dose toxicity	68 mg/m³	0.000
		PROC 2	12.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.179
		PROC 3	29.9 mg/m^3	Repeated dose toxicity	68 mg/m³	0.447
		PROC 4	24.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.357
		PROC 8a	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 8b	60.0 mg/m^3	Repeated dose toxicity	68 mg/m³	0.894
		PROC 15**	1.71 mg/m^3	Repeated dose toxicity	68 mg/m³	0.026
	Combined routes					RCR Inhalation-systemic + RCR Dermal-systemic

**Based on estimations determined by ECETOC for worst case: >4 hours worker exposure, outdoors, no respiratory protection.*
*** Based on estimations determined by ECETOC for: >4 hours worker exposure, indoors with LEV, no respiratory protection.*

10.3.1.2. Consumers

Consumers are not directly expososed to theuses of Acetonitrile in pharmaceutical, fine chemical and active substance manufacture. .Acetonitrile is only used in the production of the a.i. (active ingredient) and is not

present in the finished formulation or product.

10.3.1.3. Indirect exposure of humans via the environment

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the manufacture of acetonitrile does not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

10.3.2. Environment

10.3.2.1 Aquatic compartment (including sediment and secondary poisoning)

The PECs outlined in section 9 are compared to the derived PNECs below.

Table 156: Risk characterisation for the aquatic compartment

Compartments	PEC mg/l	PNEC mg/l or mg/kg dw	PEC/PNEC	Comments/Discussion
ERC 4*				
Tier 2 Freshwater	3.21	10.2	0.315	Safe use demonstrated for all compartments in tier 2.
Tier 2 Marine	0.321	1.02	0.315	
Tier 2 Freshwater sediment	14.2	45	0.315	
Tier 2 Marine sediment	1.42	4.5	0.315	
ERC 6a				
Tier 2 Freshwater	0.311	10.2	0.0305	Safe use demonstrated for all compartments in tier 2.
Tier 2 Marine	0.0311	1.02	0.0305	
Tier 2 Freshwater sediment	1.37	45	0.0305	
Tier 2 Marine sediment	0.137	4.5	0.0305	

*presented PECs and RCRs for ERC 4 based on a maximum permissible concentration in STP effluent of 32 mg/L

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.3.2.2 Terrestrial compartment (including secondary poisoning)

There is no direct exposure of the terrestrial compartment from the use of acetonitrile in the manufacture of pharmaceuticals, fine chemicals and active substances. Concentrations of acetonitrile in the terrestrial compartment are expected to be minimal and the PECs presented here are expected to be vast overestimations of the concentrations that will actually exist in the terrestrial compartmentdue to the fact that acetonitrile is likely to degrade rapidly in the environment.

Table 157: Risk characterisation for the terrestrial compartment

Compartments	PEC mg/kg dw	PNEC mg/kg dw	PEC/PNEC	Comments/discussion
ERC 4				
Tier 2 soil	2.47	3.02	0.818	Safe use demonstrated tier 2.
ERC 6a				
Tier 2 soil	0.0509	3.02	0.0168	Safe use demonstrated tier 2.

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.3.2.3 Atmospheric compartment

Atmospheric contamination due to the use of acetonitrile in the manufacture of pharmaceuticals, fine chemicals and active substances is minimal, and as there is no indicated effects on plants or animals from atmospheric acetonitrile no PNEC and no RCR is derived.

10.3.2.4 Microbiological activity in sewage treatment systems

A worst case PEC for the STP is presented below. As all RCRs are less than 1 it is considered that safe use has been demonstrated.

Table 158: Risk characterisation for the sewage treatment microorganisms (STP)

Compartments	PEC mg/L	PNEC mg/L	PEC/PNEC	Comments/discussion
ERC 4*				
Tier 2 Sewage treatment plant (STP)	32	32	1	Safe use demonstrated tier 2.
ERC 6a				
Tier 2 Sewage treatment plant (STP)	3.11	32	0.097	Safe use demonstrated tier 2.

*presented PECs and RCRs for ERC 4 based on a maximum permissible concentration in STP effluent of 32 mg/L

10.4. Exposure scenario 4 – Laboratory use of acetonitrile

10.4.1. Human health

10.4.1.1. Workers

The estimated concentrations for dermal exposures to acetonitrile in workers predicted by the ECETOC TRA Tier 1 model were all below the DNEL value for long-term systemic effects. A risk characterisation for acute systemic and local effects associated with dermal exposures were not carried out as an appropriate DNEL for this endpoint could not be quantified.

