SAFETY DATA SHEET

According to Regulation (EC) No 1907/2006 (REACH), Annex II (COMMISSION REGULATION (EU) No 2015/830) Page 1 of 141 First Issue : Dec. 1, 2010 Revised : May. 03, 2021 SDS No. : TS-001(EU)

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

#### 1.1 Product identifier

Substance name : Acrylonitrile

Synonyms : Acrylonitrile; Vinyl cyanide; 2-Propenitrile; 2-Propenenitrile

**EC Number** : 203-466-5

**CAS Number** : 107-13-1

Index Number from Annex VI (Part 3) of Regulation (EC) No 1272/2008 : 608-003-00-4REACH Registration Number : 01-2119474195-34-0006

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

#### 1.2.1 Identified uses

Production of acrylic and modacrylic textile fibres Production of acrylonitrile-butadiene-styrene (ABS) and styrene-acrylonitrile (SAN) plastics Monomer for production of nitrile rubbers Intermediate for the production of bulk chemicals, resins and adiponitrile/acrylamide synthesis Laboratory reagent

#### 1.2.2 Uses advised against

Not for use in any process other than an intermediate or monomer. Not for direct use by the general public. Use resulting in wide and dispersive release is not advised.

#### 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

#### Non-Community manufacturer :

Name :	Tongsuh Petrochemical Corp., ltd.		
Address :	108-70, Sapyeong-ro, Nam-gu,		
	Ulsan, 44785		
	Republic of Korea		
Telephone number :	+82-2-3215-0710		
Telefax number :	+82-2-3215-0770		
E-mail address :	tspcmail@tspc.co.kr		

## SAFETY DATA SHEET

#### 1.4 Emergency telephone number

EU-wide emergency number : 112 See section 16.6 for the list of telephone number of poison centers in the European Economic Area.

#### 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 3 Acute Toxicity (Dermal) Category 3 Acute Toxicity (Inhalation) Category 3 Skin Corrosion/Irritation Category 2 Serious eye damage/Irritation Category 1 Skin Sensitization Category 1 Carcinogenicity Category 1B Specific Target Organ Toxicity Single Exposure Category 3(Respiratory tract irritation), H335 Aquatic Toxicity Chronic 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 vapor.
- H301 Toxic if swallowed.
- H311 Toxic in contact with skin
- H315 Causes skin irritation.
- H317 May cause allergic skin reaction.
- H318 Causes serious eye damage.
- H331 Toxic if inhaled.
- H335 May cause respiratory irritation.
- H350 May cause cancer.
- H411 Toxic to aquatic life with long lasting effects.

### SAFETY DATA SHEET

#### Precautionary Phrases :

1) Prevention

- P201 Obtain special instructions before use.
- P202 Do not handle until all safety precautions have been read and understood.
- 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. Flammable liquids (chapter 2.6) 1, 2, 3
- P243 Take precautionary measures against static discharge.
- P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
- P264 Wash hands thoroughly after handling.
- P270 Do not eat, drink or smoke when using this product.
- P271 Use only outdoors or in a well-ventilated area.
- P272 Contaminated work clothing should not be allowed out of the workplace.
- P273 Avoid release to the environment.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P281 Use personal protective equipment as required.
- 2) Response
  - P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
  - P302+P352 IF ON SKIN: Wash with plenty of soap and water.
  - P303+P361+P353 IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower.
  - P304+P340 IF INHALED: Remove 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.
  - P308+P313 If exposed or concerned: Get medical advice/attention.
  - P310 Immediately call a POISON CENTER or doctor/physician.
  - P311 Call a POISON CENTER or doctor/physician.
  - P312 Call a POISON CENTER or doctor/physician if you feel unwell.
  - P321 Specific treatment
  - P322 Specific measures
  - P330 Rinse mouth.
  - P332+P313 If skin irritation occurs: Get medical advice/attention.
  - P333+P313 If skin irritation or rash occurs: Get medical advice/attention.
  - P361 Remove/Take off immediately all contaminated clothing.
  - P362 Take off contaminated clothing and wash before reuse.
  - P363 Wash contaminated clothing before reuse.
  - P370+P378 In case of fire: Use Suitable extinguishing media for extinction(Refer Section MSDS 5). P391 Collect spillage.
- 3) Storage
  - P403+P233 Store in a well-ventilated place. Keep container tightly closed.
  - P403+P235 Store in a well-ventilated place. Keep cool.
  - P405 Store locked up.
- 4) Disposal

- P501 Dispose of contents/container in accordance with local and national regulations. For full text of P precautionary statements see section 16.

## SAFETY DATA SHEET

#### 3. COMPOSITION / INFORMATION ON INGREDIENTS

#### 3.1 Substance

Substance name : Acrylonitrile

Index Number from Annex VI (Part 3) of Regulation (EC) No 1272/2008 : 608-003-00-4

Classification and Labelling Inventory Number : Not applicable

Authorisation Number : Not applicable

**EC Number** : 203-466-5

**CAS Number** : 107-13-1

**REACH Registration Number** : 01-2119474195-34-0006

Purity :  $\geq$  99.4 %

Inhibitor: 4-methoxyphenol (MEHQ) [EC Number 205-769-8; CAS Number 150-76-5]

Impurities or other constituents contributing to substance classification : Not applicable

#### 4. FIRST AID MEASURES

#### 4.1 Description of first aid measures:

#### 4.1.1 In case of inhalation:

If inhaled, remove to fresh air. Do not use mouth to mouth ventilation. Resuscitate using a mouth-to-mask with one-way valve or with Ambu Bag. Warning: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Get medical attention immediately.

#### 4.1.2 In case of skin contact:

Immediately wash exposed skin with soap and water. Get medical attention immediately. If symptoms of poisoning develop, treat as for inhalation. Remove contaminated clothing and shoes. Wash clothing before reuse. Do not use protective clothing made of leather, natural or nitrile rubber. If such clothing is contaminated with acrylonitrile, it should be destroyed by burning. Note that contaminated clothing may be a fire hazard.

#### 4.1.3 In case of eyes contact:

In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. If symptoms of poisoning develop, treat as for inhalation. Get medical attention immediately.

#### 4.1.4 In case of ingestion:

Get medical attention immediately. Make the patient drink a large quantity of water, if possible with an addition of activated carbon, immediately, and then at frequent intervals. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Keep person warm and at rest.

#### 4.2 Most important symptoms and effects, both acute and delayed:

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11. Further symptoms are possible.

#### 4.3 Indication of any immediate medical attention and special treatment needed:

## SAFETY DATA SHEET

Notes to physician: Upon absorption and metabolism Acrylonitrile 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. Take a blood sample in all cases for blood cyanide using fluoride/oxalate tube and chill immediately and arrange urgent analysis. Blood cyanide levels will take some time to become available, and are generally only useful as a retrospective indicator of exposure. Treatment decisions must therefore be based on the clinical features of each individual case, without waiting for blood cyanide results. If the patient is conscious and breathing normally, administration of oxygen is the only treatment necessary. In a deteriorating clinical situation, with a patient's conscious level decreasing, in addition to the need for cardio-pulmonary resuscitation, consideration should be given to the use of a specific cyanide antidote [dicobalt edetate (kelocyanor)]. THIS SPECIFIC ANTIDOTE IS DANGEROUS WHEN ADMINISTERED IN THE ABSENCE OF SERIOUS CYANIDE POISONING. One ampoule of dicobalt edetate (300mg) diluted in 20ml glucose solution is given by slow intravenous injection, being careful to avoid extravasation. Constant pulse and blood pressure monitoring is required, along with facilities for resuscitation, as sudden severe fall in blood pressure can occur during injection. Treatment may be repeated if there is an inadequate response to the initial injection.

#### 5. FIREFIGHTING MEASURES

#### 5.1 Extinguishing media

- 5.5.1 Suitable extinguishing media In case of fire, use water spray (fog), foam, dry chemical or CO2.
- 5.1.2 Unsuitable extinguishing media Do not use water jet.

#### 5.2 Special hazards arising from the substance or mixture

#### Unusual Fire and Explosion Hazards :

Highly flammable liquid and vapor. May explode when heated.

Explosive in the presence of open flames, sparks and static discharge. Vapors may cause flash fire. Vapors may accumulate in low or confined areas, travel a considerable distance to a source of ignition and flash back. Collect contaminated fire-fighting water separately. It must not enter the sewage stream.

Runoff to sewer may create fire or explosion hazard. Excessive heat above 500°F (260°C) may trigger exothermic reaction. May re-ignite itself after fire is extinguished.

#### Combustion Products :

Thermal decomposition products may include oxides of carbon (carbon monoxide, carbon dioxide), nitrogen oxides (NO, NO2) and hydrogen cyanide. Evolves toxic fumes when heated to the decomposition state. When heated to decomposition it emits acrid smoke and irritating fumes.

#### 5.3 Advice for fire fighters

Protection of fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode. Cool containing vessels with flooding quantities of water until well after fire is out. May re-ignite itself after fire is extinguished. Apply water from a safe distance to cool container and protect surrounding area. Special fire-fighting procedures: 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-of-sight of the scene and away from windows.

#### 6. ACCIDENTAL RELEASE MEASURES

## SAFETY DATA SHEET

#### 6.1 Personal precautions, protective equipment and emergency procedures

#### 6.1.1 For non-emergency personnel:

Eliminate all sources of ignition. Evacuate surrounding areas. Avoid breathing vapours. Immediately contact emergency personnel. Eliminate all ignition sources. Keep unnecessary personnel away; isolate hazard area and deny entry. Use suitable protective equipment (section 8). Follow all fire-fighting procedures (section 5). Do not touch or walk through spilt material. Contain and absorb using earth, sand or other inert material. Dyke large spills and use a non-sparking or explosion-proof means to transfer material to an appropriate container for disposal.

#### 6.1.2 For emergency responders:

Wear suitable protective equipment. Apply the same recommendations as above.

#### 6.2 Environmental precautions

Avoid dispersal of spilt material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

#### 6.3 Methods and material for containment and cleaning up

If emergency personnel are unavailable, contain spilled material. For small spills add absorbent (soil may be used in the absence of other suitable materials) and use non-sparking or explosion proof means to transfer material to a sealed, appropriate container for hazardous material disposal. For large spills dike spilled material or otherwise contain material to ensure that runoff does not reach a waterway. Place spilled material in an appropriate container for hazardous material disposal. Avoid contact of spilled material with soil and prevent runoff entering surface waterways. See Section 13 for Waste Disposal information.

#### 6.4 Reference to other sections

See Section 7 for information on safe handling. See Section 8 for information on personal protection equipment.

#### 7. HANDLING AND STORAGE

#### 7.1 Precautions for safe handling

#### 7.1.1 Protective measures:

Use suitable protective equipment (section 8). Avoid breathing vapours of this product. Do not get in eyes, on skin or on clothing. Cyanide first aid treatment (containing amyl nitrite capsules) must be available at site.

Keep container closed. Use only with adequate ventilation. 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.

#### 7.1.2 Advice on general occupational hygiene:

Good personal washing routines should be followed. Do not eat, drink and smoke in work areas. Wash hands after use. Remove contaminated clothing and protective equipment before entering eating areas.

#### 7.2 Conditions for safe storage, including any incompatibilities

Store in segregated and approved area. Store in a cool, well-ventilated area away from incompatible materials and ignition sources. Suitable storage materials are mild steel and stainless steel. Do not

## SAFETY DATA SHEET

store in copper and its alloys. Keep containers tightly closed and sealed until ready to use. This product must be kept in a secure storage area so that only trained authorized personnel have access. Inhibit with p-Methoxyphenol (MEHQ). To maintain inhibitor activity, oxygen must not be eliminated from the atmosphere above the product. If the explosion risk posed by storing under air is unacceptable, use oxygen depleted air (5% oxygen minimum, no greater than 8%). Check inhibitor level periodically. See Section 10: Stability and Reactivity.

Empty containers may contain toxic, flammable and explosive residue or vapors. Do not cut, grind, drill, weld or reuse containers unless adequate precautions are taken against these hazards. Packaging Materials: Use original container.

#### 7.3 Specific end uses(s)

Not applicable

#### 8. EXPOSURE CONTROLS / PERSONAL PROTECTION

#### 8.1 Control parameters

#### 8.1.1 Occupational exposure limits

	Occupational Expo	osure Limit Value	Occupation	al Exposi	ıre Limit Value		
	(8-hour reference	period)	(15-minut	(15-minute reference period)			
Country	ppm	mg/m <sup>3</sup>	ppm	mg/ m <sup>3</sup>	Note		
Belgium	2	4.4	-	_	-		
Bulgaria	_	4.5	-	_	_		
Denmark	2	4	-	_	_		
Finland	2	4.4	4	8.8	-		
Ireland	2	4.5	-	_	-		
Lithuania	2	4.5	6	13	_		
Spain	2	4.4	-	_	-		
Sweden	2	4.5	6	13	-		
EU-OSHA	2	4.5	6	13	_		
France	2	4.5	15	32.5	_		

#### 8.1.2 Additional exposrue limits under the conditions of use

Not available.

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

None established

#### 8.1.4 DNEL values

#### 8.1.4.1 Workers

Systemic effects-Long term exposure High hazard (no threshold derived) Systemic effects-Acute exposure Medium hazard (no threshold derived) Local effects-Long term exposure 1.8 mg/m<sup>3</sup> Local effects-Acute exposure 10 mg/m<sup>3</sup> Systemic effects-Long term exposure 1.4 mg/kg bw/day Systemic effects-Acute exposure Medium hazard (no threshold derived) Local effects-Long term exposure Medium hazard (no threshold derived)

### SAFETY DATA SHEET

Local effects-Acute exposure Medium hazard (no threshold derived)

#### 8.1.4.2 General population

Systemic effects-Long term exposure 0.1 mg/m<sup>3</sup> Systemic effects-Acute exposure Medium hazard (no threshold derived) Local effects-Long term exposure 0.06 mg/m<sup>3</sup> Local effects-Acute exposure 1 mg/m<sup>3</sup> Systemic effects-Long term exposure 0.009 mg/kg bw/day Systemic effects-Acute exposure Medium hazard (no threshold derived) Local effects-Acute exposure Medium hazard (no threshold derived) Local effects-Acute exposure Medium hazard (no threshold derived) Systemic effects-Long term exposure 0.009 mg/kg bw/day Systemic effects-Long term exposure 0.009 mg/kg bw/day Systemic effects-Acute exposure Medium hazard (no threshold derived) Medium hazard (no threshold derived)

#### 8.1.5 PNEC values (Predicted No Effect Concentration) for the Environment

PNEC Water (fresh and marine)	PNEC Sediment	PNEC Soil	PNEC Sewage Treatment Plant	PNEC oral (secondary poisoning)
17 μg/L	0.0188 mg/kg sediment dw	0.00268 mg/kg soil dw	5 mg/L	Exposure is not Predicted

#### 8.2 Exposure controls

#### 8.2.1 Appropriate Engineering Controls :

Handle in accordance with good industrial hygiene and safety practice.Handle only in totally enclosed systems. Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapours below their respective occupational exposure limits.

Ensure that eyewash stations and safety showers are close to the workstation location. Wash hands after handling compounds and before eating, smoking and using the lavatory and at the end of the day.

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

#### Personal Protective Measurers

#### Eye/face Protection :

Do not get in eyes. Chemical splash goggles. Wear full face respirator for eye protection if high vapor concentration or significant liquid splash potential exists.

#### Skin Protection :

Do not get on skin or clothing. Butyl rubber is the protective material of choice. Protective clothing must be made from materials specifically recommended for protection against acrylonitrile penetration. Consult your local safety specialist for a list of recommended materials. Do notuse protective clothing made of leather, natural or nitrile rubber. If such clothing is contaminated with acrylonitrile, it should be destroyed by burning.

Note that contaminated clothing may be a fire hazard. Wash thoroughly after handling.

#### Hands :

Wear gloves that cannot be penetrated by chemicals or oil. Butyl rubber gloves. 0.5 mm Breakthrough time: >=4 hr.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

### SAFETY DATA SHEET

therefore be chosen in consultation with the supplier/manufacturer and with a full assessment of the working conditions.

#### Respiratory Protection :

Use with adequate ventilation.Ensure ventilation is adequate if there is a risk of aerosol formation or vapour build-up. Wear special protective clothing and positive pressure, self-contained breathing apparatus. Do not breathe vapour or mist.Keep container closed.

#### Thermal hazards:

Wear suitable protective clothing to prevent heat.

#### 8.2.3 Environmental Exposure Controls:

Avoid discharge into the environment. According to local regulations, Federal and official regulations. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the 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 at 101.3 kPa	pH: 6.0-7.5 (5% aqueous solution)
Color: Clear and colourless	Boiling Point: 77.3°C at 1,013 hPa
Odor: Faintly pungent odour.	Evaporation Rate: Not available
Odour Threshold: Not available	Vapor Pressure: 11.5 kPa at 20°C
Melting/Freezing Point: -83.5°C at 1,013 hPa	and 133.3 hPa at 23.6 °C
Flash Point: 0 °C at 1,013 hPa	Relative Density: 0.806 g/cm <sup>3</sup> at 20 °C
Lower Flammability Limit: Not available	and 0.8004 g/cm $^3$ at 25 $^\circ\mathrm{C}$
Upper Flammability Limit: Not available	Octanol/Water Partition Coefficient
Flammability: Highly flammable	: 0.017 at 21°C
Vapor Density(Air=1): Not available	Decomposition Temperature: Not applicable
Solubilities: 73 g/L at 20 °C	Explosive Properties: Non explosive
Autoignition Temperature: 481°C 101.3 kPa	SAPT(Self-Accelerating Polymerization
Viscosity: 0.34 mPa.s at 20°C	<b>Temperature)</b> : > $75^{\circ}$ C
Oxidizing Properties: Non oxidising	

#### 9.2 Other information :

Surface tension: The surface tension of acrylonitrile is reported to be 26.6 mN/m at 25 °C (Kirk-Othmer, 2001)

#### 10. STABILITY AND REACTIVITY

#### 10.1 Reactivity

Stable at room temperature under normal storage and handling conditions.

#### 10.2 Chemical stability

Stable at room temperature in closed containers under normal storage and handling conditions.

#### 10.3 Possibility of hazardous reactions

No dangerous reaction known under conditions of standard use.

Hazardous polymerisation: Yes. Product stabilised but may polymerise readily. Avoid depletion of inhibitor. Inhibit with: p-Methoxyphenol (MEHQ). To maintain inhibitor activity, oxygen must not be eliminated from the atmosphere above the product. If the explosion risk posed by storing under air is unacceptable, use oxygen depleted air (5% oxygen minimum). Check inhibitor level periodically.

#### 10.4 Conditions to avoid

Incompatible materials. Keep away from heat and direct sunlight. Avoid all possible sources of ignition (spark or flame). Product stabilised but may polymerise readily. Avoid depletion of inhibitor. Inhibit with: p-Methoxyphenol (MEHQ). To maintain inhibitor activity, oxygen must not be eliminated from the atmosphere above the product. If the explosion risk posed by storing under air is unacceptable, use oxygen depleted air (5% oxygen minimum). Check inhibitor level periodically.

#### 10.5 Incompatible materials

Highly reactive with oxidising agents, reducing agents, acids, alkalis. This product may polymerise with explosive violence. May polymerise on exposure to sunlight, absence of oxygen, peroxides, alkalis, strong acids, Ammonia, Bromine, and Copper.

#### 10.6 Hazardous decomposition products

Decomposition products may include the following materials: carbon oxides (CO, CO2), nitrogen oxides (NO, NO2 etc.), Hydrogen cyanide (HCN). Evolves toxic fumes when heated to decomposition. Emits acrid smoke and irritating fumes when heated to decomposition.

#### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

#### Acute toxicity

Skin Irritation/Corrosivity : Causes skin irritation.

Serious eye irritation/damage : Causes serious eye damage.

Respiratory Sensitization : Not available

Skin Sensitization : May cause an allergic skin reaction.

Germ Cell Mutagenicity : Not classified

Carcinogenicity : May cause cancer.

Reproductive Toxicity : Not available

### SAFETY DATA SHEET

STOT - single exposure : May cause respiratory irritation.