No measured dermal data are available. Acetonitrile is used as a laboratory reagent and solvent where opportunity for exposure arises during transfer of the substance from small containers to reaction vessels or vice versa and during sampling. Modern laboratories have local exhaust ventilation (LEV) systems in order to comply with occupational exposure requirements and therefore, the potential for worker exposure to acetonitrile is limited. Workers involved in the handling, sampling and transfer of the substance are well-trained in these procedures and they use personal protection equipment (eg protective eye goggles, butyl rubber gloves and laboratory coats) in order to minimise exposure.

Systemic inhalation exposures to acetonitrile in workers estimated by the ECETOC TRA Tier 1 model were all below the acute systemic DNEL and acute local effects DNEL. Systemic inhalation exposures predicted by the model for activities PROC 3 and 15 were also below the DNEL for long-term systemic effects. These estimates were based on the worst-case assumption that the activities are carried out indoors, without the use of LEV and without the use of respiratory protection. Workers involved in the production, handling, sampling and transfer of materials are well-trained in the procedures and use of appropriate protective equipment in order to minimise exposure and risks.

It can be concluded that the risks to workers are adequately controlled with acceptable margins of safety when performing activities indoors without LEV and without the use of respiratory protection.

Table 159: (Semi) Quantitative risk characterisation for workers

	Route	PROC code	ES 3- exposure concentrations (EC)*		Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio	
			Without LEV	With LEV			Without LEV	With LEV
Acute - systemic effects	Dermal	-	-	-	-	Not quantifiable	-	-
	Inhalation	PROC 3	42.8 mg/m^3	8.55 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638	0.128
		PROC 15	17.1 mg/m^3	3.42 mg/m^3	Repeated dose toxicity	68 mg/m³	0.255	0.051
Acute - local effects	Dermal	-	-	-	-	Not quantifiable	-	-
	Inhalation	PROC 3	42.8 mg/m^3	8.55 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638	0.128
		PROC 15	17.1 mg/m^3	3.42 mg/m^3	Repeated dose toxicity	68 mg/m³	0.255	0.051

	Route	PROC code	ES 3- exposure concentrations (EC)*		Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio	
			Without LEV	With LEV			Without LEV	With LEV
Long-term - systemic effects	Dermal	PROC 3	0.343 mg/kg bw/d	0.034 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011	0.001
		PROC 15	0.343 mg/kg bw/d	0.034 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011	0.001
	Inhalation	PROC 3	42.8 mg/m^3	8.55 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638	0.128
		PROC 15	17.1 mg/m^3	3.42 mg/m^3	Repeated dose toxicity	68 mg/m³	0.255	0.051
	Combined routes						RCR Inhalation-systemic + RCR Dermal-systemic	
Long-term – local effects	Dermal	-	-	-	-	Not quantifiable	-	-
Long-term – local effects	Inhalation	PROC 3	42.8 mg/m^3	8.55 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638	0.128
		PROC 15	17.1 mg/m^3	3.42 mg/m^3	Repeated dose toxicity	68 mg/m³	0.255	0.051
	Combined routes						RCR Inhalation-systemic + RCR Dermal-systemic	

**all estimations determined for worst case: >4 hours worker exposure, no respiratory protection.*

10.4.1.2. Consumers

Consumers are not directly exposed to the laboratory use of Acetonitrile.

10.4.1.3. Indirect exposure of humans via the environment

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the manufacture of acetonitrile does not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

10.4.2. Environment

10.4.2.1 Aquatic compartment (including sediment and secondary poisoning)

The PECs outlined in section 9 are compared to the derived PNECs below.

Table 160: Risk characterisation for the aquatic compartment

Compartments	PEC mg/l or mg/kg dw	PNEC mg/l or mg/kg dw	PEC/PNEC	Comments/Discussion
ERC 8a				
Tier 2 Freshwater	0.0112	10.2	1.09×10^{-3}	Safe use demonstrated for all compartments in tier 2
Tier 2 Marine	1.1×10^{-3}	1.02	1.09×10^{-3}	
Tier 2 Freshwater sediment	0.0493	45	1.09×10^{-3}	
Tier 2 Marine sediment	4.87×10^{-3}	4.5	1.09×10^{-3}	

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.4.2.2 Terrestrial compartment (including secondary poisoning)

There is no direct exposure of the terrestrial compartment from laboratory use of acetonitrile. Concentrations of acetonitrile in the terrestrial compartment are expected to be minimal and the PECs presented here are expected to be vast overestimations of the concentrations that will actually exist in the terrestrial compartment due to the fact that acetonitrile is likely to degrade rapidly in the environment.

Table 161: Risk characterisation for the terrestrial compartment

Compartments	PEC mg/kg dw	PNEC mg/kg dw	PEC/PNEC	Comments/discussion
ERC 8a				
Tier 2 soil	1.53×10^{-3}	3.02	5.06×10^{-4}	Safe use demonstrated tier 2

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.4.2.3 Atmospheric compartment

Atmospheric contamination due to laboratory use of acetonitrile is minimal, and as there is no indicated effects on plants or animals from atmospheric acetonitrile no PNEC and no RCR is derived.

10.4.2.4 Microbiological activity in sewage treatment systems

A worst case PEC for the STP is presented below. As all RCRs are less than 1 it is considered that safe use has been demonstrated.

Table 162: Risk characterisation for the sewage treatment microorganisms (STP)

Compartments	PEC mg/L	PNEC mg/L	PEC/PNEC	Comments/discussion
ERC 8a				
Tier 2 Sewage treatment plant (STP)	0.0851	32	2.66×10^{-3}	Safe use demonstrated tier 2.

10.5. Exposure scenario 5 – Photographic/printing uses of acetonitrile

10.5.1. Human health

10.5.1.1. Workers

The estimated concentrations for dermal exposures to acetonitrile in workers predicted by the ECETOC TRA Tier 1 model were all below the DNEL value for long-term systemic effects. A risk characterisation for acute systemic and local effects associated with dermal exposures were not carried out as an appropriate DNEL for this endpoint could not be quantified.

No measured dermal data are available. The photographic/printing use of acetonitrile is generally performed indoors in a closed system limiting the potential for dermal exposure. Professional workers involved in the handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves) and appropriate protective clothing in order to minimise exposure.

Systemic inhalation exposures to acetonitrile in workers estimated by the ECETOC TRA Tier 1 model were all below the acute systemic DNEL and acute local effects DNEL. Systemic inhalation exposures predicted by the model for activities PROC 3 and 15 were also below the DNEL for long-term systemic effects. These estimates were based on the worst-case assumption that the activities are carried out indoors, without the use of LEV without respiratory protection. Workers involved in the handling, sampling and transfer of materials are welltrained in the procedures and use of appropriate protective equipment in order to minimise exposure. It can be concluded that the risks to workers are adequately controlled with acceptable margins of safety when performing activities indoors without LEV and without the use of respiratory protection.

Table 163: (Semi) Quantitative risk characterisation for workers

	Route	PROC code	ES 4-exposure concentrations (EC)*	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute - systemic effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 3	42.8 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638
		PROC 15	17.1 mg/m^3	Repeated dose toxicity	68 mg/m³	0.255
Acute - local effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 3	42.8 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638
		PROC 15	17.1 mg/m^3	Repeated dose toxicity	68 mg/m³	0.255
Long-term - systemic effects	Dermal	PROC 3	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
		PROC 15	0.343 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011
	Inhalation	PROC 3	42.8 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638
		PROC 15	17.1 mg/m^3	Repeated dose toxicity	68 mg/m³	0.255
	Combined routes					RCR Inhalation-systemic + RCR Dermal-systemic
	Route	**PROC code**	**ES 4-exposure concentrations (EC)***	**Leading toxic end point / Critical effect**	**DN(M)EL**	**Risk characterisation ratio**
Long-term – local effects	Dermal	-	-	-	Not quantifiable	-
	Inhalation	PROC 3	42.8 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638
		PROC 15	17.1 mg/m^3	Repeated dose toxicity	68 mg/m³	0.255
	Combined routes					RCR Inhalation-systemic + RCR Dermal-systemic

**all estimations determined for worst case: no LEV, >4 hours worker exposure, no respiratory protection.*

10.5.1.2. Consumers

Consumers are not directly exposed to the use of Acetonitrile in photographic or printing uses.