STOT - repeat exposure : Not available

Aspiration hazard : Not available

### 11.2 Other Information

Not available

#### 12. ECOLOGICAL INFORMATION

#### 12.1 Toxicity

Acute Toxicity to Fish : 96-hour LC<sub>50</sub> 5.1 mg/L (Freshwater) 96-hour LC<sub>50</sub> 8.6 mg/L (Marine water)

Acute Toxicity to Aquatic: 48-hour EC\_{50} 2.5 mg/L Daphnia magnaInvertebrates: 72-hour EC\_{50} (growth rate) 10 mg/L algaeChronic Toxicity to Fish: NOEC freshwater fish 0.17 mg/LChronic toxicity to Aquatic: NOEC freshwater invertebrates 0.5 mg/LInvertebrates: NOEC marine water algae 0.95 mg/L

#### 12.2 Persistence and degradability

Inherently biodegradable.

#### 12.3 Bioaccumulative potential

BCF (aquatic species): 1 dimensionless

#### 12.4 Mobility in soil

Koc = 9 at 20 °C

#### 12.5 Results of PBT and vPvB assessment

The substance is not considered a PBT/vPvB.

12.6 Other adverse effects : Toxic to aquatic life with long lasting effects.

#### 13. DISPOSAL CONSIDERATIONS

#### 13.1 Waste treatment methods

Dispose of in accordance with all applicable local and national regulations. Use recovery/recycling where feasible, otherwise incineration is the recommended method of disposal. Empty containers may contain hazardous residues. Do not cut, puncture or weld on or near to the container. Labels should not be removed from containers until they have been cleaned. Contaminated containers must not be treated as household waste. Containers should be cleaned by appropriate methods and then re-used or disposed of by landfill or incineration as appropriate. Do not incinerate closed containers.

#### 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
Land transport (ADR/RID)	UN1093	Acrylonitrile, Stabilized	3 (6.1)	PG I	Yes
Inland waterways (ADN)	UN1093	Acrylonitrile, Stabilized	3 (6.1)	PG I	Yes
Sea transport (IMDG)	UN1093	Acrylonitrile, Stabilized	3 (6.1)	PG I	Yes
Air transport (ICAO/IATA)	UN1093	Acrylonitrile, Stabilized	3 (6.1)	PG I	Yes

- 14.6 Special precautions for user : See section 2.2
- 14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code Not regulated

#### 15. **REGULATORY INFORMATION**

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

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 : 5.2.7.1.1.II	
Classification of Substances Hazardous	to Water (WGK): 3

#### 15.2 Chemical safety assessment

A chemical safety assessment has been performed.

#### 16. OTHER INFORMATION

#### 16.1 Indication of changes

- The Safety Data Sheet has been reviewed and the data therein were revised and laid out according the requirements of the Commission Regulation (EU) No. 2015/830

**NOTICE**: This 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.

## SAFETY DATA SHEET

#### 16.2 Abbreviations and acronyms

ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road								
ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways								
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								
IATA	International Air Transport Association								
ICAO	International Civil Aviation Organization								
LC50	Median lethal concentration								
NOAEL	No observed adverse effect level								
NOEC	No Observed Effect Concentration								
PBT	Persistent, bioaccumulative and toxic								
PNEC	Predicted no effect concentration								
REACH	Registration, evaluation, authorisation and restriction of chemicals (Regulation (EC) 1907/2006)								
RID	Regulation for rail International transportation of Dangerous goods								
STOT	Specific target organ toxicity								
STP	Sewage treatment plant								
vPvB	Very persistent and very bioaccumulative								

#### 16.3 Key literature references and sources for data

This Safety Data Sheet has been prepared in accordance with Commission Regulation (EU) No 2015/830. 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 Classification procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]

Flammable Liquid Category 2 Acute Toxicity (Oral) Category 3 Acute Toxicity (Dermal) Category 3 Acute Toxicity (Inhalation) Category 3 Skin Corrosion/Irritation Category 2 Serious eye damage/Irritation Category 1 Skin Sensitization Category 1 Carcinogenicity Category 1B Specific Target Organ Toxicity Single Exposure Category 3(Respiratory tract irritation), H335 Aquatic Toxicity Chronic Category 2

#### 16.5. Relevant H-statements (number and full text):

- H225 Highly flammable liquid and vapor.
- H301 Toxic if swallowed.
- H311 Toxic in contact with skin

### SAFETY DATA SHEET

- H315 Causes skin irritation.
- H317 May cause allergic skin reaction.
- H318 Causes serious eye damage.
- H331 Toxic if inhaled.
- H335 May cause respiratory irritation.
- H350 May cause cancer.
- H411 Toxic to aquatic life with long lasting effects.
- 16.6 Training advice
  - Not applicable

#### 16.7. Further information

- The SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered. This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only.
- for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product. Contact a poison control centre, List of Telephone Numbers : AUSTRIA (Vienna Wien) +43 1 406 43 43; BELGIUM (Brussels Bruxelles) +32 70 245 245; BULGARIA (Sofia) +359 2 9154 409; CZECH REPUBLIC (Prague Praha) +420 224 919 293; DENMARK (Copenhagen) 82 12 12 12; ESTONIA (Tallinn) 112; FINLAND (Helsinki) +358 9 471 977; FRANCE (Paris) +33 1 40 0548 48; GERMANY (Berlin) +49 30 19240; GREECE (Athens Athinai) +30 10 779 3777; HUNGARY (Budapest) 06 80 20 11 99; ICELAND (Reykjavik) +354 525 111, +354 543 2222; IRELAND (Dublin) +353 1 8379964; ITALY (Rome) +39 06 305 4343; LATVIA (Riga) +371 704 2468; LITHUANIA (Vilnius) +370 5 236 20 52 or +370 687 53378; MALTA (Valletta) 2425 0000; NETHERLANDS (Bilthoven) +31 30 274 88 88; NORWAY (Oslo) 22 591300; POLAND (Gdansk) +48 58301 65 16 or +48 58 349 2831; PORTUGAL (Lisbon Lisboa) 808 250 143; ROMANIA (Bucharest) +40 21 3183606 SLOVAKIA (Bratislava) +421 2 54 77 4166; SLOVENIA (Ljubljana) + 386 41 650 500; SPAIN (Barcelona) +34 93 227 98 33 or +34 93 227 54 00 bleep 190; SWEDEN (Stockholm) 112 or +46 8 33 12 31 (mon-fri 9.00-17.00); UNITED KINGDOM (London) 112 or 0845 4647 (NHS Direct).

The exposure scenario section is extracted from the CSR.

#### **9** EXPOSURE ASSESSMENT

Overview of exposure scenarios

Engineering controls:

Reflecting the hazard profile of acrylonitrile and the possibility of exposure to acrylonitrile during production/processing, the following conditions are in place: (EU RAR, based on Industry data.)

The use of strictly closed systems; The enclosure of specific parts of plant equipment; The use of the highest technically available safety valves and glands; The use of rotary mechanical double acting seals with fluidpackage; The use of technical exhaust systems (engineering controls including local exhaust ventilation); The use of vent gas systems with connection to incineration; The use of cleaning/washing procedures for waste gas streams; Transportation of raw polymer in closed systems under reduced pressure; Cleaning of systems prior to maintenance work by rinsing with steam, air, nitrogen; together with adequate latency periods.

#### PPE requirements:

Preventive protection is only resistant to acrylonitrile for a short time and is used in activities where none of the substance is normally released, but the risk of this happening cannot be completely ruled out altogether. As a general principle, if acrylonitrile is released (accidentally) during work, activities should be stopped immediately, following which clothing should first be rinsed with plenty of water and then removed. An overall with a close-fitting hood and elastic fitting around the wrists and ankles is used for body protection. Disposable gloves are used to protect the hands.

Repressive protective clothing is highly resistant to acrylonitrile for longer periods. This clothing is used for work in places where acrylonitrile is released and the workers may come in contact with it, e.g. during disaster control. In such instances an attempt must first be made to halt the release of the product from a distance. Repressive protection clothing for acrylonitrile consists of a gas-tight suit, e.g. of butyl rubber. The wearing of this repressive clothing can give riseto a high level of physical and mental stress and such suits must not be worn for longer than 20 minutes.

#### Breathing protection

### SAFETY DATA SHEET

For work purposes, air masks should be equipped with a clear view face piece, speaking diaphragm and air demand regulator. Theair will be supplied from a 30-45 minutes capacity air cylinder, or medical air supply hose from air tanks or long duration cylinders. The use of the mask in the positive pressure mode affords greater protection and is preferred. Masks with carbon filter cartridges may be worn in emergencies, but only for a very limited period of time, especially if the concentrations of acrylonitrile are fairly high. Escape masks should only be used for escape purposes and during short exposure time.

Respiratory protection should be used during the installation of engineering controls, during routine maintenance and repair activities, during reactor cleaning where use of engineering controls is not feasible, when available engineering controls are not sufficient to reduce exposure below permissible exposure limitd and during emergencies.

#### Eye protection

This is incorporated into the full-face mask as mentioned above. A pair of close-fitting goggles may be used in emergencies. However attention should be paid to the fact that acrylonitrile can attack the skin, eyes and unprotected parts of the face.

#### Hand protection

For preventive clothing purposes, disposable gloves, made of high quality butyl rubber or neoprene, must be worn, while for repressive clothing requirement the hand protection element is incorporated into the need to wear a complete butyl-rubber gas-tight suit with independent air supply.

#### Foot protection

Neoprene rubber boots.

#### Body protection

For preventive clothing purposes a PVC overall with a close-fitting hood and an elastic fitting around wrists and ankles should be worn, while for repressive clothing purposes a butyl rubber gas-tight suit with an independent air supply must be worn.

### SAFETY DATA SHEET

#### Table 1: Overview on exposure scenarios and coverage of substance life cycle

			Id	entifi uses	ed	Resul life cy stag	ycle						
ES number	Volume (tonnes)*	Manufacture	Formulation	End use	Consumer use	Service life (for articles)	Waste stage	Linked to Identified Use	Sector of Use Preparation (SU) Category (PC)		Process category (PROC)	Environment al Release Category (ERC)	Article category (AC)
ES 1Production of acrylic and modacrylic textile fibres	314700			x					SU 5	PC 32	PROC 1, 2, 3, 4,8b and 9	ERC 6C	AC 5-1 AC 5-2
ES 2 Production of acrylonitrile-butadi ene-styrene (ABS) and styrene-acrylonitrile (SAN) plastics	179300			x					SU 11 and 12	PC 32	PROC 1, 2, 3, 4, 8b and 9	ERC 6C	AC 1-1, AC 1-2, AC 2, AC 3-1, AC 3-3 and AC 13
ES 3 Monomer for production of nitrile rubbers	53,000			x					SU 11	PC 32	PROC 1, 2, 3, 8b and 9	ERC 6C	AC 10-1, AC 10-2, AC 10-3, AC 10-4 and AC 10-5
ES 4 Intermediate for the manufacture of bulk chemicals, materials and resins	136,000			x					SU 8 and 12	PC 19 and 32	PROC 1, 2, 3, 8b and 9	ERC 6A, 6C and 6D	N/A
ES 5 Laboratory reagent	<1			x					SU 22	PC 19	PROC 15	ERC 6A	N/A
ES 6 Manufacture	750,000	x							SU 8, 9, 10	n.a	PROC 1, 2, 8b and 9	ERC 1	

\*average tonnage for years 2008, 2009 and 2010 (predicted).

9.1 Exposure scenario 1: Use as a monomer in the production of acrylic and modacrylic textile fibres

#### 9.1.1 Exposure scenario

The largest use of acrylonitrile is the production of acrylic and modacrylic textile fibres. These fibres are used in clothing, domestic furnishing and other industrial purposes such as a precursor to carbon fibres, concrete reinforcement fibre and asbestos replacement.

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

The following description is taken from the EU RAR (2004). Production and processing of acrylonitrile polymers to fibres

The process is fully continuous, with precipitation polymerisation occurring in a single stage. Polymerisation is an exothermic reaction process and is preferentially carried out without pressure at 40-70°C. Normal conversion levels of the polymerisation reaction under process conditions amount to about 80-90%. The average chain length of the macromolecules is adjusted through catalyst concentration, the reaction time, the temperature and possibly polymerisation modifiers. In order to obtain the desired fibre properties, it is necessary to co-polymerise co-monomers such as acrylic acid methyl ester, vinyl acetate, methacrylic acid methyl ester and sulphonate group-containing olefin. Halogen-containing monomers may be used in special cases to reduce flammability of the fibres.

#### Polymerisation

Polymerisation is usually carried out as a continuously operating precipitation with subsequent filtration and drying, although polymer may also be produced by solution polymerisation. Precipitation polymerisation is carried out in a stirred tank reactor into which the liquid acrylonitrile, co-monomers, catalysts and auxiliary products as well as water are continuously fed prior to polymerisation It may be necessary to destabilise the acrylonitrile by distillation after stabilisation for storage purposes with polymerisation inhibitors. The polymer suspension is continuously withdrawn from the reactor; the polymerisation heat is removed by jacket cooling. The output from this stage of the fibre manufacture is a very viscous solution (dope). After polymerisation may be stopped by appropriate agents. Depending on the process, the suspension can be subject to intensive degasification whereby the quality requirements to be met by the polymer have to be taken into account. In the subsequent continuously operated washing filter the solids content is separated, washed and sent to a dryer. The filtrate from the washing filter has a residual monomer content of about 1 to 3% and is processed in an acrylonitrile

## SAFETY DATA SHEET

recovery plant. The polyacrylonitrile powder obtained is subsequently conveyed to intermediate storage in silos by screw conveyor or pneumatically with inert gas as the conveying agent. The waste gases from vent pipes of the stirred-tank reactor and the suspension collector as well as the waste gases of the washing filter and intensive degassing, are sent for waste gas scrubbing or adsorption. The main part of the acrylonitrile trapped in the waste gases can be recovered as solution from acrylonitrile-rich partial streams by previous cooling. aqueous The acrylonitrile-containing waste air of the dryers is emitted. The acrylonitrile content in these large volumes of air is relatively low. The reactors are opened only in case of repair and breakdown, so that emissions during these operations are negligible. The acrylonitrile/water mixtures contain the residual acrylonitrile, which was not converted during polymerisation. The effluent of the purification and cooling plants have different acrylonitrile contents varying with the process. They are either recycled into the process or sent to a stripping column together with the filtrate of the washing filter. The acrylonitrile recovered here is also returned to the polymerisation process. The vent pipes of the stripping columns are connected to the central disposal system.

#### Spinning of polymers to fibres

In the case of fibre production, a homogeneous solution is produced from the polymer and asolvent. This solution is spun in hot inert gas in the case of dry spinning or in coagulation baths in the case of wet spinning. The acrylonitrile polymers still contain residual amounts of acrylonitrile monomer, dependent on polymer type. They are mainly washed out (wet spinning) or released (dry spinning) in the spinning machines. The viscous solution is extruded through multi-holed jets and thin streams of dope coagulate to form gelatinous filaments. Depending on the technology used, extrusion is into long baths of a suitable aqueous liquid or into vertical towers where the filaments are formed in air. The filaments are collected together and taken through a succession of stages including partial stretch in a pre-heat bath, further stretching in a steam stretch tube, washing out residual impurities. The enclosed spinning machines are vented, resulting in large volumes of air with a relatively low acrylonitrile content. The waste gases are treated by scrubbers and emitted.

### 9.1.1.2 Operational conditions related to frequency, duration and amount of use Table 2: Duration, frequency and amount (for industrial use) [ES1]

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	kg/d	No specific data are available and are not required for risk assessment or risk characterisation
Duration of exposure per day at workplace [for one worker]	8h/day	Default value
Frequency of exposure at workplace [for one worker]	220 d/y	220 [default]
Emission days per site	300 d/y	Default value

### 9.1.1.3 Operational conditions and risk management measures related to product characteristics Table 3: Characteristics of the substance or preparation [ES1]

Information type	Data field	Explanation
Physical state	Liquid	Substance is a liquid
For solids: Categorisation of dust grades	Not applicable	Substance is a liquid
Concentration of substance in preparation	Not applicable	Undiluted substance is used
Concentration after dilution for use (if relevant)	Not applicable	-
Risk management measures related to the design of product	-	Not applicable

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

#### Table 4: Operational conditions related to respiration and skin contact [ES1]

Information type	Data field	Explanation
Respiration volume under conditions of use	$10 m^{3}/d$	Default value for light-work
Room size and ventilation rate	m3 ; exchange per hour	Room size and general ventilation are not employed to control risk
Area of skin contact with the substance under conditions of use	cm <sup>2</sup>	Not applicable. The substance is used under largely enclosed conditions. The substance is an irritant and sensitizer; RMMs and protective equipment should be used to eliminate or minimise dermal contact with the substance.
Body weight	65 kg	Default for workers

#### 9.1.1.5 Other operational conditions of use

Table 5: Technical fate of substance and losses from process/use to waste, waste water and air [ES1]

Information type	Data field	Explanation		
Fraction of applied amount lost from process/use to waste gas,	0.05 kg/kg	Default release to air for ERC 6c.		
Fraction of applied amount lost from process/use to waste water	0.05 kg/kg	Default release to waste water for ERC 6c.		
Fraction of applied amount lost from process/use to waste	0 kg/kg	No additional waste is predicted		
Fraction consumed in process/use	0.9 kg/kg	The substance is consumed during the process of polymer manufacture.		
Fraction of applied amount leaving the site with products	0 kg/kg	The substance is consumed during the process of polymer manufacture and is only present in the manufactured polymer in trace amounts.		

#### 9.1.1.6 Risk management measures

#### Table 6: Risk management measures for industrial site [ES1]

Information type	Data field Explanation						
Containment and local exhaust ve	entilation						
Containment plus good work practice required	Effectiveness in terms of residual exposure: Unknown	The production of acrylic and modacrylic textile fibres occurs either in a closed system or partially closed system. In the case of the partially enclosed system, local exhaust ventilation is used.					
Local exhaust ventilation required plus good work practise	Effectiveness in terms of reduction factor against situation without LEV or residual exposure: Unknown	A fully closed system or partially closed system is used. In the case of the partially enclosed system local exhaust ventilation is used.					
Personal protective equipment (PI	PE)						
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness Gloves : 90% (dermal) RPE required for open systems.	Protective gloves and face-shield are routinely worn to prevent accidental contact with the substance. RPE used unless a fully enclosed system is used					
Other risk management measures	related to workers						
		Workers received specific training and instruction in order to ensure minimal contact with the substance.					
		Airborne concentrations of acrylonitrile are routinely monitored to ensure compliance with occupational exposure standards.					
Risk management measures relate	Risk management measures related to environmental emissions from industrial sites						
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost						

Information type	Data field	Explanation
	form the technical process)	-
Resulting fraction of initially applied amount in waste water released from site	0.000165 kg/kg	Only a very small proportion is released from STP. In the STP, the substance is degraded by 95% according to biodegradation tests (see section 4.1.3). Waste water from the purification and cooling plants containing residual acrylonitrile (i.e. not converted during polymerisation) are either recycled into the process or sent to a stripping column prior to return to the process.
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	
Resulting fraction of applied amount in waste gas released to environment	0.0005 kg/kg	Emissions during the polymerisation process are negligible as the process is enclosed. Waste gases are subjected to scrubber systems which oxidises the residual acrylonitrile and are effectively combusted. For the purposes of the model the efficiency has been modelled as 99%. In reality, the removal of atmospheric emissions is highly efficient and negligible amounts of acrylonitrile are released.
Onsite waste treatment	Effectiveness (fraction after on-site treatment compared to the fraction entered into waste treatment.	
Fraction of initially applied amount sent to external waste treatment. This is the sum of direct losses from processes to waste, and the residues from onsite waste water and waste gas treatment.	0.000165 kg/kg 0.0495 kg/kg	Release to water (including removal by STP) Scrubber residues are treated on site The value shown represents the proportion (99 %) of particulate substance (5% default assumption for loss to waste gas) removed by scrubber systems.
Municipal or other type of external waste water treatment	Effectiveness of substance removal [fraction of substance in treated waste water compared to entering the waste water treatment plant]	Not applicable
Effluent (of the waste water treatment plant) discharge rate	2000 m3/d	Default: 2000 m3/d
Recovery of sludge for agriculture or horticulture	No	Sludge is not recovered for agriculture or horticulture

#### 9.1.1.7 Waste related measures

 Table 7: Fractions of substance in waste and waste management measures [ES1]

Information type	Data field	Explanation	
Amount of substances in waste	0.000165 kg/kg	Release to water	
resulting from identified uses covered in the exposure scenario	0.0005 kg/kg	Release to air.	
Amount of substances in waste resulting from service life of articles	0 kg/y	Not relevant	
Type of waste, suitable waste codes	Suitable EWC code(s)	Not relevant	
Type of external treatment aiming at recycling or recovery of substances	Not relevant	Not relevant	
Fraction of the initially applied amount of substance recovered.	0 kg/kg	Not relevant	
Type of external treatment aiming at final disposal of the waste	Not relevant	Not relevant	
Fraction of substance released into the environment via air from waste handling	0 kg/kg	Not relevant	
Fraction of substance released into the environment via waste water from waste handling	0 kg/kg	Not relevant	
Fraction of substance disposed of as secondary waste	0 kg/kg	Not relevant	

#### 9.1.2 Exposure estimation

#### 9.1.2.1 Worker exposure

#### 9.1.2.1.1 Acute/Short term exposure

The exposure estimates were generated using the ECETOC TRA exposure model. The RMM efficiency used in the model were based on ECETOC (2009) so the estimate obtained represents a full shift and the  $90^{\text{m}}$  percentile of the exposure distribution. Acute worst-case values for inhalation can be derived from fullshift values by using a multiplication factor which is detailed in Table R.14-3 of Guidance document R.14: Occupational exposure estimation. It is recommended to multiply a full shift ECETOC estimate by a factor of 2 to obtain the related short-term inhalation exposure distribution. These results are shown in the table below.

Routes of exposure	PROC	Estimated E Concentratio	xposure ns	Measured e	exposure ons	Explanation / source of measured data	
		value	unit	Value	unit	of measured data	
	PROC 1	0.343	mg/kg bw/d	-	-		
	PROC 2	0.137	mg/kg bw/d	-	-		
	PROC 3	0.0343	mg/kg bw/d	-	-		
Dermal exposure	PROC 4	0.686	m g / k g bw/d	-	-	No measured data	
	PROC 8b	0.686	m g / k g bw/d	-	-		
	PROC 9	0.686	m g / k g bw/d	-	-		
	PROC 1	0.1376 (without LEV and RP)	mg/m3				
Inhalation exposure	PROC 2	0.688	mg/m3	0105		Data obtained from	
	PROC 3	1.72	mg/m3	0.1-0.5	ppm	EU RAR.	
	PROC 4	1.376	mg/m3				
	PROC 8b	1.032	mg/m3				
	PROC 9	3.44	mg/m3				

Table 8: Acute exposure concentrations to workers [ES1]

\*all values generated with RP and LEV unless otherwise stated in ECETOC TRA.

Polymerisation to produce acrylic and modacrylic fibres is an exothermic reaction process and carried out without pressure at40-70 °C in a closedor partially closed system. Local exhaust ventilation (LEV) is used where the system is not fully enclosed. Inhalation exposure is therefore minimised and significant exposure occurs only through accident or poor working practice.

Specific exposure data are reported in the EU RAR for a European fibre processing plant during the 1990s. A mean measured occupational exposure of 0.2 ppm is reported (n=270).

The manufacturing process for acrylic fibres comprises 4 principal steps:

- Monomer receipt into bulk storage
- Polymerisation
- Spinning
- Finishing including drying and baling.

Typical levels for selected tasks within the manufacturing of acrylic fibres are 0.4 ppm for polymerisation operators, 0.5 ppm for spinners, 0.4 ppm for jet room operators, 0.1 ppm forfinish and 0.2 ppm for maintenance. However the recent introduction / improvement of the following engineering controls in the workplace has resulted in much lower levels of acrylonitrile exposure:

• Delivery of raw material acrylonitrile by pipeline, this eliminating the hazard of the risk of exposure during unloading

### SAFETY DATA SHEET

- · Redirection of vents coming from storage facilities away from areas occupied by personnel
- Continuous air monitoring in areas of greater risk
- Engineering controls to pump seals so as to reduce the leakage potential
- Improvement in ventilation including extract ventilation at critical locations

These improvements have dramatically reduced the extent of inhalation exposure. As a result, the measured data quoted in the EU RAR for acrylonitrile is considered to be unrealistically high and the estimated values will be used in the risk assessment.

Dermal exposure to workers could potentially occur during the handling of the fibres as the acrylonitrile polymers may still contain residual amounts of acrylonitrile monomer. In order to minimise the amount of acrylonitrile monomer residues they are washed out (wet spinning) or released (dry spinning) in the spinning machines. Appropriate PPE (gloves, overcoat, safety goggles) are also used in order to minimise dermal exposure to this irritant and sensitising substance.

Table 9: Summary of acute exposure concentrations to workers [ES1]

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data are available. Estimated values are used for risk characterisation.
Inhalation exposure (in mg/m3)	0.22-1.08	Measured values quoted in the EU RAR converted to mg/m3.

#### 9.1.2.1.2 Long-term exposure

Table 10: Long-term exposure concentrations t	to	to work	ers	[ES1]	
---	----	---------	-----	-------	--

Routes of exposure	PROC	Estimated Exposure Concentrations		Measured e		Explanation / source of measured data	
-		value	unit	Value	unit	of measured data	
	PROC 1	0.343	mg/kg bw/d	-	-		
	PROC 2	0.137	mg/kg bw/d	-	-		
Dermal experies	PROC 3	0.0343	mg/kg bw/d	-	-	No measured data	
Dermal exposure	PROC 4	0.686	mg/kg bw/d	-	-	No measured data	
	PROC 8b	0.686	mg/kg bw/d	-	-		
	PROC 9	0.686	mg/kg bw/d	-	-		
	PROC 1	0.0688 (without LEV and RP)	mg/m3				
Inhalation exposure	PROC 2	0.344	mg/m3	0.1-0.5	ppm	Data from EU RAR	
	PROC 3	0.860	mg/m3	0.1-0.5	Phu		
	PROC 4	0.688	mg/m3				
	PROC 8b	0.516	mg/m3				
	PROC 9	1.72	mg/m3				

Table	11:	Summary	of	long-term	exposure	concentration	to	workers	[ES1]	
-------	-----	---------	----	-----------	----------	---------------	----	---------	-------	--

Routes of exposure	Concentrations	Justification			
Dermal exposure	0.686	No measured dermal data are available. Estimated values are used			
(in mg/kg bw/d)	0.080	for risk characterisation.			
Measured Inhalation					
exposure	0.22-1.08	Measured values quoted in the EU RAR converted to mg/m3.			
(in mg/m3)					
Inhalation exposure	1.72	Worst again actimated inhelation averaging			
(in mg/m3)	1./2	Worst case estimated inhalation exposure.			

#### 9.1.2.2 Consumer exposure

Acrylonitrile polymer fibres are widely used in consumer products. The main potential routes of exposure to acrylonitrile in consumer products are via inhalation or though dermal contact and absorption through the skin.

#### Dermal exposure

Relevant exposure scenarios to consider include the release of residual acrylonitrile monomer from acrylic fibres used in themanufacture of clothes.

The results of a survey carried out by the US Consumer Product Safety Commission in 1978 (and reported) in the EU RAR on the potential for monomer migration or extraction from consumer products containing acrylonitrile indicated that levels offresidual monomer in acrylonitrile fibres were extremely low. The survey also indicated that the release of acrylonitrile in consumer products will not occur under normal conditions of use; this is confirmed by fibre manufacturers. The EU RAR notes no transmission (lod: 1 ppm) of acrylonitrile from a sampleof fabric to a 1% saline solution (designed to simulate human perspiration) even under extreme conditions of 120 烈 and an extraction time of 1 month. A further study reported in the EU RAR similarly demonstrated no diffusion of acrylonitrile (lod: 0.04 ppm) from only at elevated temperatures of greater than 130 怼. In addition, the levels of residual acrylonitrile monomer present in acrylic and modacrylic fibres are well below 1 ppm. Even levels of acrylonitrile in freshly spun fibres are less than 1 ppm and levels in fabrics (following subsequent processing) were considered by the EU RAR more realistically to be <0.1 ppm. The unreacted acrylonitrile present in polymers is tightly bound and diffuses slowly even, at elevated temperatures. The results of exposure modelling reported in the EU RAR also indicates that, even if residual acrylonitrile were released from clothing fabrics, only a very small proportion ( $\leq 0.5\%$ ) would be absorbed through the skin.

The EU RAR considers a scenario of a consumer wearing 1 kg acrylic fibres containing 1 ppm free acrylonitrile and calculates dermal exposure of 0.18 ng/kg bw/d (0.00000018 mg/kg bw/d) over a period of 30 days. Even using a number of worst-case assumptions including an acrylonitrile level of 1 ppm (considerably in excess of the levels seen even in freshly-spun fibre with no loss due to subsequent processing) and continuous dermal contact over a 30-day period, calculated levels of exposure were shown to be very low.

Inhalation exposure

### SAFETY DATA SHEET

Inhalation exposure of consumers may also occur. Relevant exposure scenarios to consider would include the inhalation of residual acrylonitrile monomer from fibres present in acrylic carpets. The EU RAR calculates an average air concentration of 0.00023 mg/m3acrylonitrile in a room with an acrylic fibre carpet, assuming the total release of free acrylonitrile over a one-year time period.

Modelled consumer exposures to acrylonitrile are shown below. ECETOC TRA modelled exposure values are considered to be unrealistic as the very low levels of residual acrylonitrile monomer present in manufactured polymer are very low and are effectively bound. Actual levels of consumer exposurewill therefore be minimal, as discussed above.

Routes of exposure	AC code	Estimated Exposure Concentrations		Measured exposure concentrations		Explanation / source of	
		value	unit	Value	unit	measured data	
01	AC 5-1	4.30	mg/kg/d	-	-	No	
Oral exposure $A$	AC 5-2	0.1	mg/kg/d	-	-	No measured data	
D	AC 5-1	1030	mg/kg/d	-	-	N	
Dermal exposure	AC 5-2	23.9	mg/kg/d	-	-	No measured data	
Inhalation annoanna	AC 5-1	$1.08 \times 10^4$	mg/kg/d	-	-	No maggined data	
Inhalation exposure	AC 5-2	$1.25 \times 10^5$	mg/kg/d	-	-	No measured data	

 Table 12: Exposure concentrations to consumers (ECETOC TRA) [ES1]

\*values generated using the ECETOC TRA exposure model TRA

 Table 13: Summary of exposure concentrations to consumers [ES1]

Routes of exposure	Concentrations	Justification
Oral exposure (in mg/kg bw/d)	-	Not relevant for this exposure scenario
Dermal exposure (in mg/kg bw/d)	0.00000018 mg/kg bw/d	Value taken from the EU RAR, based on the assumption of a consumer wearing 1 kg acrylic fibre for 30 days.
Inhalation exposure (in mg/m3)	0.00023	Value taken from the EU RAR; modelled value based on average air concentrations over a 1-year period.

#### 9.1.2.3 Indirect exposure of humans via the environment

Indirect exposure of the general public via the environment from consumption of biota or drinking water and exposure to air containing residual acrylonitrile is theoretically possible but will be very low as negligible amounts of acrylonitrile are released to air and water. In addition, acrylonitrile will be extensively degraded following a short acclimation period in water, air and soil plus bioaccumulation is not predicted. The EU RAR concluded that 'exposure of humans via the food chain is therefore anticipated to be extremely small and is not considered further in this risk assessment'. For indirect exposure via the air, the EU RAR estimates an average level of acrylonitrile in the atmosphere of 0.0005 mg/m<sup>3</sup>, equivalent to a systemic inhalation exposure of 0.000000007 mg/kg bw/d.

	Estimated exposure concentrations		Measured expo concentrations	sure	Explanation / source of
	value	unit	value	unit	measured data
Wet fish	0.0198	mg/kg	-	-	No measured data
Drinking water	0.014	mg/L	-	-	No measured data
Meat	1.26 x 10 <sup>-6</sup>	mg/kg	-	-	No measured data
Milk	1.26 x 10 <sup>-5</sup>	mg/L	-	-	No measured data

#### Table 14: Concentration for exposure of humans via the environment [ES1]

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 22 sites across Europe, the local release fraction was changed to 0.045 for a total EU tonnage of 314,700 t/a.

#### 9.1.2.4 Environmental exposure

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented.

For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acrylonitrile 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 6c covers the production of acrylic and modacrylic textile fibres. As there are 22 sites across Europe producing acrylic and modacrylic textile fibres, the local fraction was set to 0.045 asthe figure of 314700 tpa has been quoted as the maximum total EU tonnage.

It is proposed that the use of ERC 6c to estimate emissions to the environment will result in an unrealistic assessment for acrylonitrile. This is because the default emissions fractions in ERC 6c represent a worst case and does not take into account the efficiency of the waste water treatment or atmospheric scrubber systems used. Release of Acrylonitrile to the environment is strictly controlled by local and national pollution control. Specific process technology is required to limit and control release at each site. An average efficiency for all sites is not known. Based on the conservative standard risk assessment model, the maximum release to waste water before processing must not exceed 7.9 kg/d in a standard waste water treatment plant limited to 2000 m3per day. This is equivalent to a sewage influent of 3.5 mg/L.An average efficiency for all sites is not known but the maximum release to water must not exceed 7.9 kg/d. The table below shows the parameters entered into the EUSES model:

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	53.06	g/mol	-
Vapour Pressure	11500	Pa	-
Water Solubility	73000	mg/L	-
Octanol/water partition coefficient	0.25	logKow	-
Biodegradability	Ready biodegradable	-	-
Life Cycle Step	Use	-	-
Tonnage	314700	Tonnes	-
Number of sites	22	-	-
Environmental Release Class	ERC6c	-	-
Fraction of Tonnage for Region	0.045	-	1.0
STP	On-site STP	-	
Emission events per year	300	Days	20
Release to Air	0.05 (takes into account 99% efficiency of scrubber systems)	%	5
Release to Water	7.86 kg/d	%	5
Dilution factor applied for PEC derivation	-	-	10 (2,000 m3/d)
% fraction degraded in STP	95	%	86
% fraction released to water after STP	4.3	%	12.1
% fraction released to air after STP	0.65	%	1.83
% fraction released to sludge after STP	0.0475	%	0.133

#### Table 15: Input Parameters [ES1]

#### 9.1.2.4.1 Environmental releases

In the table below are the estimates generated using the parameters above for ERC 6C using EUSES:

Table 16: Releases to the environment generated by EUSES [ES1]

Compartments ERC 6C	Predicted releases	Required release (kg/d)	Explanation / source of measured data
Aquatic (after STP)	0.0169 mg/L	7.86	No measured data.
Air (direct + STP)	0.00656 mg/m3	-	No measured data.
Soil (direct only)	5.13 x 10 <sup>-4</sup> mg/kg	-	No measured data.

\* estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 22 sites across Europe, the local release fraction was changed to 0.045 for a total EU tonnage of 314,700 t/a.

9.1.2.4.2 Exposure concentration in sewage treatment plants (STP)

The use of ERC 6c default values to estimate emissions is considered to be unrealistic for acrylonitrile. Following polymerisation, the unreacted monomer is recovered and recycled to the reactor. In addition, an industrial sewage treatment plant with a fully acclimated microbial population is highly efficient and causes at least 95% degradation (see section 4.1.3) of the remaining Acrylonitrile. Only 4.3% of the fraction treated in the STP is released to waste water. As a result, the release to waste water is negligible.

Table 17: Concentrations in sewage using the EUSES exposure model [ES1]

Compartments	Estimated exposure Measured exposure concentrations		sure	Explanation / source of measured data	
•	value	unit	value	unit	•
Sewage (STP effluent)	0.169	mg/L	-	-	No measured data
Sewage sludge	4.73	mg/kg	-	-	No measured data

\* estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 22 sites across Europe, the local release fraction was changed to 0.045 for a total EU tonnage of 314,700 t/a. The following values will be used in the risk assessment:

Table 18: Predicted Exposure Concentrations (PEC) in sewage [ES1]

	Value	Justification
Concentration in sewage (PECstp)(in mg/l)	0.169	Worst case modelled concentration in sewage. No measured data.
Concentration in sewage sludge (in mg/kg d.w.)	4.73	Estimated worst case value. No measured data available.

#### 9.1.2.4.3 Exposure concentration in aquatic pelagic compartment

Following polymerisation, any unreacted monomer is recovered and recycled to the reactor. As a result, the releases to waste water are minimal. Furthermore, a large number of acrylonitrile fibre production sites have dedicated wastewater treatment plants which degrade >95% of the remaining acrylonitrile monomer.

Table 19: Loca	l concentrations	in	water	determined	using	the	EUSES	exposure	model	[ES1]	1

Compartments	Estimated exposure concentration		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Freshwater	0.0169	mg/L	-		No measured data.
Marine water	0.00169	mg/L	-		No measured data.
Intermittent releases to water	NA		-		No measured data

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kgin order to allow for the fact that the sludge is incinerated or landfilled. As there are 22 sites across Europe, the local release fraction was changed to 0.045 for a total EU tonnage of 314,700 t/a. The following data will be used for risk assessment and characterisation:

Table 20: Predicted Exposure Concentrations (PEC) in aquatic compartment [ES1]	Table 2	0: Predicted	Exposure	Concentrations	(PEC)	in	aquatic	compartment	[ES1]
--	---------	--------------	----------	----------------	-------	----	---------	-------------	-------

Compartments	Local concentration	PEC aquatic (local+regional)	Justification
Freshwater (in mg/l)	0.0169	0.0169	Worst case predicted freshwater concentration. No measured data for freshwater concentrations.
Marine water (in mg/l)	0.00169	0.00169	Default dilution of 10.
Intermittent releases to water (in mg/l)	NA	-	-

#### 9.1.2.4.4 Exposure concentration in sediments

#### Table 21: Local concentrations in sediment [ES1]

Compartments	Estimated exposure concentrations		concentrations		exposure concentrations		Explanation / source of measured data
	value	unit	value	unit			
Freshwater sediments	0.0185	mg/kg	-	-	-		
Marine water sediments	0.00184	mg/kg	-	-	-		

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 22 sites across Europe, the local release fraction was changed to 0.045 for a total EU tonnage of 314,700 t/a. The following values will be used for the risk assessment and risk characterisation:

Table	22:	Predicted	Exposure	Concentrations	(PEC)	in	sediments	[ES1]
-------	-----	-----------	----------	----------------	-------	----	-----------	-------

Compartments	PEC sediment (local+regional)	Justification
Freshwater sediments (in mg/kg d.w)	0.0185	Worst case predicted value. No measured values available.
Marine water sediments (in mg/kg d.w.)	0.00184	Assumed 10-fold reduction factor for marine sediment

#### 9.1.2.4.5 Exposure concentrations in soil and groundwater

Acrylonitrile can be potentially be deposited onto/into the soil from the atmosphere and aqueous compartments. Information from industry indicates that industrial sludge from acrylonitrile fibre producing plants is not spread onto land. The sewage is normally incinerated with other wastes. Therefore the only potential route of exposure to soil is indirect, via the atmosphere. Atmospheric emissions are kept to a minimum by the use of scrubbers therefore exposure to the soil and groundwater is expected to be minimal. The predicted exposure concentration for soil have been calculated using the EUSES exposure model and are given below:

Table 23: Local concentrations in soil [ES1]

Compartments	ents Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Agricultural soil averaged	5.13 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data
Grassland averaged	6.92 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data
Groundwater	0.0014	mg/L	-	-	No measured data

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 22 sites across Europe, the local release fraction was changed to 0.045 for a total EU tonnage of 314,700 t/a. The following values will be used for risk assessment and characterisation:

#### Table 24: Predicted Exposure Concentrations (PEC) in soil and groundwater [ES1]

	Local concentration	PEC soil/groundwater (local+regional)	Justification
Agricultural soil averaged (mg/kg ww)	5.13 x 10 <sup>-4</sup>	5.13 x 10 <sup>-4</sup>	
Grassland averaged (mg/kg ww)	6.92 x 10 <sup>-4</sup>	6.92 x 10 <sup>-4</sup>	Estimated values. No measured data.
Groundwater(mg/l)	-	0.0014	

#### 9.1.2.4.6 Atmospheric compartment

Acrylonitrile is volatile and therefore the atmospheric compartment is likely to be a major compartment of distribution of acrylonitrile. Releases are reduced by the scrubbing of gaseous and volatile waste before discharging to the atmosphere. The predicted exposure concentration (PEC) in air has been estimated using the EUSES exposure model to gain an approximation.