10.5.1.3. Indirect exposure of humans via the environment

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment. Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the manufacture of acetonitrile does not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

10.5.2. Environment

10.5.2.1 Aquatic compartment (including sediment and secondary poisoning)

The PECs outlined in section 9 are compared to the derived PNECs below.

Table 164: Risk characterisation for the aquatic compartment

Compartments	PEC mg/l or mg/kg dw	PNEC mg/l or mg/kg dw	PEC/PNEC	Comments/Discussion
Tier 1 Freshwater	8.52×10^{-3}	10.2	8.35×10^{-4}	Safe use demonstrated for all compartments in tier 1.
Tier 1 Marine	8.52×10^{-4}	1.02	8.35×10^{-4}	
Tier 1 Freshwater sediment	0.0376	45	8.35×10^{-4}	
Tier 1 Marine sediment	3.76×10^{-3}	4.5	8.35×10^{-4}	

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.5.2.2 Terrestrial compartment (including secondary poisoning)

There is no direct exposure of the terrestrial compartment from photographic/printing uses of acetonitrile. Concentrations of acetonitrile in the terrestrial compartment are expected to be minimal and the PECs presented here are expected to be vast overestimations of the concentrations that will actually exist in the terrestrial compartmentdue to the fact that acetonitrile is likely to degrade rapidly in the environment.

Table 165: Risk characterisation for the terrestrial compartment

Compartments	PEC mg/kg dw	PNEC mg/kg dw	PEC/PNEC	Comments/discussion
Tier 1 soil	1.38×10^{-3}	3.02	4.56×10^{-4}	Safe use demonstrated tier 1.

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.5.2.3 Atmospheric compartment

Atmospheric contamination due to photographic/printing uses of acetonitrile is minimal, and as there is no indicated effects on plants or animals from atmospheric acetonitrile no PNEC and no RCR is derived.

10.5.2.4 Microbiological activity in sewage treatment systems
A worst case PEC for the STP is presented below. As all RCRs are less than 1 it is considered that safe use has been demonstrated.

Table 166: Risk characterisation for the sewage treatment microorganisms (STP)

Compartments	PEC mg/L	PNEC mg/L	PEC/PNEC	Comments/discussion
Tier 1 Sewage treatment plant (STP)	0.851	32	2.66×10^{-3}	Safe use demonstrated tier 1.

10.6. Exposure scenario 6 – Repackaging/dilution (Azeotrope creation) of acetonitrile

10.6.1. Human health

10.6.1.1. Workers

The estimated concentrations for dermal exposures to acetonitrile in workers predicted by the ECETOC TRA Tier 1 model were all below the DNEL value for long-term systemic effects. A risk characterisation for acute systemic and local effects associated with dermal exposures were not carried out as an appropriate DNEL for this endpoint could not be quantified.

No measured dermal data are available. Acetonitrile can be mixed with various solvents including water (azeotropes) and repackaged for sale for professional uses (e.g. laboratory uses). The dilution/mixing applications take place at dedicated facilities in a closed batch reactor where opportunity for exposure can arise (*i.e.* taking samples at different points of the process, when transferring or loading the substance to/from reactor, when mixing or blending). Transfer or drumming to smaller vessels is conducted in a closed system with a vapour return at dedicated facilites. For tasks where opportunity for exposure arises, use of personal protection equipment is required; protective eye goggles, gloves/gauntlets (eg butyl rubber gloves) and protective coveralls to minimise skin exposure . . These processes are largely conducted outside under cover from precipitation. Use of local exhaust ventilation (LEV) should also be employed if conducted indoors, given the flammability of Acetonitrile and the potential for significant inhalation exposure.

The systemic inhalation exposure predicted by the ECETOC model for activity PROC 3 was below the DNEL for acute and long-term systemic effects and for acute and long-term local effects when performing this activity indoors without LEV and without respiratory protection. However, systemic inhalation exposures to acetonitrile estimated by the model for activities PROC 5 and 9 were found to exceed the DNEL for acute and long-term systemic effects and for acute and long-term local effects when performing these tasks indoors without LEV and without repiratory protection. When these tasks are performed indoors without LEV but with the use of respiratory protective equipment, the estimated inhalation exposures will then be below the DNELs. Workers involved in the handling, sampling and transfer of materials are well-trained in the procedures and use of appropriate protective equipment in order to minimise exposure and risks.