Table 25: Local concentrations in air [ES1]

		Estimated exposure concentrations		ocal ns	Explanation / source of measured	
	value	unit	value	unit	data data	
During emission	0.00656	mg/m <sup>3</sup>	-	-	Measured atmospheric release must not exceed 0.2 mg/m3 according to BREF document of acrylonitrile.	
annual average	0.00539	mg/m <sup>3</sup>	-	-	No measured data	
Annual total deposition	0.00778	mg/m <sup>3</sup>	-	-	No measured data	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 22 sites across Europe, the local release fraction was changed to 0.045 for a total EU tonnage of 314,700 t/a.

#### Table 26: Predicted Exposure Concentration (PEC) in air [ES1]

	Local concentration	PEC air (local+regional)	Justification
During emission (mg/m <sup>3</sup> )	0.00656	-	Worst case calculated PEC.
annual average (mg/m <sup>3</sup> )	0.00539	0.0054	Worst case calculated concentration.
Annual deposition (mg/m <sup>2</sup> /d)	0.00778	-	Worst case calculated release.

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

Exposure of aquatic species to low levels of acrylonitrile in the aquatic environment is possible. The predicted concentrations relevant for the food chain have been generated using the EUSES exposure model.

	Predicted exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Concentration in food of fish eating predator	0.00986 (freshwater) 0.000985 (marine water)	mg/kg	-	-	No measured data are available	
Concentration in food of fish eating top-predator (marine)	0.0002	mg/kg	-	-	No measured data are available	
Concentration in earthworm	0.000567	mg/kg	-	-	No measured data are available	

#### Table 27: Local concentration relevant for secondary poisoning [ES1]

# 9.2 Exposure Scenario 2- Production of acrylonitrile-butadiene-styrene (ABS) and styrene-acrylonitrile (SAN) plastics

#### 9.2.1 Exposure scenario

The second largest use of acrylonitrile is in the production of acrylonitrile-butadiene-styrene (ABS) and styrene-acrylonitrile (SAN) plastics. Reaction of acrylonitrile with butadiene and/or styrene in an emulsion or solution polymerisation systems gives a rigid plastic product after further processing. The plastic can be used in a wide variety of products including automotive parts, household appliances and food containers.

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

ABS plastic consists of a homogeneous physical mixture of a butadiene-acrylonitrile-styrene (ABS) graft polymer and a styrene-acrylonitrile (SAN) copolymer. ABS is placed on the market as plastic granulate which is ready for processing. The technical production of ABS may be carried out via different processes including pure emulsion polymerisation or combined solution/emulsion polymerisation.

#### Production of ABS plastics by emulsion polymerisation

The process consists of four steps:

1. Butadiene Polymerisation distribution.

#### 2. Graft polymerisation

In the presence of the polybutadiene latex, a styrene acrylonitrile monomer mixture is graft polymerised by means of anionic emulsifiers. Production takes place without pressure in stirred tank reactors. Water, polybutadiene latex and the initiator are introduced and heated to 50-80°C.

## SAFETY DATA SHEET

The emulsifier, acrylonitrile and styrene are added to the aqueous phase while the polymerisation temperature is controlled with a heating/cooling cycle. At the end of the feeding, the mixture is polymerised at a higher temperature. After polymerisation the latex is stored until further processing. The stored latex still contains low amounts of unreacted volatile acrylonitrile, styrene and butadiene. The acrylonitrile withdrawn during polymerisation and during reactor cleaning is passed to a waste gas combustion plant. The acrylonitrile, styrene and butadiene-containing displacement air of stored latex is connected to the same disposal system. Here the acrylonitrile is combusted with greater than 99% efficiency (EU RAR).

#### 3. Resin polymerisation

The resin component is produced via emulsion polymerisation of styrene or alpha-methyl styrene and acrylonitrile. Resin polymerisationis carried out in stirred-tank reactors at temperatures range of 50-80°C without pressure, while water, emulsifier and auxiliary products are fed into the reactor and the monomer mixture is added under stirring. The polymerisation heat is removed via a heating/cooling cycle. The resin polymer latex is pumped off into storage tanks. Prior to processing, the resin polymer latex is kept at intermediate storage in the same way as the graft latex. Emissions of acrylonitrile occur at the vent pipes of the reactors and intermediate storage tanks. The acrylonitrile-containing waste gases are sucked off prior to the opening of the stirred-tank reactors for repair or cleaning purposes. They are also sent to the vent pipes. The polymer generated during wet reactor cleaning releases volatile acrylonitrile practically completely to the aqueous phase. The wastes from the vent pipes of the reactors and from the intermediate storage tanks are sent to a waste gas combustion plant via a centralwaste gas pipe.

#### 4. ABS Powder production

During the first processing stage the graft polymer latex is mixed with the resin polymer latex in predetermined proportions, and stabilisers are added. In other stages the mixed latex is coagulated, the solids are separated from water and the wet ABS is dried and granulated to powder at 100-180°C. Acrylonitrile-containing waste gases arise when the mixing tanks are filled, in the precipitation and in the washing and drying process. Waste air produced during powder conveying, compounding/granulating and granulate conveying may contain low levels of acrylonitrile. While the tank vent pipes and the suction pipes of the washing stage permit an integration into the waste air combustion system due to comparatively high acrylonitrile loads, the dryer waste air is emitted due to the high volume flows involved.

#### Production of ABS polymers

The production of ABS polymers by combined solution/emulsion polymerisation involves three steps:

## SAFETY DATA SHEET

#### 1. SAN polymer production

The starting materials acrylonitrile and styrene or alpha-methylstyrene are continuously fed to the reactor with a solvent. The reaction is conducted at 90 and 170°C at pressures of up to 6 bars. The reaction heat can be removed from the pressurised reaction mixture via evaporative coolers. The polymer solution is continuously discharged from the reactor. In the subsequent solvent recovery plant, the solvent and the non-converted monomers are withdrawn by heat increase and pressure reduction. After condensation they are recycled into the polymerisation process. The degassed polymer melt is sent to the mixing unit. Acrylonitrile-containing inert gas streams escape from the solvent recovery and are sent for combustion.

#### 2. Latex production

Latex production takes place in two stages. In the first stage, a base dispersion is polymerised in the reactor without involvement of acrylonitrile. In the second polymerisation stage, acrylonitrile and styrene are fed and grafted onto the base dispersion in another reactor. The polymerisation takes place at this stage at 50-80°C without pressure. The resulting aqueous dispersion with solid contents of between 30 and 50% (graft dispersion) is sent to an intermediate storage tank for further processing. During polymerisation the monomer-laden inert gases are removed. Suction systems at the openings for reactor filling, sampling and cleaning convey among others acrylonitrile-containing waste gases, which are emitted. In order to avoid emissions as a result of non-converted monomers, the reactors and intermediate storage tanks are connected by gas displacement ducts to shift the displacement of air. Any excessive displacement air is sent for combustion.

#### 3. Latex processing

The aqueous dispersion is sent via an intermediate storage tank to the precipitation and de-watering plant. The resulting product together with the SAN melt is continuously fed into the mixing unit and homogenised. The crude ABS is granulated. Near the discharge device of the mixing unit and during granulation, acrylonitrile-containing waste gases arise and are emitted. The acrylonitrile-containing waste gases from the precipitation and dewatering plants and from the mixing unit are sent for combustion.

#### 9.2.1.2 Operational conditions related to frequency, duration and amount of use Table 28: 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	kg/d	No specific data: not required for risk assessment or risk characterisation
Duration of exposure per day at workplace [for one worker]	8h/day	Default value
Frequency of exposure at workplace [for one worker]	220 d/y	220 [default value]
Emission days per site	365 d/y	Assumed continuous process

#### 9.2.1.3 Operational conditions and risk management measures related to substance characteristics Table 29: Characteristics of the substance or preparation

Information type	Data field	Explanation
Physical state	Liquid	The substance is a liquid
For solids: Categorisation of dust grades	Not applicable	Not relevant: the substance is a liquid
Concentration of substance in preparation	Not applicable	The substance is used undiluted
Concentration after dilution for use (if relevant)	Not applicable	Not relevant: the substance is used undiluted
Risk management measures related to the design of product	Not applicable	Not relevant

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

For exposure scenarios covering workeruses, the following example table for reporting information is available:

#### Table 30: 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		
Room size and ventilation rate	m <sup>3</sup> ; exchange per hour	Room size and general ventilation are not employed to control risk		
Area of skin contact with the substance under conditions of use	cm <sup>2</sup>	Not relevant. The substance is a skin irritant and skin sensitizer. RMMs must therefore be used to eliminate the potential for skin contact under normal conditions of use.		
Body weight	65 kg	Default for workers		

#### 9.2.1.5 Other operational conditions of use

Table 31: 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,	0.05 kg/kg	Default (worst-case) assumption for ERC 6C		
Fraction of applied amount lost from process/use to waste water	0.05 kg/kg	Default (worst-case) assumption for ERC 6C		
Fraction of applied amount lost from process/use to waste	0 kg/kg	No additional waste		
Fraction consumed in process/use	0.9 kg/kg	Assumes worst-case losses to waste gas and waste water		
Fraction of applied amount leaving the site with products	0 kg/kg	The substance is polymerised and hence is chemically transformed during the plastic manufacture process. Only trace amounts of unreacted monomer are present in the products		

#### 9.2.1.6 Risk management measures

#### Table 32: 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	The production of ABS and SAN plastics occurs either in a closed system or partially closed system. In the case of the partially enclosed system, local exhaust ventilation is used.						
Local exhaust ventilation required plus good work practise	Effectiveness in terms of reduction factor against situation without LEV or residual exposure	A fully closed system or partially closed system is used. In the case of the partially enclosed system local exhaust ventilation is used.						
Personal protective equipment (PPE)								
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness	Personal protective equipment (PPE)						
		Protective gloves and face-shield are routinely worn to prevent accidental contact with the substance.						
		RPE used unless a fully enclosed system is used						
Other risk management measures related	ed to workers							
		Workers received specific training and instruction in order to ensure minimal contact with the substance.						

Information type	Data field	Explanation
		Airborne concentrations of acrylonitrile are routinely monitored to ensure compliance with occupational exposure standards.
Risk management measures related to	environmental emissions from in	dustrial sites
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	
Resulting fraction of initially applied amount in waste water released from site	0.000237 kg/kg	Only a very small proportion is released from STP. In the STP, the substance is degraded by 95% according to biodegradation tests (see section 4.1.3). Waste water from the purification and cooling plants containing residual acrylonitrile (i.e. not converted during polymerisation) are either recycled into the process or
		sent to a stripping column prior to return to the process.
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	
Resulting fraction of applied amount in waste gas released to environment	0.0005 kg/kg	Emissions during the polymerisation process are negligible as the process is enclosed. Waste gases are subjected to scrubber systems which oxidises the residual acrylonitrile and are effectively combusted. For the purposes of the model the efficiency has been modelled as 99%. In reality, the removal of atmospheric emissions is highly efficient and negligible amounts of acrylonitrile are released.
Onsite waste treatment	Effectiveness (fraction after on-site treatment compared to the fraction entered into waste treatment.	
Fraction of initially applied amount	0.000237 kg/kg	Release to water (including removal by STP)
sent to external waste treatment. This is the sum of direct losses from processes to waste, and the residues from onsite waste water and waste gas treatment.	0.0495 kg/kg	Scrubber residues are treated on site The value shown represents the proportion (99 %) of particulate substance (5% default assumption for loss to waste gas) removed by scrubber systems.
Municipal or other type of external waste water treatment	Effectiveness of substance removal [fraction of substance in treated waste water compared to entering the waste water treatment plant]	Short description of technique

Information type	Data field	Explanation
Effluent (of the waste water treatment plant) discharge rate	2000 m <sup>3</sup> /d	Default: 2.000 m <sup>3</sup> /d
Recovery of sludge for agriculture or horticulture	No	Sludge from acrylonitrile processing plants is not recovered for agriculture or horticulture

#### 9.2.1.7 Waste related measures

#### Table 33: Fractions of substance in waste and waste management measures

Information type	nation type Data field	
Amount of substances in waste resulting from service life of articles	0 kg/y	Not applicable: plastic articles only contain trace amounts of bound unreacted monomer
Type of waste, suitable waste codes	-	-
Type of external treatment aiming at recycling or recovery of substances	-	Not applicable
Fraction of the initially applied amount of substance recovered.	0 kg/kg	Not applicable
Type of external treatment aiming at final disposal of the waste	-	Not applicable
Fraction of substance released into the environment via air from waste handling	0 kg/kg	Not applicable
Fraction of substance released into the environment via waste water from waste handling	0 kg/kg	Not applicable
Fraction of substance disposed of as secondary waste	0 kg/kg	Not applicable; primary waste only is generated from this exposure scenario

#### 9.2.2 Exposure estimation

#### 9.2.2.1 Workers exposure

#### 9.2.2.1.1 Acute/Short term exposure of workers:

The exposure estimates were generated using the ECETOC TRA exposure model. The RMM efficiency used in the model were based on ECETOC (2009) so the estimate obtained represents a full shift and the  $90^{\text{th}}$  percentile of the exposure distribution. Acute worst-case values for inhalation can be derived from full shift values by using a multiplication factor which is detailed in Table R.14-3 of Guidance document R.14: Occupational exposure estimation. It is recommended to multiply a full shift ECETOC estimate by a factor of 2 to obtain the related short-term inhalation exposure distribution. These results are shown in the table below.

Routes of exposure	PROC	Estimated Exposure Concentrations		Measured exposure concentrations		Explanation / source	
F		value	unit	Value	unit	of measured data	
	PROC 1	0.343	mg/kg bw/d	-	-		
	PROC 2	0.137	mg/kg bw/d	-	-		
Dermal exposure	PROC 3	0.0343	mg/kg bw/d	-	-	NT 114	
	PROC 4	0.686	mg/kg bw/d	-	-	No measured data	
	PROC 8b	0.686	mg/kg bw/d	-	-		
	PROC 9	0.686	mg/kg bw/d	-	-		
	PROC 1	[0.1376] (without LEV and RP)	mg/m <sup>3</sup>				
Inhalation exposure	PROC 2	[0.688]	mg/m <sup>3</sup>			No measured data are	
	PROC 3	[1.72]	mg/m <sup>3</sup>	] -	-	available	
	PROC 4	[1.376]	mg/m <sup>3</sup>				
	PROC 8b	[1.032]	mg/m <sup>3</sup>				
	PROC 9	[3.44]	mg/m <sup>3</sup>				

Table 34: Acute exposure concentrations to workers

\*all values generated with RP and LEV unless otherwise stated

[Values for acute inhalation exposures are modelled TWA values with a factor of 2 applied]

The production of plastics including resin processing and ABS powder production all involve processes in a closed system with full containment. For plastic production the processing temperature is 80 °C and for ABS powder production the temperature is 180 °C. For the closed system, both dermal and inhalation exposures is therefore minimal. Exposure could occur during the sampling of the reactor. In this case, suitable local ventilation extraction or respiratory protection is used to minimise inhalation exposure. Appropriate PPE (gloves, overcoat, safety goggles) are also used in order to minimise dermal exposure.

Specific exposure data has been provided in the EU RAR from five European ABS processing plant during the 1990s. The mean level of occupational exposure was quoted as 0.046-0.3 ppm.

More recently, improvements in the workplace have been introduced, including:

- Delivery of raw material acrylonitrile by pipeline eliminating the hazard of the risk of exposure during unloading.
- Redirection of vents coming from storage facilities away from areas occupied by personnel.
- Continuous air monitoring in areas of greater risk
- Engineering controls to pump seals so as to reduce the leakage potential.
- Improvement in ventilation including extract ventilation at critical locations

These improvements have dramatically reduced the extent of inhalation and dermal exposure. As a result, the quoted measured data is unrealistically high and the estimated values will be used in the risk assessment.

Table 35: Summary of acute exposure concentrations to workers	Table	35:	Summary	of	acute	exposure	concentrations	to	workers
---	-------	-----	---------	----	-------	----------	----------------	----	---------

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data. Modelled values are therefore used.
Estimated Inhalation exposure (in mg/m <sup>3</sup> )	3.44	Worst case modelled data.
Measured Inhalation exposure (in mg/m <sup>3</sup> )	0.0997-0.65	Measured data from EU RAR.

#### 9.2.2.1.2 Long-term exposure

Table 36:	Long-term	exposure	concentrations	to	workers
-----------	-----------	----------	----------------	----	---------

Routes of exposure	PROC	Estimated E Concentration		Measured e		Explanation / source of	
		value	unit	Value	unit	measured data	
	PROC 1	0.343	mg/kg bw/d	-	-		
	PROC 2	0.137	mg/kg bw/d	-	-		
Dormal aveagura	PROC 3	0.0343	mg/kg bw/d	-	-	No manufacto	
Dermal exposure	PROC 4	0.686	mg/kg bw/d	-	-	No measured data	
	PROC 8b	0.686	mg/kg bw/d	-	-		
	PROC 9	0.686	mg/kg bw/d	-	-		
	PROC 1	0.0688 (without LEV and RP)	mg/m <sup>3</sup>	Mean 0.046-0.3; 95% CL 0.64 ppm	ppm		
	PROC 2	0.344	mg/m <sup>3</sup>			Data from EU RAR (p.	
Inhalation exposure	PROC 3	0.860	mg/m <sup>3</sup>			85) for five ABS plants (n>700)	
	PROC 4	0.688	mg/m <sup>3</sup>	Mean		(11-700)	
	PROC 8b	0.516	mg/m <sup>3</sup>	0.1-0.65;			
	PROC 9	1.72	mg/m <sup>3</sup>	95% CL 1.4	mg/m <sup>3</sup>		

#### Table 37: Summary of long-term exposure concentration to workers

Routes of exposure	Concentrations	Justification			
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data. Estimated values used.			
Inhalation exposure (in mg/m3)	1.72	Worst case modelled data.			
Measured Inhalation exposure (in mg/m3)	0.0997-0.65	Measured data from EU RAR.			

#### 9.2.2.2 Consumer exposure

The relevant route of consumer exposure for this exposure scenario is oral. Acrylonitrile polymers (ABS, SAN) are used in food packaging materials. The levels of migration of acrylonitrile into are limited to 0.02 mg/kg food under separate legislation (Directive 90/128/EEC). The EU RAR estimates human intake of no more than 2  $\frac{1}{2}$ /day (0.00003 mg/kg bw/d) acrylonitrile, based on the assumption that 5% of food intake is packagedin ABS.

 Table 38: Exposure concentrations to consumers

Routes of exposure	AC code	Estimated Exposure Concentrations		Measured exposure concentrations		Explanation / source of	
-		value	unit	Value	unit	measured data	
Oral exposure		0.00003	mg/kg bw/d			No measured data are available	
Dermal exposure	Not relevan	Not relevant for this exposure scenario					
Inhalation exposure	Not relevan	Not relevant for this exposure scenario					

#### 9.2.2.3 Indirect exposure of humans via the environment

Indirect exposure of the general public via the environment from consumption of biota or drinking water and exposure to air containing residual acrylonitrile is theoretically possible but will be very low as negligible amounts of acrylonitrile are released to air and water. In addition, acrylonitrile will be extensively degraded following a short acclimation period in water, air and soil plus bioaccumulation is not predicted. The EU RAR concluded that 'exposure of humans via the food chain is therefore anticipated to be extremely small and isnot considered further in this risk assessment'. For indirect exposure via the air, the EU RAR estimates an average level of acrylonitrile in the atmosphere of  $0.0005 \mu m/m^3$ , equivalent to a systemic inhalation exposure of 0.00000007 mg/kg bw/d.