It can be concluded that the risks to workers are adequately controlled with acceptable margins of safety when performing these tasks indoors without LEV and with the use of respiratory protection. If LEV is used, respiratory prtection will not be required.

Table 167: (Semi) Quantitative risk characterisation for workers

	Route	PROC code	ES 5- exposure concentrations (EC)*			Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio		
			Without LEV*	Without LEV**	With LEV*			With-out LEV*	With-out LEV**	With LEV*
Acute - systemic effects	Dermal	-	-	-	-	-	NQ	-	-	-
	Inhalation	3	42.8 mg/m^3	4.28 mg/m^3	8.55 mg/m^3	Repeated dose toxicity	68 mg/m³	0.638	0.064	0.128
		5	171 mg/m^3	17.1 mg/m^3	34.2 mg/m^3	Repeated dose toxicity	68 mg/m³	2.55	0.255	0.511
		9	171 mg/m^3	17.1 mg/m^3	34.2 mg/m^3	Repeated dose toxicity	68 mg/m³	2.55	0.255	0.511

	Route	PROC code	ES 5- exposure concentrations (EC)*			Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio		
			Without LEV*	Without LEV**	With LEV*			With-out LEV*	With-out LEV**	With LEV*
Acute - local effects	Dermal	-	-		-	-	NQ	-	-	-
	Inhalation	3	42.8 mg/m³	4.28 mg/m³	8.55 mg/m³	Repeated dose toxicity	68 mg/m³	0.638	0.064	0.128
		5	171 mg/m³	17.1 mg/m³	34.2 mg/m³	Repeated dose toxicity	68 mg/m³	2.55	0.255	0.511
		9	171 mg/m³	17.1 mg/m³	34.2 mg/m³	Repeated dose toxicity	68 mg/m³	2.55	0.255	0.511
Long-term - systemic effects	Dermal	3	0.343 mg/kg bw/d	0.343 mg/kg bw/d	0.034 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.011	0.011	0.001
		5	13.7 mg/kg bw/d	13.7 mg/kg bw/d	0.0686 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.429	0.429	0.002
		9	6.86 mg/kg bw/d	6.86 mg/kg bw/d	0.686 mg/kg bw/d	Repeated dose toxicity	32 mg/kg bw/d	0.214	0.214	0.021
	Inhalation	3	42.8 mg/m³	4.28 mg/m³	8.55 mg/m³	Repeated dose toxicity	68 mg/m³	0.638	0.064	0.128
		5	171 mg/m³	17.1 mg/m³	34.2 mg/m³	Repeated dose toxicity	68 mg/m³	2.55	0.255	0.511
		9	171 mg/m³	17.1 mg/m³	34.2 mg/m³	Repeated dose toxicity	68 mg/m³	2.55	0.255	0.511
	Combined routes							RCR Inhalation- systemic + RCR Dermal- systemic		
Long-term – local effects	Dermal	-	-		-	-	NQ	-	-	-
Long-term – local effects	Inhalation	3	42.8 mg/m³	4.28 mg/m³	8.55 mg/m³	Repeated dose toxicity	68 mg/m³	0.638	0.064	0.128
		5	171 mg/m³	17.1 mg/m³	34.2 mg/m³	Repeated dose toxicity	68 mg/m³	2.55	0.255	0.511
		9	171 mg/m³	17.1 mg/m³	34.2 mg/m³	Repeated dose toxicity	68 mg/m³	2.55	0.255	0.511
	Combined routes							RCR Inhalation- systemic + RCR Dermal- systemic		

**all estimations determined for worst case: indoors, >4 hours worker exposure, no respiratory protection.*
***all estimations determined for: indoors, >4 hours worker exposure, with respiratory protection.*
NQ = Not quantifiable.

10.6.1.2. Consumers

Consumers are not directly exposed to the repackaging/dilution or drumming of acetonitrile.

10.6.1.3. Indirect exposure of humans via the environment

Indirect exposure of humans via the environment is unlikely due to lifecycle of substance, its physico-chemical properties and it is readily biodegradable in water. Therefore, it is expected to be negligible in the environment.
Acetonitrile is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore the manufacture of acetonitrile does not involve any targeted environmental emissions or application and the primary receiving compartment is the STP. Removal in the STP is expected to be highly efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

10.6.2. Environment

10.6.2.1 Aquatic compartment (including sediment and secondary poisoning)

The PECs outlined in section 9 are compared to the derived PNECs below.