	Estimated exposure concentrations		Measured expo concentrations	osure	Explanation / source of
	value	unit	value	unit	measured data
Wet fish	0.0197	mg/kg	-	-	No measured data
Drinking water	0.0139	mg/L	-	-	No measured data
Meat	1.06 x 10 <sup>-6</sup>	mg/kg	-	-	No measured data
Milk	1.06 x 10 <sup>-5</sup>	mg/L	-	-	No measured data

#### Table 39: Concentration for exposure of humans via the environment

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 18 sites across Europe, the local release fraction was changed to 0.056 for a total EU tonnage of 179,300 t/a.

#### 9.2.2.4 Environmental exposure

The environmental releases are determined primarily by tonnage and the ERC with conservative estimations and defaults being implemented. For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acrylonitrile 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 6C covers the use of acrylonitrile in theproduction of acrylonitrile-butadiene-styrene (ABS) and styrene-acrylonitrile (SAN) plastics. As there are 18 sites across Europe producing ABS/SAN plastics, the local fraction was set to 0.056 asthe figure of 179,300tpa has been quotedas the maximum total EU tonnage.

It is proposed that the use of ERC 6c to estimate emissions to the environment will result in an unrealistic assessment for acrylonitrile. This is because the default emissions fractions in ERC 6c represent a worst case and does not take into account the efficiency of the waste water treatment or atmospheric scrubber systems used. Release of Acrylonitrile to the environment is strictly controlled by local and national pollution control. Specific process technology is required to limit and control release at each site. An average efficiency for all sites is not known. Based on the conservative standard risk assessment model, the maximum release to waste water before processing must not exceed 7.9 kg/d in a standard waste water treatment plant limited to 2000 m3per day. This is equivalent to a sewage influent of 3.5 mg/L. The table below shows the parameters entered into the EUSES model:

### Acrylonitrile

### SAFETY DATA SHEET

### Table 40: Input Parameters

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	53.06	g/mol	-
Vapour Pressure	11500	Ра	-
Water Solubility	73000	mg/L	-
Octanol/water partition coefficient	0.25	logKow	-
Biodegradability	Ready biodegradable	-	-
Life Cycle Step	Use	-	-
Tonnage	179,300	Tonnes	-
Number of sites	18	-	-
Environmental Release Class	ERC6c	-	-
Fraction of Tonnage for Region	0.056	-	1.0
STP	On-site STP	-	
Emission events per year	300	Days	20
Release to Air	0.05 (takes into account 99% efficiency of scrubber systems)	%	5
Release to Water	7.86 kg/d	%	5
Dilution factor applied for PEC derivation	-	-	10 (2,000 $m^3/d$ )
% fraction degraded in STP	95	%	86
% fraction released to water after STP	4.3	%	12.1
% fraction released to air after STP	0.65	%	1.83
% fraction released to sludge after STP	0.0475	%	0.133

#### 9.2.2.4.1 Environmental releases

Table 41 Releases to the environment generated using the EUSES exposure model

Compartments ERC 6C	Predicted releases	Required release (kg/d)	Explanation / source of measured data
Aquatic (after STP)	0.0169 mg/L	7.86	No measured data available
Air (direct + STP)	$0.00462 \text{ mg/m}^3$	-	No measured data available
Soil (direct only)	3.61 x 10-4 mg/kg	-	No measured data.

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 18 sites across Europe, the local release fraction was changed to 0.056 for a total EU tonnage of 179,300 t/a.

#### 9.2.2.4.2 Exposure concentration in sewage treatment plants (STP)

The use of ERC 6c default values to estimate emissions is considered to be unrealistic for acrylonitrile. Following polymerisation, the unreacted monomer is recovered and recycled to the reactor. In addition, an industrial sewage treatment plant with a fully acclimated microbial population is highly efficient and causes at least 95% degradation (see section 4.1.3) of the remaining Acrylonitrile. Only 4.3% of the fraction treated in the STP is released to waste water. As a result, the release to waste water is negligible.

Compartments	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Sewage (STP effluent)	0.169	mg/L	-	-	No measured data	
Sewage sludge	4.73	mg/kg	-	-	No measured data	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 18 sites across Europe, the local release fraction was changed to 0.056 for a total EU tonnage of 179,300 t/a. The following values will be used in the risk assessment:

Table 43: Predicted Exposure Concentrations (PEC) in sewage

	Value	Justification
Concentration in sewage (PECstp) (in mg/l)	0.169	Worst case sewage effluent concentration.
Concentration in sewage sludge (in mg/kg d.w.)	4.73	Worst case estimated value. No measured data available.

**9.2.2.4.3 Exposure concentration in aquatic pelagic compartment** Following polymerisation, the unreacted monomer is recovered and recycled to the reactor. As a result, the release to waste water is negligible. Furthermore, a large number of sites have dedicated wastewater treatment plants which degrade any of the acrylonitrile monomer remaining. The standard rate of degradation is >95%.

Compartments	exposure expos		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Freshwater	0.0169	mg/L	-		No measured data	
Marine water	0.00169	mg/L	-		No measured data	
Intermittent releases to water	NA		-		No measured data	

#### Table 44: Local concentrations in water using EUSES exposure model

#### Table 45: Predicted Exposure Concentrations (PEC) in aquatic compartment

Compartments	Local concentration	PEC aquatic (local+regional)	Justification
Freshwater (in mg/l)	0.0169	0.0169	Worst case predicted freshwater concentration. No measured data for freshwater concentrations.
Marine water (in mg/l)	0.00169	0.00169	Default dilution of 10 applied to the freshwater concentration
Intermittent releases to water (in mg/l)	NA	-	-

#### 9.2.2.4.4 Exposure concentration in sediments

Risk management measures such as waste water treatment and atmospheric scrubbers are implemented in order to reduce emissions to the environment. The exposure concentration in sediments is therefore negligible.

Table 46: Predicted exposure concentration in sediments using measured effluent data

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Freshwater sediments	0.0185	mg/kg	-	-		
Marine water sediments	0.00185	mg/kg	-	-	No measured data are available	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 18 sites across Europe, the local release fraction was changed to 0.056 for a total EU tonnage of 179,300 t/a.

The following values will be carried forward to the risk assessment and risk characterisation:

Table 47: Predicted Exposure Concentrations (PEC) in sediments

Compartments	PEC sediment (local+regional)	Justification
Freshwater sediments (in mg/kg d.w)	0.0185	Worst case predicted value. No measured values available.
Marine water sediments (in mg/kg d.w.)	0.00185	Assumed 10-fold reduction factor.

#### 9.2.2.4.5 Exposure concentrations in soil and groundwater

Acrylonitrile can potentially be deposited onto/into the soil from the atmosphere and aqueous from Information industry indicates thatlittle compartments. industrial sludge from Acrylonitrileprocessingplantsis spread onto land. The sewage is normally incinerated with other wastes. Therefore the only potential route of exposure to soil is (indirect) via the atmosphere. The predicted exposure concentration for soil was calculated using the EUSES exposure model. The results are given in the table below:

Table	<b>48:</b>	Local	concentrations	in	soil

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Agricultural soil averaged	3.61 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data	
Grassland averaged	4.88 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data	
Groundwater	9.86 x 10 <sup>-4</sup>	mg/L	-	-	No measured data	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set

#### Acrylonitrile

### SAFETY DATA SHEET

to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 18 sites across Europe, the local release fraction was changed to 0.056 for a total EU tonnage of 179,300 t/a.

The following values will be carried forward to the risk assessment and risk characterisation:

	Local concentration	PEC soil/groundwater (local+regional)	Justification
Agricultural soil averaged (mg/kg ww)	3.61 x 10 <sup>-4</sup>	3.61 x 10 <sup>-4</sup>	Estimated values using measured data for
Grassland averaged (mg/kg ww)	4.88 x 10 <sup>-4</sup>	4.88 x 10 <sup>-4</sup>	sewage effluent, atmospheric releases and dilution factor. Represents worst case out of the sites with waste water treatment.
Groundwater(mg/l)	-	9.86 x 10	of the sites with waste water treatment.

Table 49: Predicted Exposure Concentrations (PEC) in soil and groundwater

#### 9.2.2.4.6 Atmospheric compartment

Acrylonitrile is volatile and therefore the atmospheric compartment is the major compartment of distribution of acrylonitrile. Releases are reduced by the combustion or scrubbing of gaseous and volatile waste before discharging to the atmosphere. The predicted exposure concentration (PEC) in air has been estimated using the EUSES exposure model to gain an accurate approximation. It has been assumed that the efficiency of the atmospheric scrubbers is 99%.

Table 50: Local concentrations in air

	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured
	value	unit	value	unit	data
During emission	0.00462	mg/m <sup>3</sup>	-	-	No measured data
annual average	0.0038	mg/m <sup>3</sup>	-	-	No measured data
Annual total deposition	0.00548	mg/m <sup>3</sup>	3.6	t/y	EU RAR

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 18 sites across Europe, the local release fraction was changed to 0.056 for a total EU tonnage of 179,300 t/a.

Table   5	1:	Predicted	Exposure	Concentration	(PEC)	in	air	
-----------	----	-----------	----------	---------------	-------	----	-----	--

	Local concentration	PEC air (local+regional)	Justification
During emission (mg/m <sup>3</sup> )	0.00462	-	Worst case calculated PEC
annual average (mg/m <sup>3</sup> )	0.0038	0.0038	Worst case calculated concentration
Annual deposition (mg/m <sup>2</sup> /d)	0.00548	-	Worst case calculated concentration

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

Exposure of aquatic species to low levels of acrylonitrile in the aquatic environment is possible. The predicted concentrations relevant for the food chain have been generated using the EUSES exposure model using the measured data for water and atmospheric releases.

	Predicted exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Concentration in food of fish eating predator	0.00986 (freshwater) 0.00986 (marine water)	mg/kg	-	-	No measured data
Concentration in food of fish eating top-predator (marine)	0.0002	mg/kg	-	-	No measured data
Concentration in earthworm	0.0004	mg/kg	-	-	No measured data

Table 52: Local concentration relevant for secondary poisoning

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. As there are 18 sites across Europe, the local release fraction was changed to 0.056 for a total EU tonnage of 179,300 t/a.

#### 9.3 Exposure Scenario 3: Monomer for production of nitrile rubbers

#### 9.3.1 Exposure scenario

Acrylonitrile can be co-polymerised with butadiene to produce nitrile rubber, nitrile rubber latex and elastomers. Production in this sector in Western Europe in 1995 amounted to 134,000 tonnes (46,000 tonnes of acrylonitrile). Although some traditional uses for nitrile rubber are in decline these polymers are still widely used in products which are likely to come in contact with petroleum products, solvents, oil etc and in personal protective equipment.

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

Nitrile butadiene (NB) rubber is a co-polymer of acrylonitrile and butadiene. The exothermal reaction of the monomers is carried out in aqueous emulsifier solutions by means of initiators. When producing NB rubber in a continuous polymerisation process 5 steps are involved as follows:

#### 1. Latex polymerisation

The continuous production of precursor latex is done at temperatures below  $35^{\circ}$  and at a pressure of up to 10 bars in reactors installed in cascades. All chemicals required for the

#### Acrylonitrile

### SAFETY DATA SHEET

reaction (monomers, activators, emulsifier solutions and modifiers) are fed into the cascades via dosing devices. In order to preserve certain polymer properties, the polymerisation is stopped at a conversion of about 70%. The reaction heat is removed in evaporators with liquid ammonia. No waste gas arises during polymerisation since it takes place in a closed system.

#### 2. Latex degassing

The latex is continuously withdrawn from the polymerisation tank via pressurised valves; it is introduced into the degassing tanks, which operate at reduced pressure and are degassed with steam. A mixture of acrylonitrile, butadiene and steam is withdrawn during degassing and sent for recovery to the separation unit. The steam displaced from the buffer tank is also sent to the separation unit. The displacement air of the latex tanks is sent to a combustion unit.

#### 3. Monomer recovery

In the separation unit, acrylonitrile and liquid butadiene are separated in several steps from the volatile degassing mixture. The aqueous acrylonitrile is concentrated by distillation and both monomers are returned to polymerisation. The intermediate storage tanks required for the aqueous acrylonitrile release their displacement air into the separation unit. The buffer containers for recovered acrylonitrile are connected to a scrubber in which the displacement air is purified. The scrubbing water is circulated after stripping of the acrylonitrile. The waste gas from this scrubbing has a low acrylonitrile content and is emitted.

#### 4. Intermediate storage of latex

The intermediate storage with its selective latex mixing provides special product qualities or general homogenising; it guarantees continuous supplies of material to the precipitation units. Despite degassing, the latex contains residual monomers which might escape during storage (one to three days). The displacement air and the released monomer vapours are sent to a thermal combustion unit.

#### 5. Solid rubber processing

The processing steps are precipitation, washing, screw-dewatering, drying and assembly. The coagulation of the NBR latex with electrolyte solutions takes place in a closed system. Polymerisation auxiliaries and precipitation agents have to be washed from the precipitated rubber. The main water content is pressed off in screws to a large extent, and the rubber is then mechanically reduced to pellet size and dried in hot air streams to a residual moisture of less than

0.5%. The NB rubber is then pressed into bales or assembled as pellets or powder. No acrylonitrile-containing waste gas will escape during coagulation, with the exception of fugitive emissions. During drying the residual volatile acrylonitrile is stripped. This waste air is emitted

#### Acrylonitrile

### SAFETY DATA SHEET

because of the large volumes of air involved. During the washing of the coagulate, the acrylonitrile-containing waste gases are sucked off the headspace of the enclosed washing tanks and sent to a combustion unit. The efficiency of acrylonitrile combustion amounts to greater than 99%. The acrylonitrile-laden precipitation and washing waters are discharged into the sewage plant.

#### 9.3.1.2 Operational conditions related to frequency, duration and amount of use Table 53: 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	kg/d	No specific data: not required for risk assessment
Duration of exposure per day at workplace [for one worker]	8h/day	Default value
Frequency of exposure at workplace [for one worker]	220 d/y	Default value
Emission days per site	365 d/y	Assumed continuous process.

#### 9.3.1.3 Operational conditions and risk management measures related to substance characteristics Table 54: Characteristics of the substance or preparation

Information type Data field		Explanation
Physical state	Liquid	The substance is a liquid
For solids: Categorisation of dust grades	Not applicable	Not relevant: the substance is a liquid
Concentration of substance in preparation	Not applicable	Not relevant
Concentration after dilution for use (if relevant)	Not applicable	Not relevant
Risk management measures related to the design of product		Not relevant

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

For exposure scenarios covering worker uses, the following example table for reporting information is available:

Table 55: Operati	onal conditions	related to	respiration	and skin c	contact
Tuble cer operad	ondi conditions	renative to	respination	which statin c	onace

Information type	Data field	Explanation
Respiration volume under conditions of use	$10 m^{3}/d$	Default value for light-work
Room size and ventilation rate	m <sup>3</sup> ; exchange per hour	Not relevant: room size and general ventilation are not employed to control risk.
Area of skin contact with the substance under conditions of use	cm <sup>2</sup>	Not relevant. The process takes place under enclosed conditions. The substance is a skin irritant and skin sensitizer, therefore dermal exposure must be eliminated or minimised through the use of RMMs.
Body weight	65 kg	Default for workers

#### 9.3.1.5 Other operational conditions of use

Releases to air, water and waste before risk management.

#### Table 56: 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,	0.05 kg/kg	Default value for ERC 6C
Fraction of applied amount lost from process/use to waste water	0.05 kg/kg	Default value for ERC 6C
Fraction of applied amount lost from process/use to waste	0.1 kg/kg	Total loss to waste water and gas based on default values for ERC 6C
Fraction consumed in process/use	0.9 kg/kg	The substance is chemically transformed during the polymerisation reaction
Fraction of applied amount leaving the site with products	0 kg/kg	The substance is chemically transformed during the polymerisation reaction; products only contain trace amounts of unreacted monomer

#### 9.3.1.6 Risk management measures

#### Table 57: Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilat	ion	
Containment plus good work practice required	Effectiveness in terms of residual exposure	The process is largely enclosed, with limited potential for worker exposure.
Local exhaust ventilation required plus good work practise	Effectiveness in terms of reduction factor against situation without LEV or residual exposure	LEV is required for processes that are not totally enclosed
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness	Protective gloves and face-shield are routinely worn to prevent accidental contact with the substance.
		RPE used unless a fully enclosed system is used
Other risk management measures related	ed to workers	
		Workers received specific training and instruction in order to ensure minimal contact with the substance.
		Airborne concentrations of acrylonitrile are routinely monitored to ensure compliance with occupational exposure standards.
Risk management measures related to	environmental emissions from in	dustrial sites
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	0.00044 kg/kg	5% default release for ERC 6C taking into account the rate of degradation at 85%.
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Air emissions are limited through the use of scrubbers or the combustion of waste gases with efficiency of >99%.
Resulting fraction of applied amount in waste gas released to environment	0.0005 kg/kg	5% default release for ERC 6C; treatment by combustion or scrubbers with >99% efficiency
Onsite waste treatment	Effectiveness (fraction after on-site treatment compared to the fraction entered into waste treatment.	
Fraction of initially applied amount sent to external waste treatment. This is the sum of direct losses from processes to waste, and the	0.000044 kg/kg	Release to water after STP.

Information type	Data field	Explanation
residues from onsite waste water and waste gas treatment.	0.0495 kg/kg	Scrubber residues may be treated on site, sent to external waste treatment or recycled. Value represents the proportion (99%) of particulate substance (5% default assumption for loss to waste gas) removed by scrubber systems.
Municipal or other type of external waste water treatment	Effectiveness of substance removal [fraction of substance in treated waste water compared to entering the waste water treatment plant]	No further STP performed.
Effluent (of the waste water treatment plant) discharge rate	$2000 \text{ m}^{3}/\text{d}$	Default: 2.000 m <sup>3</sup> /d
Recovery of sludge for agriculture or horticulture	No	Sludge from plants handling acrylonitrile is not recovered for use in agriculture or horticulture

#### 9.3.1.7 Waste related measures

The following example table for reporting information is available.

#### Table 58: Fractions of substance in waste and waste management measures

Information type	Data field	Explanation
Amount of substances in waste resulting from service life of articles	0 kg/y	The substance is chemically transformed during the polymerisation reaction; products only contain trace amounts of unreacted monomer
Type of waste, suitable waste codes	-	Not applicable
Type of external treatment aiming at recycling or recovery of substances	-	Not applicable
Fraction of the initially applied amount of substance recovered.	0 kg/kg	Not applicable
Type of external treatment aiming at final disposal of the waste	-	Not applicable
Fraction of substance released into the environment via air from waste handling	0 kg/kg	Not applicable
Fraction of substance released into the environment via waste water from waste handling	0 kg/kg	Not applicable
Fraction of substance disposed of as secondary waste	0 kg/kg	Not applicable: primary waste only

#### 9.3.2 Exposure estimation

#### 9.3.2.1 Workers exposure

#### 9.3.2.1.1 Acute/Short term exposure

The exposure estimates were generated using the ECETOC TRA exposure model. The RMM efficiency used in the model were based on ECETOC (2009) so the estimate obtained represents a full shift and the 90<sup>th</sup>percentile of the exposure distribution. Acute worst-case values for inhalation can be derived from full shift values by using a multiplication factor which is detailed in Table R.14-3 of Guidance document R.14: Occupational exposure estimation. It is recommended to multiply a full shift ECETOC estimate by a factor of 2 to obtain the related short-term inhalation exposure distribution. These results are shown in the table below.

Routes of exposure	PROC	Estimated E Concentration		Measured exposure concentrations		Explanation / source of measured data
		value	unit	Value	unit	of measured data
	PROC 1	0.343	mg/kg bw/d	-	-	
	PROC 2	0.137	mg/kg bw/d	-	-	
Dermal exposure	PROC 3	0.0343	mg/kg bw/d	-	-	No measured data
	PROC 8b	0.686	mg/kg bw/d	-	-	_
	PROC 9	0.686	mg/kg bw/d	-	-	
	PROC 1	[0.1376] (without LEV and RP)	mg/m <sup>3</sup>			
Inhalation exposure	PROC 2	[0.688]	mg/m <sup>3</sup>		-	No measured data
	PROC 3	[1.72]	mg/m <sup>3</sup>			
	PROC 8b	[1.032]	mg/m <sup>3</sup>			
	PROC 9	[3.44]	mg/m <sup>3</sup>			

Table 59: Acute exposure concentrations to workers

\*all values generated with RP and LEV unless otherwise stated

[Acute inhalation values estimated from the modelled TWA values, applying a factor of 2]

The production of nitrile rubber occurs in a closed system with full containment at a temperature of 35 °C. The main route of potential occupational exposure to acrylonitrile is by inhalation of the vapour of this volatile substance. However, due to the closed nature of the production system, both dermal and inhalation exposure is therefore minimal. Exposure could occur during the sampling activities. In this case, suitable local ventilation extraction or respiratory protection is used to minimise inhalation exposure. Appropriate PPE (gloves, overcoat, safety goggles) are also used in order to minimise dermal exposure. As there are no measured values available, the estimated values will be used in the risk assessment.

#### Table 60: Summary of acute exposure concentrations to workers

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data. Estimated values used.
Inhalation exposure (in mg/m <sup>3</sup> )	3.44	No measured value. Estimated values will therefore be used in the risk assessment.

#### 9.3.2.1.2 Long-term exposure

#### Table 61: Long-term exposure concentrations to workers

Routes of exposure	PROC	Estimated Exposure Concentrations		Measured e		Explanation / source
		value	unit	Value	unit	of measured data
	PROC 1	0.343	mg/kg bw/d	-	-	
	PROC 2	0.137	mg/kg bw/d	-	-	
Dermal exposure	PROC 3	0.0343	mg/kg bw/d	-	-	No measured data
	PROC 8b	0.686	mg/kg bw/d	-	-	
	PROC 9	0.686	mg/kg bw/d	-	-	
	PROC 1	0.0688 (without LEV and RP)	mg/m <sup>3</sup>			
	PROC 2	0.344	mg/m <sup>3</sup>			
Inhalation exposure	PROC 3	0.860	mg/m <sup>3</sup>		-	No measured data
	PROC 8b	0.516	mg/m <sup>3</sup>			
	PROC 9	1.72	mg/m <sup>3</sup>			

#### Table 62: Summary of long-term exposure concentration to workers

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data. Estimated values used.
Inhalation exposure (in mg/m3)	1.72	No measured value. Estimated values will therefore be used in the risk assessment.

#### 9.3.2.2 Consumer exposure

Nitrile rubber is used to manufacture a large number of articles including those which could potentially result in consumer exposure, such as protective gloves and flooring. However, unreacted acrylonitrile is

#### Acrylonitrile

### SAFETY DATA SHEET

only present in the manufactured polymer at trace amounts (if at all) and is considered to be bound within the polymer. Consumer exposure to acrylonitrile resulting from the use of nitrile rubber articles is therefore considered to be negligible and will be less than the very low exposures to residual acrylonitrile monomer calculated above for inhalation and dermal exposure to acrylic fibres and oral exposure to residual acrylonitrile monomer calculated above for oral exposure resulting from the use of ABS plastics for food packaging.

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

Indirect exposure of the general public via the environment from consumption of biota or drinking water and exposure to air containing residual acrylonitrile is theoretically possible although considered to be of low risk due to the extremely low levels calculated.

	Estimated exposure concentrations		Measured expo concentrations	sure	Explanation / source of	
	value	unit	value	unit	measured data	
Wet fish	0.0197	mg/kg	-	-	No measured data	
Drinking water	0.0139	mg/L	-	-	No measured data	
Meat	8.51 x 10 <sup>-7</sup>	mg/kg	-	-	No measured data	
Milk	8.51 x 10 <sup>-6</sup>	mg/L	-	-	No measured data	

Table 63: Concentration for oral exposure of humans via the environment

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 53,000 t/a.

#### 9.3.2.4 Environmental exposure

The environmental releases are determined primarily by tonnage and the ERC with conservative estimations and defaults being implemented. For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acrylonitrile 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 6C covers the use of acrylonitrile in theproduction of nitrile rubbers. In initial assessments for this use the 53,000 tpa has been quoted as the maximum tonnage used in the EU over several sites.

It is proposed that the use of ERC 6c to estimate emissions to the environment will result in an unrealistic assessment for acrylonitrile. This is because the default emissions fractions in ERC 6c represent a worst case and does not take into account the efficiency of the waste water treatment or atmospheric scrubber systems used. Release of Acrylonitrile to the environment is strictly controlled by local and national pollution control. Specific process technology is required to limit and control release at each site. An average efficiency for all sites is not known. Based on the conservative standard risk

assessment model, the maximum release to waste water before processing must not exceed 7.9 kg/d in a standard waste water treatment plant limited to 2000 m3per day. This is equivalent to a sewage influent of 3.5 mg/L. The table below shows the parameters entered into the EUSES model:

#### Table 64: Input Parameters [ES3]

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	53.06	g/mol	-
Vapour Pressure	11500	Ра	-
Water Solubility	73000	mg/L	-
Octanol/water partition coefficient	0.25	logKow	-
Biodegradability	Ready biodegradable	-	-
Life Cycle Step	Use	-	-
Tonnage	53000	Tonnes	-
Environmental Release Class	ERC6c	-	-
Fraction of Tonnage for Region	0.01	-	
STP	On-site STP	-	
Emission events per year	300	Days	20
Release to Air	0.05 (takes into account 99% efficiency of scrubber systems)	%	5
Release to Water	7.86 kg/d	%	5
Dilution factor applied for PEC derivation	-	-	10 (2,000 m3/d)
% fraction degraded in STP	95	%	86
% fraction released to water after STP	4.3	%	12.1
% fraction released to air after STP	0.65	%	1.83
% fraction released to sludge after STP	0.0475	%	0.133

#### 9.3.2.4.1 Environmental releases

In the table below are the estimates generated using the parameters abovefor ERC 6C using EUSES:

 Table 65: Releases to the environment generated using the ECETOC TRA exposure model

 [ES3]

Compartments ERC 6C	Predicted releases	Required release (kg/d)	Explanation / source of measured data
Aquatic (after STP)	0.0169 mg/L	7.86	No measured data.
Air (direct + STP)	$0.00246 \text{ mg/m}^3$	-	No measured data.
Soil (direct only)	0.000193 mg/kg	-	No measured data.

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration wasset to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 53,000 t/a.

#### 9.3.2.4.2 Exposure concentration in sewage treatment plants (STP)

Following the polymerisation of acrylonitrile to form nitrile rubber, the unreacted monomer is recovered and recycled to the reactor. As a result, the releases to waste water will be minimal.

Compartments	Estimated exposure concentrations				Explanation / source of measured data
	value	unit	value	unit	
Sewage (STP effluent)	0.169	mg/L	-	-	
Sewage sludge	4.73	mg/kg	-	-	

Table 66: Concentrations in sewage using the EUSES exposure model

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 53,000 t/a.

The following values will be used for the risk assessment and risk characterisation in Section 10.3:

Table 67: Predicted Exposure Concentrations (PEC) in sewage

	Value	Justification
Concentration in sewage (PECstp)(in mg/l)	0.169	Worst case modelled sewage effluent concentration.
Concentration in sewage sludge (in mg/kg d.w.)	4.73	Estimated value. No measured data available.

#### 9.3.2.4.3 Exposure concentration in aquatic pelagic compartment

Following polymerisation, the unreacted monomer is recovered and recycled to the reactor. As a result, the release to waste water is minimal. Furthermore, a large number of sites have dedicated wastewater treatment plants which degrade (>95%) any of the acrylonitrile monomer remaining. The risk management measures can be implemented into EUSES to obtain an accurate prediction.

Table 68: Local concentrations in water based on measured data

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Freshwater	0.0169	mg/L	-		No measured data
Marine water	0.00169	mg/L	-		No measured data
Intermittent releases to water	NA		-		No measured data

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded of 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 53,000 t/a.

The following value will be used for the risk assessment and risk characterisation in Section 10.3:

Table 69: Predicted Exposure Concentrations (PEC) in aquatic compartment

Compartments	Local concentration	PEC aquatic (local+regional)	Justification
Freshwater (in mg/l)	0.0169	0.0169	Worst case predicted freshwater concentration. No measured data.
Marine water (in mg/l)	0.00169	0.00169	Default dilution of 10.
Intermittent releases to water (in mg/l)	NA		

#### 9.3.2.4.4 Exposure concentration in sediments

The use of ERC 6c default (worst case) values to estimate environmental emissions of acrylonitrile for this exposure scenariois considered to be unrealistic. Following polymerisation, the unreacted monomer is recovered and recycled to the reactor. In addition, any remaining monomer is degraded by >95% in the on-site STP. Exposure to sediment is therefore minimal.

Table	70:	Local	concentrations	in	sediment	[EUSES]
-------	-----	-------	----------------	----	----------	---------

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Freshwater sediments	0.0185	mg/kg	-	-	No measured data are available
Marine water sediments	0.00184	mg/kg	-	-	No measured data are available

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 53,000 t/a.

The following values willbe used for the risk assessment and risk characterisation in Section 10.3:

Table 71: Predicted Exposure Concentrations (PEC) in sediment

Compartments	PEC sediment (local+regional)	Justification
Freshwater sediments (in mg/kg d.w)	0.0185	Worst case predicted value.
Marine water sediments (in mg/kg d.w.)	0.00184	Assumed 10-fold reduction factor based on freshwater

#### 9.3.2.4.5 Exposure concentrations in soil and groundwater

Acrylonitrile can potentially be deposited onto/into the soil from the atmosphere and aqueous compartments. Information from industry indicates that sludge from acrylonitrile is not spread onto land. The sewage is normally incinerated with other wastes. Therefore the only potential route of exposure to soil is (indirect) via the atmosphere. The predicted exposure concentration for soil was calculated using the EUSES exposure model. The results are given in the table below:

Table 72: Local concentrations in soil	Table	72:	Local	concentrations	in	soil
--	-------	-----	-------	----------------	----	------

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Agricultural soil averaged	1.93 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data
Grassland averaged	2.6 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data
Groundwater	5.26 x 10 <sup>-4</sup>	mg/L	_	-	No measured data

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of

### Acrylonitrile

### SAFETY DATA SHEET

#### 53,000 t/a.

The following values will be used for the risk assessment and risk characterisation in Section 10.3:

	Local concentration	PEC soil/groundwater (local+regional)	Justification
Agricultural soil averaged (mg/kg ww)	1.93 x 10 <sup>-4</sup>	1.93 x 10 <sup>-4</sup>	
Grassland averaged (mg/kg ww)	2.6 x 10 <sup>-4</sup>	2.6 x 10 <sup>-4</sup>	Estimated values. No measured values available.
Groundwater(mg/l)	-	5.26 x 10 <sup>-4</sup>	

Table 73: Predicted Exposure Concentrations (PEC) in soil and groundwater

#### 9.3.2.4.6 Atmospheric compartment

Acrylonitrile is volatile and therefore the atmospheric compartment is the major compartment of distribution of acrylonitrile. Releases are reduced by the combustion and scrubbing of gaseous waste before discharging to the atmosphere. The predicted exposure concentration (PEC) in air has been estimated using EUSES exposure model to gain an accurate approximation.

Table 74: Local concentra	tions in	air
---------------------------	----------	-----

	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	uata
During emission	0.00246	mg/m <sup>3</sup>	-	-	No measured data
annual average	0.00202	mg/m <sup>3</sup>	-	-	No measured data
Annual total deposition	0.00292	mg/m <sup>2</sup> /d	-	-	No measured data

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe isnot known so the local release fraction was changed to 0.1 for a total EU tonnage of 53,000 t/a.

The following values will be used for the risk assessment and risk characterisation in Section 10.3:

#### Table 75: Predicted Exposure Concentration (PEC) in air

	Local concentration	PEC air (local+regional)	Justification
During emission (mg/m <sup>3</sup> )	0.00246	-	Worst case estimated concentration.
annual average (mg/m <sup>3</sup> )	0.00202	0.00202	Worst case calculated concentration.
Annual deposition (mg/m <sup>2</sup> /d)	0.00292	-	Worst case calculated emission.

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

Exposure of aquatic species to acrylonitrile in the aquatic environment is possible, however levels will be low due to the limited emissions and the treatment of waste water containing acrylonitrile prior to release.

	Predicted exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Concentration in food of fish eating predator	9.86 x $10^{-3}$ (freshwater) 9.85 x $10^{-3}$ (marine water)	mg/kg	-	-	No measured data	
Concentration in food of fish eating top-predator (marine)	0.0002	mg/kg	-	-	No measured data	
Concentration in earthworm	2.14 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data	

Table 76: Local concentration relevant for secondary poisoning

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 53,000 t/a.

## 9.4 Exposure scenario 4: Intermediate for the manufacture of bulk chemicals, materials and resins.

#### 9.4.1 Exposure estimation

#### 9.4.1.1 Description of activities and processes covered in the exposure scenario

Acrylonitrile can be used as an industrial intermediate: for example the substance is dimerised to make adiponitrile which is used in the synthesis of certain Nylons. Acrylonitrile is also used as a precursor in the industrial manufacture of acrylamide and acrylic acid. Acrylamide is produced from acrylonitrileby a catalytic hydration process in solution in which unreacted acrylonitrile is recovered and recycled.

#### 9.4.1.2 Operational conditions related to frequency, duration and amount of use Table 77: 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	kg/d	No specific data are available: not required for risk assessment
Duration of exposure per day at workplace [for one worker]	8h/day	Default value

Information type	Data field	Explanation
Frequency of exposure at workplace [for one worker]	220 d/y	Default value
Emission days per site	365 d/y	Assumed continuous process.

#### 9.4.1.3 Operational conditions and risk management measures related to substance characteristics

For substances used on their own or in preparation, the following example table for reporting information is available:

Table 78: Characteristics of the substance or preparation

Information type	Data field	Explanation
Physical state	Liquid	The substance is a liquid
For solids: Categorisation of dust grades	Not applicable	Not relevant: the substance is a liquid
Concentration of substance in preparation	Not applicable	The substance is not used in a preparation
Concentration after dilution for use (if relevant)	Not applicable	Not relevant: the substance is not used in a preparation
Risk management measures related to the design of product		Not applicable

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

Table 79: 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
Room size and ventilation rate	m <sup>3</sup> ; exchange per hour	Not relevant: room size and general ventilation are not employed to control risk
Area of skin contact with the substance under conditions of use	cm <sup>2</sup>	Not applicable. The process operates under largely enclosed conditions with little potential for dermal exposure. Any activities potentially resulting in dermal exposure will be performed using appropriate RMMs to eliminate or minimise dermal exposure to this irritant and sensitising substance.
Body weight	65 kg	Default for workers

#### 9.4.1.5 Other operational conditions of use

Releases to air, water and waste before risk management:

#### Table 80: 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,	0.05 kg/kg	Default value for ERC6C (worst environmental releases from the following environmental release categories: ERC 6A, 6C and 6D). Will be lower as unreacted acrylonitrile monomer is recovered and recycled.
Fraction of applied amount lost from process/use to waste water	0.05 kg/kg	Default value for ERC6C (worst environmental releases from the following environmental release categories: ERC 6A, 6C and 6D). Will be lower as unreacted acrylonitrile monomer is recovered and recycled.
Fraction of applied amount lost from process/use to waste	0.1 kg/kg	Total loss.
Fraction consumed in process/use	0.9 kg/kg	The substance is consumed (chemically transformed) during the production process. This will be higher as unreacted acrylonitrile monomer is recovered and recycled.
Fraction of applied amount leaving the site with products	0 kg/kg	The substance is consumed (chemically transformed) during the production process.

#### 9.4.1.6 Risk management measures

#### Table 81: 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	The process is largely contained. For activities not involving containment, LEV or RP are used.			
Local exhaust ventilation required plus good work practise	Effectiveness in terms of reduction factor against situation without LEV or residual exposure	LEV or RP are used for those activities not involving containment.			
Personal protective equipment (PPE)					
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness	Protective gloves and a face-shield are routinely used to prevent accidental contact with the substance.			
,		RP is used for activities not involving containment.			
Other risk management measures related	ed to workers				
		Workers received specific training and instruction in order to ensure minimal contact with the substance.			

Information type	Data field	Explanation
		Airborne concentrations of acrylonitrile are routinely monitored to ensure compliance with occupational exposure standards.
Risk management measures related to	environmental emissions from in	dustrial sites
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	There is limited release of waste water as residual acrylonitrile monomer is recovered and recycled into the process. Waste water is treated typical effectiveness 99%.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	0.000017 kg/kg	Assumes default release of 5% and 95% breakdown in on-site STP.
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Air emissions are minimised though the recovery and recycling of acrylonitrile monomer into the process. Waste air is treated using scrubbers or combustion with >99% efficiency.
Resulting fraction of applied amount in waste gas released to environment	0.0005 kg/kg	Assumes default release of 5% and 99% efficiency of scrubbers
Onsite waste treatment	Effectiveness (fraction after on-site treatment compared to the fraction entered into waste treatment.	Not applicable
Fraction of initially applied amount sent to external waste treatment. This is the sum of direct losses from processes to waste, and the residues from onsite waste water and	0.000017 kg/kg 0.0495	Release to water Scrubber residues sent for on-site treatment or recycling.
waste gas treatment. Municipal or other type of external waste water treatment	Effectiveness of substance removal [fraction of substance in treated waste water compared to entering the waste water treatment plant]	Emissions to municipal STP will be further degraded (95%).
Effluent (of the waste water treatment plant) discharge rate	2000 m <sup>3</sup> /d	Default: 2.000 m <sup>3</sup> /d
Recovery of sludge for agriculture or horticulture	No	Sewage sludge from acrylonitrile processing plants is not recovered for agriculture or horticulture.

#### 9.4.1.7 Waste related measures

The following example table for reporting information is available.

#### Table 82: Fractions of substance in waste and waste management measures

Information type	Data field	Explanation
Amount of substances in waste resulting from identified uses covered in the exposure scenario	0 kg/y	Not applicable: intermediate use
Amount of substances in waste resulting from service life of articles	0 kg/y	Not applicable: intermediate use
Type of waste, suitable waste codes	-	Not applicable
Type of external treatment aiming at recycling or recovery of substances	-	Not applicable
Fraction of the initially applied amount of substance recovered.	0 kg/kg	Not applicable
Type of external treatment aiming at final disposal of the waste	-	Not applicable
Fraction of substance released into the environment via air from waste handling	0 kg/kg	Not applicable
Fraction of substance released into the environment via waste water from waste handling	0 kg/kg	Not applicable
Fraction of substance disposed of as secondary waste	0 kg/kg	Not applicable: primary waste only

#### 9.4.2 Exposure estimation

#### 9.4.2.1 Worker exposure

#### 9.4.2.1.1 Acute/Short term exposure

The exposure estimates were generated using the ECETOC TRA exposure model. The RMM efficiency used in the model were based on ECETOC (2009) so the estimate obtained represents a full shift and the 90<sup>th</sup>percentile of the exposure distribution. Acute worst-case values for inhalation can be derived from full shift values by using a multiplication factor which is detailed in Table R.14-3 of Guidance document R.14: Occupational exposure estimation. It is recommended to multiply a full shift ECETOC estimate by a factor of 2 to obtain the related short-term inhalation exposure distribution. These results are shown in the table below.