Table 168: Risk characterisation for the aquatic compartment

Compartments	PEC mg/l	PNEC mg/l or mg/kg dw	PEC/PNEC	Comments/Discussion
Tier 1 Freshwater	0.0311	10.2	3.04×10^{-3}	Safe use demonstrated for all compartments in tier 1.
Tier 1 Marine	3.11×10^{-3}	1.02	3.04×10^{-3}	
Tier 1 Freshwater sediment	0.137	45	3.04×10^{-3}	
Tier 1 Marine sediment	0.0137	4.5	3.04×10^{-3}	

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.6.2.2 Terrestrial compartment (including secondary poisoning)

There is no direct exposure of the terrestrial compartment from repackaging/dilution uses of acetonitrile. Concentrations of acetonitrile in the terrestrial compartment are expected to be minimal and the PECs presented here are expected to be vast overestimations of the concentrations that will actually exist in the terrestrial compartmentdue to the fact that acetonitrile is likely to degrade rapidly in the environment.

Table 169: Risk characterisation for the terrestrial compartment

Compartments	PEC mg/kg dw	PNEC mg/kg dw	PEC/PNEC	Comments/discussion
Tier 1 soil	4.86×10^{-3}	3.02	1.61×10^{-3}	Safe use demonstrated tier 1.

As all RCRs are less than 1 it is considered that safe use has been demonstrated.

10.6.2.3 Atmospheric compartment

Atmospheric contamination due to repackaging dilution uses of acetonitrile is minimal, and as there is no indicated effects on plants or animals from atmospheric acetonitrile no PNEC and no RCR is derived.

10.6.2.4 Microbiological activity in sewage treatment systems

A worst case PEC for the STP is presented below. As all RCRs are less than 1 it is considered that safe use has been demonstrated.

Table 170: Risk characterisation for the sewage treatment microorganisms (STP)

Compartments	PEC mg/L	PNEC mg/L	PEC/PNEC	Comments/discussion
Tier 1 Sewage treatment plant (STP)	0.311	32	$9.7x10^{-3}$	Safe use demonstrated tier 1.

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

10.7.1. Human health (combined for all exposure routes)

Combination of exposures is appropriate where a population may be exposed in more than one way *i.e.* to more than one source. In theory, a worker at a factory could be exposed during production, during use (if the factory rotated its workers through several parts of the plant), as a consumer handling the materials produced outside of work, and via food grown locally, if local soils are affected by emissions from the factory. In the case of acetonitrile, worker exposure during production is considered the worst case, so that any worker changing to other areas using acetonitrile would be either less or similarly exposed to a worker spending all their time on acetonitrile production. There is no significant consumer exposure to acetonitrile, and no anticipated exposure of soils or potential for exposure via the food chain or drinking water. Therefore there is no combination of exposure routes: total exposure is as described for exposure scenario 1.

10.7.2. Environment (combined for all emission sources)

A combined regional risk assessment may be performed to determine the regional risk based on production and uses of acetonitrile. In order to carry out this assessment combined regional PEC values from all exposure scenarios. As all derived PECs are below the relevant PNEC and so no further assessment or refinements are required.

Table 171: Combined regional concentrations in the environment covering all exposure scenarios

	Predicted regional tier 2 exposure Concentrations	
	PEC value	**unit**
Freshwater	0.0173	mg/l
Marine water	1.64×10^{-3}	mg/l
Freshwater sediments	0.0662	mg/kg dw
Marine sediments	6.37×10^{-3}	mg/kg dw
Agricultural soil	6.28×10^{-4}	mg/kg dw
Grassland	9.08×10^{-4}	mg/kg dw
Air	3.26×10^{-4}	mg/m^3

Table 172: Combined regional RCRs in the environment covering all exposure scenarios

	Predicted regional tier 2 exposure Concentrations			
	PEC value	**PNEC**	**Unit**	**RCR**
Freshwater	0.0173	10.2	mg/l	0.00169
Marine water	1.64×10^{-3}	1.02	mg/l	0.00161
Freshwater sediments	0.0662	45	mg/kg dw	0.00147
Marine sediments	6.37×10^{-3}	4.5	mg/kg dw	0.00142
Agricultural soil	6.28×10^{-4}	3.02	mg/kg dw	2.1×10^{-4}
Grassland	9.08×10^{-4}	3.02	mg/kg dw	3×10^{-4}