Routes of exposure	PROC	Estimated Exposure Concentrations		Measured exposure concentrations		Explanation / source
-		value	unit	Value	unit	of measured data
	PROC 1	0.343	mg/kg bw/d	-	-	No measured data
	PROC 2	0.137	mg/kg bw/d	-	-	
Dermal exposure	PROC 3	0.0343	mg/kg bw/d	-	-	
	PROC 8b	0.686	mg/kg bw/d	-	-	
	PROC 9	0.686	mg/kg bw/d	-	-	
		[0.1376]			-	No measured data
Inhalation exposure	PROC 1	(without LEV and RP)	mg/m <sup>3</sup>			
	PROC 2	[0.688]	mg/m <sup>3</sup>	-		
	PROC 3	[1.72]	mg/m <sup>3</sup>			
	PROC 8b	[1.032]	mg/m <sup>3</sup>			
	PROC 9	[3.44]	mg/m <sup>3</sup>			

 Table 83: Acute exposure concentrations to workers [ES4]

\*all values generated with RP and LEV unless otherwise stated in ECETOC TRA

[Acute inhalation estimates are based on the application of a factor of 2 to the modelled (TWA) value]

The production of acrylamide and adiponitrile occurs in a closed system with full containment. The main potential route of occupational exposure to acrylonitrile is by inhalation of the vapour of this volatile substance. However, due to the closed nature of the production system, both dermal and inhalation exposure is therefore minimal. Exposure may potentially occur during the sampling of the reactor. In this case, suitable local ventilation extraction or respiratory protection is used to minimise inhalation exposure. Appropriate PPE (gloves, overcoat, safety goggles) are also used in order to minimise dermal exposure. As there are no measured values available, the estimated values will be used in the risk assessment.

#### Table 84: Summary of acute exposure concentrations to workers

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data. Estimated values used.
Inhalation exposure (in mg/m3) <sup>1</sup> )	3.44	No measured value. Estimated values will therefore be used in the risk assessment.

#### 9.4.2.1.2 Long-term exposure

#### Table 85: Long-term exposure concentrations to workers

Routes of exposure PROC		Estimated E Concentration			exposure ons	Explanation / source
-		value	unit	Value	unit	of measured data
	PROC 1	0.343	mg/kg bw/d	-	-	
	PROC 2	0.137	mg/kg bw/d	-	-	
Dermal exposure	PROC 3	0.0343	mg/kg bw/d	-	-	No measured data
	PROC 8b	0.686	mg/kg bw/d			
	PROC 9	0.686	mg/kg bw/d	-	-	
Inhalation exposure	PROC 1	0.0688 (without LEV and RP)	mg/m <sup>3</sup>			
	PROC 2	0.344	mg/m <sup>3</sup>	-	-	No measured data
	PROC 3	0.860	mg/m <sup>3</sup>			
	PROC 8b	1.032	mg/m <sup>3</sup>			
	PROC 9	1.72	mg/m <sup>3</sup>			

\*all values generated with RP and LEV unless otherwise stated in ECTOC TRA.

#### Table 86: Summary of long-term exposure concentration to workers

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data. Estimated values used.
Inhalation exposure $(in mg/m^3)^{2}$	1.72	No measured value. Estimated values will therefore be used in the risk assessment.

<sup>1)</sup> during short-term exposure, air concentration at the workplace

<sup>2)</sup> during short-term exposure, air concentration at the workplace

#### 9.4.2.2 Consumer exposure

There will be no direct consumer exposure to acrylonitrile resulting from this use as an industrial intermediate.

#### 9.4.2.3 Indirect exposure of humans via the environment

Indirect exposure of the general public via the environment from consumption of biota or drinking water and exposure to air containing residual acrylonitrile is theoretically possible although considered to be of low risk due to the negligible amounts released to the environment.

	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of
	value	unit	value	unit	measured data
Wet fish	0.0197	mg/kg	-	-	No measured data
Drinking water	0.0139	mg/L	-	-	No measured data
Meat	1.23 x 10 <sup>-6</sup>	mg/kg	-	-	No measured data
Milk	1.23 x 10 <sup>-5</sup>	mg/L	-	-	No measured data

#### Table 87: Concentration for oral exposure of humans via the environment

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 136,000 t/a. The release to air was set at 0.0005 (taking into account the efficiency of the scrubbers at 99%).

#### 9.4.2.4 Environmental exposure

The environmental releases are determined primarily by tonnage and the ERC with conservative estimations and defaults being implemented. For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acrylonitrile 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 6C covers the use of acrylonitrile in the production of nitrile rubbers. In initial assessments for this use the 136,000 tpa has been quoted as the maximum tonnage used in the EU over several sites.

It is proposed that the use of ERC 6c to estimate emissions to the environment will result in an unrealistic assessment for acrylonitrile. This is because the default emissions fractions in ERC 6c represent a worst case and does not take into account the efficiency of the waste water treatment or atmospheric scrubber systems used. Release of Acrylonitrile to the environment is strictly controlled by local and national pollution control. Specific process technology is required to limit and control release at each site. An average efficiency for all sites is not known. Based on the conservative standard risk assessment model, the maximum release to waste water before processing must not exceed 7.9 kg/d in a standard waste water treatment plant limited to 2000 m3per day. This is equivalent to a sewage influent of 3.5 mg/L.The table below shows the parameters entered into the EUSES model:

### Acrylonitrile

### SAFETY DATA SHEET

#### Table 88: Input Parameters [ES4]

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	53.06	g/mol	-
Vapour Pressure	11500	Ра	-
Water Solubility	73000	mg/L	-
Octanol/water partition coefficient	0.25	logKow	-
Biodegradability	Ready biodegradable	-	-
Life Cycle Step	Use	-	-
Tonnage	136000	Tonnes	-
Environmental Release Class	ERC6c	-	-
Fraction of Tonnage for Region	0.01	-	
STP	On-site STP	-	
Emission events per year	300	Days	20
Release to Air	0.05 (takes into account 99% efficiency of scrubber systems)	%	5
Release to Water	7.86 kg/d	%	5
Dilution factor applied for PEC derivation	-	-	10 (2,000 $m^{3}/d$ )
% fraction degraded in STP	95	%	86
% fraction released to water after STP	4.3	%	12.1
% fraction released to air after STP	0.65	%	1.83
% fraction released to sludge after STP	0.0475	%	0.133

### 9.4.2.4.1 Environmental releases

### Table 89: Releases to the environment generated using EUSES exposure model [ES4]

Compartments ERC 6C	Predicted releases	Required release (kg/d)	Explanation / source of measured data
Aquatic (after STP)	0.0169 mg/L	7.86 kg/d	
Air (direct + STP)	$0.006 \text{ mg/m}^3$		
Soil (direct only)	0.000493 mg/kg	-	-

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnageof 136,000 t/a. The release to air was set at 0.0005 (taking into account the efficiency of the scrubbers at 99%).

### 9.4.2.4.2 Exposure concentration in sewage treatment plants (STP)

The use of ERC 6c default (worst case) parameters to estimate the environmental emissions of acrylonitrile is considered to be unrealistic as the assumptions do not take into account RMMs. Following polymerisation to form acrylamide or adiponitrile, the unreacted monomer is recovered and recycled to the reactor. As a result, the release to waste water is lower than predicted using the default values. The efficiency of the atmospheric scrubbers and the sewage treatment plant can be incorporated into the EUSES model to obtain an accurate prediction.

Compartments	Estimated exconcentration	mated exposure Measured exposure concentrations		sure	Explanation / source of measured data	
	value	unit	value	unit		
Sewage (STP effluent)	0.169	mg/L	-	-	No measured values	
Sewage sludge	4.73	mg/kg	-	-	No measured values	

Table 90: Concentrations in sewage using the EUSES exposure model

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration wasset to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 136,000 t/a. The release to air was setat 0.0005 (taking into account the efficiency of the scrubbers at 99%).

The following values will be used for the risk assessment and risk characterisation in Section 10.4:

### Table 91: Predicted Exposure Concentrations (PEC) in sewage

	Value	Justification
Concentration in sewage (PECstp)(in mg/l)	0.169	No measured data. Therefore estimated data will be used in risk assessment.
Concentration in sewage sludge (in mg/kg d.w.)	4.73	The majority of unreacted acrylonitrile is recovered and recycled. However, no measured data available so the estimated data will be used in the risk assessment.

### 9.4.2.4.3 Exposure concentration in aquatic pelagic compartment

Following the production of adiponitrile and acrylamide, the unreacted monomer is recovered and recycled to the reactor. As a result, the release to waste water is lower than predicted using the default releases. In addition, on-site STP causes degradation of the remaining material by 95%. Further predictions by EUSES give a more accurate estimation of the release to water.

Table 92: Local concentrations in water determined using EUSES exposure model [ES4]

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Freshwater	0.0169	mg/L	-		No measured data	
Marine water	0.00169	mg/L	-		No measured data	
Intermittent releases to water	NA		-		No measured data	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 136,000 t/a. The release to air was set at 0.0005 (taking into account the efficiency of the scrubbers at 99%).

The following values will be used for the risk assessment and risk characterisation in Section 10.4: **Table 93: Predicted Exposure Concentrations (PEC) in aquatic compartment** 

#### Local **PEC** aquatic Compartments Justification concentration (local+regional) No measured data. Estimated Freshwater (in mg/l) 0.0169 0.0169 data to be used in risk assessment. 0.00169 0.00169 Default dilution of 10. Marine water (in mg/l) Intermittent releases to water (in mg/l) NA

### 9.4.2.4.4 Exposure concentration in sediments

The use of ERC 6c default (worst case) parameters to estimate the environmental emissions of acrylonitrile is considered to be unrealistic as the assumptions do not take into account RMMs.

Following polymerisation to form acrylamide or adiponitrile, the unreacted monomer is recovered and recycled to the reactor. Further predictions by EUSES give a more accurate estimation of the exposure to sediment.

Table 94: Local concentrations in sediment by EUSES [ES4]

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data	
	value unit value unit					
Freshwater sediments	0.0185	mg/kg	-	-	No measured data are available	
Marine water sediments	0.00185	mg/kg	-	-	No measured data are available	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 136,000 t/a. The release to air was set at 0.0005 (taking into account the efficiency of the scrubbers at 99%).

The following values will be used for the risk assessment and risk characterisation in Section 10.4

 Table 95: Predicted Exposure Concentrations (PEC) in sediments

Compartments PEC sediment (local+regional)		Justification				
Freshwater sediments (in mg/kg d.w)	0.0185	No measured values available. Predicted exposure concentration in sediment.				
Marine water sediments (in mg/kg d.w.)	0.00185	Assumed 10-fold reduction factor from freshwater				

### 9.4.2.4.5 Exposure concentrations in soil and groundwater

Acrylonitrile can potentially be deposited onto/into the soil from the atmosphere and aqueous compartments. Information from industry indicates that industrial sludge from Acrylonitrile waste water processing plants is not spread onto land but is normally incinerated with other wastes. Therefore the only potential route of exposure to soil is indirectly, via the atmosphere. The results are given in the table below:

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Agricultural soil averaged	4.93 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data	
Grassland averaged	6.65 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data	
Groundwater	1.34 x 10 <sup>-3</sup>	mg/L	-	-	No measured data	

 Table 96: Local concentrations in soil [ES4]

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 136,000 t/a. The release to air was set at 0.0005 (taking into account the efficiency of the scrubbers at 99%).

The following values will be used for the risk assessment and risk characterisation in Section 10.4:

	Local concentration	PEC soil/groundwater (local+regional)	Justification
Agricultural soil averaged (mg/kg ww)	4.93 x 10 <sup>-4</sup>	4.93 x 10 <sup>-4</sup>	Estimated values represents worst case out
Grassland averaged (mg/kg ww)	6.65 x 10 <sup>-4</sup>	6.65 x 10 <sup>-4</sup>	of all the sites producing adiponitrile and acrylamide
Groundwater(mg/l)	-	1.34 x 10 <sup>-3</sup>	

Table 97: Predicted Exposure Concentrations (PEC) in soil and groundwater

### 9.4.2.4.6 Atmospheric compartment

Acrylonitrile is volatile and therefore the atmospheric compartment is the major potential compartment of distribution of acrylonitrile. Releases are reduced by the combustion or scrubbing of gaseous and volatile waste before discharging to the atmosphere. The predicted exposure concentration (PEC) in air has been estimated using EUSES exposure model to gain an accurate approximation.

 Table 98: Local concentrations in air [ES4]

	Estimated exposure concentrations		Measured exposure concentrat		Explanation / source of measured	
	value	unit	value	unit	data	
During emission	6.3 x 10 <sup>-3</sup>	mg/m <sup>3</sup>	-	-	No measured data	
annual average	5.18 x 10 <sup>-3</sup>	mg/m <sup>3</sup>	-	-	No measured data	
Annual total deposition	7.47 x 10 <sup>-3</sup>	mg/m <sup>2</sup> /d	-	-	No measured data	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded of 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 136,000 t/a. The release to air was set at 0.0005 (taking into account the efficiency of the scrubbers at 99%).

	Local concentration	PEC air (local+regional)	Justification
During emission (mg/m <sup>2</sup> )	6.3 x 10 <sup>-3</sup>	-	Worst case calculated concentration.
annual average (mg/m <sup>2</sup> )	5.18 x 10 <sup>-3</sup>	5.18 x 10 <sup>-3</sup>	Worst case calculated concentration.
Annual deposition (mg/m <sup>2</sup> /d)	7.47 x 10 <sup>-3</sup>	-	Worst case calculated concentration .

### Table 99: Predicted Exposure Concentration (PEC) in air [ES4]

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

Exposure of aquatic species to low levels of acrylonitrile in the aquatic environment is possible. The predicted concentrations relevant for the food chain have been generated using the EUSES exposure model using the measured data for water and atmospheric releases.

Table	100:	Local	concentration	relevant	for	secondary	poisoning	
-------	------	-------	---------------	----------	-----	-----------	-----------	--

	Predicted exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value unit			
Concentration in food of fish eating predator	9.86 x 10 <sup>-3</sup> (freshwater) 9.85 x 10 <sup>-4</sup> (marine water)	mg/kg	-	-	No measured data	
Concentration in food of fish eating top-predator (marine)	0.0002	mg/kg	-	-	No measured data	
Concentration in earthworm	5.45 x 10 <sup>-3</sup>	mg/kg	-	-	No measured data	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is not known so the local release fraction was changed to 0.1 for a total EU tonnage of 136,000 t/a. The release to air was set at 0.0005 (taking into account the efficiency of the scrubbers at 99%).

### 9.5 Exposure Scenario 5: Laboratory Reagent

### 9.5.1 Exposure estimation

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

Acrylonitrile can be routinely analysed in laboratories producing or using acrylonitrile. Alternatively, it could be used ineducational institutes in research.

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

### Table 101: 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	kg/d	No specific data are available: not required for risk assessment
Duration of exposure per day at workplace [for one worker]	8h/day	Default value
Frequency of exposure at workplace [for one worker]	220 d/y	Default value
Emission days per site	365 d/y	Assumed continuous process.

### 9.5.1.3 Operational conditions and risk management measures related to substance characteristics

For substances used on their own or in preparation, the following example table for reporting information is available:

Table 102: Characteristics of the substance or p	preparation
--	-------------

Information type	Data field	Explanation		
Physical state	Liquid	The substance is a liquid		
For solids: Categorisation of dust grades	Not applicable	Not relevant: the substance is a liquid		
Concentration of substance in preparation	Not applicable	The substance is not used in a preparation		
Concentration after dilution for use (if relevant)	Not applicable	Not relevant: the substance is not used in a preparation		
Risk management measures related to the design of product		Not applicable		

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

Information type	Data field	Explanation		
Respiration volume under conditions of use	$10 m^{3}/d$	Default for light-work		
Room size and ventilation rate	m3 ; exchange per hour	Not relevant: room size and general ventilation are not employed to control risk		
Area of skin contact with the substance under conditions of use	cm <sup>2</sup>	Not applicable. The process operates under largely enclosed conditions with little potential for dermal exposure. Any activities potentially resulting in dermal exposure will be performed using appropriate RMMs to eliminate or minimise dermal exposure to this irritant and sensitising substance.		
Body weight	65 kg	Default for workers		

### 9.5.1.5 Other operational conditions of use

Releases to air, water and waste before risk management:

# Table 104: 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,	0.05 kg/kg	Default value for ERC6a. Will be lower as unreacted acrylonitrile monomer is recovered and recycled.		
Fraction of applied amount lost from process/use to waste water	0.02 kg/kg	Default value for ERC6a. Will be lower as unreacted acrylonitrile monomer is recovered and recycled.		
Fraction of applied amount lost from process/use to waste	0.1 kg/kg	Default values for ERC6a (waste water and waste gas). Will be lower as unreacted acrylonitrile monomer is recovered and recycled.		
Fraction consumed in process/use	0.93 kg/kg	The substance is consumed (chemically transformed) during the production process. This will be higher as unreacted acrylonitrile monomer is recovered and recycled.		
Fraction of applied amount leaving the site with products	0 kg/kg	The substance is consumed (chemically transformed) during the production process.		

### 5.1.6 Risk management measures

### Table 105: Risk management measures for industrial site

Information type Data field		Explanation		
Containment and local exhaust ventilat	ion			
Containment plus good work practice required	Effectiveness in terms of residual exposure	The process is largely contained. For activities not involving containment, LEV or RP are used.		
Local exhaust ventilation required plus good work practise	Effectiveness in terms of reduction factor against situation without LEV or residual exposure	LEV or RP are used for those activities not involving containment.		
Personal protective equipment (PPE)	-			
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness	Protective gloves and a face-shield are routinely used to prevent accidental contact with the substance.		
		RP is used for activities not involving containment.		
Other risk management measures relat	ed to workers			
		Workers received specific training and instruction in order to ensure minimal contact with the substance.		
		Airborne concentrations of acrylonitrile are routinely monitored to ensure compliance with occupational exposure standards.		
Risk management measures related to	environmental emissions from in	dustrial sites		
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	There is limited release of waste water as all acrylonitrile is consumed during analysis. In addition, any waste produced is sent for special waste disposal. There are no releases into the environment.		
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	0 kg/kg	No releases to the environment. All waste is sent in containers for special waste disposal.		
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Air emissions are minimised though the recovery and recycling of acrylonitrile monomer into the process, waste air is treated using scrubbers or combustion with >99% efficiency.		
Resulting fraction of applied amount in waste gas released to environment	0.0005 kg/kg	Assumes default release of 5% and 99% efficiency of scrubbers		
Onsite waste treatment	Effectiveness (fraction after on-site treatment compared to the fraction entered into waste treatment.			

Information type	Data field	Explanation
Fraction of initially applied amount sent to external waste treatment. This is the sum of direct losses	0 kg/kg	No releases to the environment. All waste is sent in containers for special waste disposal.
from processes to waste, and the residues from onsite waste water and waste gas treatment.	0.0495 kg/kg	Scrubber residues sent for special waste disposal.
Municipal or other type of external waste water treatment	Effectiveness of substance removal [fraction of substance in treated waste water compared to entering the waste water treatment plant]	Not relevant.
Effluent (of the waste water treatment plant) discharge rate	$2000 m^{3}/d$	Default: 2.000 m3/d
Recovery of sludge for agriculture or horticulture	No	Sewage sludge from acrylonitrile processing plants is not recovered for agriculture or horticulture.

### 9.5.1.7 Waste related measures

The following example table for reporting information is available.

### Table 106: Fractions of substance in waste and waste management measures

Information type	Data field	Explanation
Amount of substances in waste resulting from service life of articles	0 kg/y	Not applicable: intermediate use
Type of waste, suitable waste codes	-	Not applicable
Type of external treatment aiming at recycling or recovery of substances	-	Not applicable
Fraction of the initially applied amount of substance recovered.	0 kg/kg	Not applicable
Type of external treatment aiming at final disposal of the waste	-	Not applicable
Fraction of substance released into the environment via air from waste handling	0 kg/kg	Not applicable
Fraction of substance released into the environment via waste water from waste handling	0 kg/kg	Not applicable
Fraction of substance disposed of as secondary waste	0 kg/kg	Not applicable: primary waste only

### 9.5.2 Exposure estimation

### 9.5.2.1 Worker exposure

### 9.5.2.1.1 Acute/Short term exposure

The exposure estimates were generated using the ECETOC TRA exposure model. The RMM efficiency used in the model were based on ECETOC (2009) so the estimate obtained represents a full shift and the 90thpercentile of the exposure distribution. Acute worst-case values can be derived from full shift values by using a multiplication factor which is detailed in Table R.14-3 of Guidance document R.14: Occupational exposure estimation. It is recommended to multiply a full shift ECETOC TRA estimate by a factor of 2 to obtain the related short-term exposure distribution. The acute exposure estimates has been derived for all activities which involve short-term exposure to hydrogen fluoride. These results are shown in the table below.

Routes of exposure	PROC	Estimated E Concentration		Measured exposure concentrations		Explanation / source	
-		value	unit	Value	unit	of measured data	
Dermal exposure	PROC 15	0.0343	mg/kg bw/d	-	-	No measured data	
Inhalation exposure	PROC 15	0.688	mg/m <sup>3</sup>	-	-	No measured data	

 Table 107: Acute exposure concentrations to workers [ES5]

all values generated with RP and LEV unless otherwise stated.

Suitable local ventilation extraction and respiratory protection is used to minimise inhalation exposure. Appropriate PPE (gloves, overcoat, safety goggles) are also used in order to minimisedermal exposure. As there are no measured values available, the estimated values will be used in the risk assessment.

Table 108: Summary of acute exposure concentrations to workers

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.0343	No measured dermal data. Estimated values used.
Inhalation exposure $(in mg/m^3)^{3)}$	0.688	No measured value. Estimated values will therefore be used in the risk assessment.

<sup>3)</sup> during short-term exposure, air concentration at the workplace

### 9.5.2.1.2 Long-term exposure

Routes of exposure					Explanation / source	
-		value	unit	Value	unit	of measured data
Dermal exposure	PROC 15	0.0343	mg/kg bw/d	-	-	No measured data
Inhalation exposure	PROC 15	0.344	mg/m <sup>3</sup>	-	-	No measured data

Table 109: Long-term exposure concentrations to workers

all values generated with RP and LEV unless otherwise stated in ECETOC TRA.

Table 110: Summary of long-term exposure concentration to workers

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.0343	No measured dermal data. Estimated values used.
Inhalation exposure $(in mg/m^3)^{4)}$	0.344	No measured value. Estimated values will therefore be used in the risk assessment.

### 9.5.2.2 Consumer exposure

There will be no direct consumer exposure to acrylonitrile resulting from its use in the laboratory.

### 9.5.2.3 Indirect exposure of humans via the environment

Indirect exposure of the general public via the environment from consumption of biota or drinking water and exposure to air containing residual acrylonitrile is theoretically possible although considered to be of low risk due to the negligible amounts released to the environment.

Table 111: Concentration for oral exposure of humans via the environment

	Estimated expo concentrations	osure	Measured expo concentrations	sure	Explanation / source of
	value	unit	value	unit	measured data
Wet fish	5.21 x 10 <sup>-5</sup>	mg/kg	-	-	No measured data
Drinking water	3.69 x 10 <sup>-5</sup>	mg/L	-	-	No measured data
Meat	1.9 x 10 <sup>-9</sup>	mg/kg	-	-	No measured data
Milk	1.9 x 10 <sup>-8</sup>	mg/L	-	-	No measured data

\*generated in EUSES using the default releases of ERC 6a taking into account the use of scrubbers and WWTP: emission to air=0.0005 and emission to water=0.0. As there is no direct application of sewage sludge to the ground the concentration of sewage sludge was changed to 0 mg/kg. The tonnage was set at 1 ton/year and the local fraction to 0.1 to represent many laboratory sites throughout Europe.

### 9.5.2.4 Environmental exposure

The environmental releases are determined primarily by tonnage and the ERC in the first tier with

<sup>4)</sup> during short-term exposure, air concentration at the workplace

### Acrylonitrile

## SAFETY DATA SHEET

conservative estimations and defaults being implemented.

For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acrylonitrile 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 6a covers the use of acrylonitrile in the laboratory. In initial assessments for production the 10% rule has been employed as the figure of 1 tpa has been quoted as the maximum tonnage used in many laboratories in the EU.

It is proposed that the use of ERC 6a to estimate emissions to the environment will result in an unrealistic assessment for acrylonitrile. The Acrylonitrile used within laboratory processes will not be released to waste water but collected from the laboratory system and reacted as an intermediate before disposal. Therefore no release of Acrylonitrile to waste water from laboratory occurs as all waste is sent for special waste disposal.

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	53.06	g/mol	-
Vapour Pressure	11500	Pa	-
Water Solubility	73000	mg/L	-
Octanol/water partition coefficient	0.25	logKow	-
Biodegradability	Ready biodegradable	-	-
Life Cycle Step	Use	-	-
Tonnage	1	Tonnes	-
Environmental Release Class	ERC6a	-	-
Fraction of Tonnage for Region	0.01	-	
STP	On-site STP	-	
Emission events per year	300	Days	20
Release to Air	0.05 (takes into account 99% efficiency of scrubber systems)	%	5
Release to Water	0 (all sent to special waste)	%	5
Dilution factor applied for PEC derivation	-	-	10 (2,000 m3/d)
% fraction degraded in STP	95	%	86
% fraction released to water after STP	4.3	%	12.1
% fraction released to air after STP	0.65	%	1.83
% fraction released to sludge after STP	0.0475	%	0.133

### Table 112: Input Parameters [ES5]

### 9.5.2.4.1 Environmental releases

The use of the defaults for ERC 6a to estimate emissions to the environment will result in an unrealistic assessment for acrylonitrile. The Acrylonitrile used within laboratory processes will not be released to waste water but collected from the laboratory system and reacted as an intermediate before disposal. Therefore no release of Acrylonitrile to waste water from laboratory occurs as all waste is sent for special waste disposal.

Table 113: Releases	to th	ne environment	generated	using	the	EUSES	exposure	model	[ES5]	L
---------------------	-------	----------------	-----------	-------	-----	-------	----------	-------	-------	---

Compartments ERC 6a	Predicted releases (mg/L)	Measured release (t/y)	Explanation / source of measured data
Aquatic (after STP)	0	-	No measured releases
Air (direct + STP)	6.95 x 10 <sup>-7</sup>	-	No measured releases
Soil (direct only)	3.6 x 10 <sup>-9</sup>	-	No measured releases

\*generated in EUSES using the default releases of ERC 6a taking into account the use of scrubbers and WWTP: emission to air=0.0005 and emission to water=0. As there is no direct application of sewage sludge tothe ground the concentration of sewage sludge was changed to 0 mg/kg. The tonnage was set at 1 ton/year and the local fraction to 0.1 to represent many laboratory sites throughout Europe.

### 9.5.2.4.2 Exposure concentration in sewage treatment plants (STP)

The use of ERC 6a default (worst case) parameters to estimate the environmental emissions of acrylonitrile is considered to be unrealistic. The Acrylonitrile used within laboratory processes will not be released to waste water but collected from the laboratory system and reacted as an intermediate before disposal. Therefore no release of Acrylonitrile to waste water from laboratory use occurs, as all waste is sent for special waste disposal. There is no treatment via STP.

The following values will be used for the risk assessment and risk characterisation in Section 10.4:

Table 114: Predicted Exposure Concentrations (PEC) in sewage

	Value	Justification
Concentration in sewage (PECstp)(in mg/l)	0	No release to water. All waste is collected and disposed of via special waste.
Concentration in sewage sludge (in mg/kg d.w.)	0	No release to water. All waste is collected and disposed of via special waste.

### 9.5.2.4.3 Exposure concentration in aquatic pelagic compartment

In the laboratory the majority of acrylonitrile is consumed in the analytical process or collected and reacted before specialist waste collection and disposal. As a result, there is minimal acrylonitrile waste which is collected and disposed ofvia special waste. There is norelease to waste water.

### Table 115: Local concentrations in water determined using measured data [ES5]

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Freshwater	0	mg/L	-		No measured data
Marine water	0	mg/L	-		No measured data
Intermittent releases to water	NA		-		No measured data

### Table 116: Predicted Exposure Concentrations (PEC) in aquatic compartment

Compartments	Local concentration	PEC aquatic (local+regional)	Justification		
Freshwater (in mg/l)	0	3.69 x 10 <sup>-5</sup>	PEC for regional contributions.		
Marine water (in mg/l)	0	3.02 x 10 <sup>-6</sup>	Default dilution of 10.		
Intermittent releases to water (in mg/l)	NA	-	-		

### 9.5.2.4.4 Exposure concentration in sediments

The use of ERC 6a default (worst case) parameters to estimate the environmental emissions of acrylonitrile is considered to be unrealistic as the assumptions do not take into account RMMs. In the laboratory the majority of acrylonitrile is consumed in the analytical process or reaction. As a result, there is minimal acrylonitrile waste which is collected and disposed of via special waste. There is no release to waste water. An accurate approximation has been generated using EUSES.

Table 117: Predicted exposure concentration in sediments using EUSES

Compartments	Estimated exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data		
	value	unit	value	unit			
Freshwater sediments	4.02 x 10 <sup>-5</sup>	mg/kg	-	-	No measured data are available		
Marine water sediments	3.29 x 10 <sup>-6</sup>	mg/kg	-	-	No measured data are available		

\*generated in EUSES using the default releases of ERC 6a taking into account the use of scrubbers and WWTP: emission to air=0.0005 and emission to water=0. As there is no direct application of sewage sludge to the ground the concentration of sewage sludge was changed to 0 mg/kg. The tonnage was set at 1 ton/year and the local fraction to 0.1 to represent many laboratory sites throughout Europe.

The following values will be used for the risk assessment and risk characterisation in Section 10.5

Compartments	PEC sediment (local+regional)	Justification					
Freshwater sediments (in mg/kg d.w)	6.5 x 10 <sup>-6</sup>	No measured values available. Predicted exposure concentration in sediment.					
Marine water sediments (in mg/kg d.w.)	5.22 x 10 <sup>-7</sup>	No measured values available. Predicted exposure concentration in sediment.					

### Table 118: Predicted Exposure Concentrations (PEC) in sediments

### 9.5.2.4.5 Exposure concentrations in soil and groundwater

Acrylonitrile can potentially be deposited onto/into the soil from the atmosphere and aqueous compartments. Information from industry indicates that industrial sludge from Acrylonitrile is not generated from laboratories as Acrylonitrile is used within laboratory processes and will not be released to waste water but collected from the laboratory system and reacted as an intermediate before disposal. Therefore the only potential route of exposure to soil is indirectly, via the atmosphere. The predicted exposure concentration for soil was calculated using the EUSES exposure model. The results are given in the table below:

### Table 119: Local concentrations in soil [ES5]

Compartments	Estimated exposu concentrations	Measured exposure concentra		Explanation / source of measured data			
	value	unit	value	unit			
Agricultural soil averaged	3.61 x 10 <sup>-9</sup>	mg/kg	-	-	No measured data		
Grassland averaged	4.88 x 10 <sup>-9</sup>	mg/kg	-	-	No measured data		
Groundwater	1.15 x 10 <sup>-6</sup>	mg/L			No measured data		

\*generated in EUSES using the default releases of ERC 6a taking into account the use of scrubbers and WWTP: emission to air=0.0005 and emission to water=0. As there is no directapplication of sewage sludge to the ground the concentration of sewage sludge was changed to 0 mg/kg. The tonnage was set at 1 ton/year and the local fraction to 0.1 to represent many laboratory sites throughout Europe.

The following values will be used for the risk assessment and risk characterisation in Section 10.5:

Tabla	120.	Dradiated	Fynosuro	Concentrations	(DEC)	in	coil	and	groundwator
I adic	140.	Treatteu	Exposure	Concent ations	(I LC)	111	<b>5011</b>	anu	groundwater

	Local concentration	PEC soil/groundwater (local+regional)	Justification
Agricultural soil averaged (mg/kg ww)	3.61 x 10 <sup>-9</sup>	4.21 x 10 <sup>-7</sup>	
Grassland averaged (mg/kg ww)	4.88 x 10 <sup>-9</sup>	4.22 x 10 <sup>-7</sup>	Represents worst case estimated value.
Groundwater(mg/l)	-	1.15 x 10 <sup>-6</sup>	

### 9.5.2.4.6 Atmospheric compartment

Acrylonitrile is volatile and therefore the atmospheric compartment is the major potential compartment of distribution of acrylonitrile. Releases are reduced by the combustion or scrubbing of gaseous and volatile waste before discharging to the atmosphere.

	Estimated expo concentrations	Measured exposure concentrati		Explanation / source of measured	
	value	unit	value	unit	data
During emission	6.95 x 10 <sup>-7</sup>	mg/m <sup>3</sup>	-	-	No measured data
annual average	3.81 x 10 <sup>-8</sup>	mg/m <sup>3</sup>	-	-	No measured data
Annual total deposition	5.48 x 10 <sup>-8</sup>	mg/m <sup>2</sup> /d	4.5	t/y	EU RAR

Table 121: Local concentrations in air [ES5]

\*generated in EUSES using the default releases of ERC 6a taking into account the use of scrubbers and WWTP: emission to air=0.0005 and emission to water=0. As there is no direct application of sewage sludge to the ground the concentration of sewage sludge was changed to 0 mg/kg. The tonnage was set at 1 ton/year and the local fraction to 0.1 to represent many laboratory sites throughout Europe.

Table	122:	Predicted	Exposure	Concentration	(PEC)	in	air	[ES5]	
-------	------	-----------	----------	---------------	-------	----	-----	-------	--

	Local concentration	PEC air (local+regional)	Justification
During emission (mg/m <sup>3</sup> )	6.95 x 10 <sup>-7</sup>	-	Worst case estimated atmospheric release.
annual average (mg/m <sup>3</sup> )	3.81 x 10 <sup>-8</sup>	2.42 x 10 <sup>-6</sup>	Worst case estimated atmospheric release.
Annual deposition (mg/m <sup>2</sup> /d)	5.48 x 10 <sup>-8</sup>	-	Worst case estimated atmospheric release.

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

Exposure of aquatic species to low levels of acrylonitrile in the aquatic environment is possible. The predicted concentrations relevant for the food chain have been generated using the EUSES exposure model using the measured data for water and atmospheric releases.

Table 123: Local concent	ration relevant for	secondary poi	isoning
--------------------------	---------------------	---------------	---------

	Predicted exposure		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Concentration in food of fish eating predator	5.21 x $10^{-5}$ (freshwater) 4.26 x $10^{-6}$ (marine water)	mg/kg	-	-	No measured data
Concentration in food of fish eating	4.26 x 10 <sup>-6</sup>	mg/kg	-	-	No measured data

	Predicted exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
top-predator (marine)					
Concentration in earthworm	7.97 x 10 <sup>-7</sup>	mg/kg	-	-	No measured data

\*generated in EUSES using the default releases of ERC 6a taking into account the use of scrubbers and WWTP: emission to air=0.0005 and emission to water=0. As there is no direct application of sewage sludge to the ground the concentration of sewage sludge was changed to 0 mg/kg. The tonnage was set at 1 ton/year and the local fraction to 0.1 to represent many laboratory sites throughout Europe.

### 9.6 Exposure scenario 6: Manufacture of Acrylonitrile

### 9.6.1 Exposure estimation

Acrylonitrile is produced from ammonia and propylene via catalytic ammoxidation in a closed system. Fractional distillation of the crude product following scrubbing to remove ammonia results in 99.9% pure acrylonitrile, which may be used directly on-site for the production of polymers or transported in stabilised monomeric form to end-users.

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

Acrylonitrile is produced by the conversion of propylene, ammonia and air in the gaseous phase on appropriate fluidized bed catalysts. Operating conditions vary from 20-200kPa gauge pressures (2.9-20 psig) and  $400-500_{\circ}$ C temperatures. Owing to the high conversion of propylene to acrylonitrile, a once-through operation with a residence time of <10s under slight excess pressure (1.3 to 2.5 bar) is employed. The reaction heat is utilised for the generation of high-pressure steam. After cooling down the reaction gases by indirect heat exchange, the temperature is further lowered by quenching with water; at the same time polymers and the discharged catalyst dust are scrubbed. In the next step the residual ammonia is removed by saturation crystallisation with sulphuric acid. In a water-operated absorber, acrylonitrile and by-products are washed out and sent to crude nitrile distillation where crude acrylonitrile composed of about 80% acrylonitrile, 10% HCN, 5% water and other by-products is recovered. Acetonitrile formed can be recovered from a side-stream of the crude distillation or fed to the absorber waste gas. The separation of HCN as well as the water removal and pure distillation occur in the three downstream distillation columns. The whole processing unit of an acrylonitrile plant is operated under atmospheric pressure. Water removal and pure distillation are carried out under reduced pressure. During start-up and shut-down of the plant, any reaction gas which does not meet specifications must be flared for safety reasons.

During the production of acrylonitrile the reactions take place in closed systems, so there are no defined emissions and exposure to acrylonitrile of workers will not occur. Waste gas produced at the separation of the reaction products consists mainly of nitrogen, carbon dioxide, carbon monoxide, propane, propylene, acetonitrile, HCN and low amounts of acrylonitrile and is typically sent to a combustion plant. Thermal combustion requires a combustion temperature of at least 800 and results in almost complete destruction of residual acrylonitrile. The waste gas from distillation (purification of the reaction products) and the tanks is sent through scrubbers. Acrylonitrile is usually stabilised at normal temperatures and normal pressure and stored under nitrogen. For long-distance transportation acrylonitrile is preferentially carried in rail or road tank wagons or barges. Acrylonitrile-containing waste gases arise during filling and emptying operations and possibly during the purging of the tanks. The transfer of acrylonitrile from

## Acrylonitrile

## SAFETY DATA SHEET

stationary to mobile tanks and vice versa is carried out via articulated arms or pressure-resistant hose-pipes with gas displacement devices or in combination with waste gas purification by scrubbers. Delivery hose connectors are used for the loading and delivery of Acrylonitrile, in the EU are NATO Standard "dry disconnect couplings" to limit operator exposure and environmental release.

Table	124:	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	kg/d	Not relevant: parameter not used for risk assessment
Duration of exposure per day at workplace [for one worker]	8h/day	Default value
Frequency of exposure at workplace [for one worker]	220d/y	Default value
Annual amount used per site	< 1 t/y	Not relevant for this exposure scenario. Only a small amount used in analytical laboratories.
Emission days per site	365 d/y	Assumed continuous process.

### 9.6.1.2 Operational conditions and risk management measures related to substance characteristics Table 125: Characteristics of the substance

Information type	Data field	Explanation
Physical state	Liquid	Acrylonitrile is a liquid substance
For solids: Categorisation of dust grades	Not applicable	Not relevant: acrylonitrile is a liquid substance
Concentration of substance in preparation	Not applicable	Not relevant: acrylonitrile is not present in a preparation
Concentration after dilution for use (if relevant)	Not applicable	Not relevant
Risk management measures related to the design of product		Not applicable

# 9.6.1.3 Operational conditions related to available dilution capacity and characteristics of exposed humans

Information type	Data field	Explanation
Respiration volume under conditions of use	$10 m^{3}/d$	Default for light-work
Room size and ventilation rate	m <sup>3</sup> ; exchange per hour	Not applicable: the process is enclosed. Room size and general ventilation are not employed to control risk.
Area of skin contact with the substance under conditions of use	cm <sup>2</sup>	Not relevant. The process is enclosed and there is little potential for dermal exposure. The potential for dermal exposure during some activities (loading) must be eliminated or minimised through the use of protective equipment as the substance is a skin irritant and skin sensitizer.
Body weight	65 kg	Default for workers

### 9.6.1.4 Other operational conditions of use

Releases to air, water and waste before risk management:

Table 127: 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	0.05 kg/kg	Default value of 5% for ERC 1
Fraction of applied amount lost from process/use to waste water	0.06 kg/kg	Default value of 6% for ERC 1
Fraction of applied amount lost from process/use to waste	0.11 kg/kg	Sum of default losses to waste gas and waste water
Fraction consumed in process/use	-	Not relevant for manufacture
Fraction of applied amount leaving the site with products	0.89 kg/kg	Manufactured acrylonitrile may leave the production site for further processing elsewhere or may be processed (e.g. by polymerisation) on-site.

### 9.6.1.5 Risk management measures

### Table 128: Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilat	ion	·
Containment plus good work practice required	Effectiveness in terms of residual exposure	The manufacturing process is essentially enclosed, with only limited opportunity for exposure during loading etc, where exposure is reduced through the use of LEV and RP.
Local exhaust ventilation required plus good work practise	Effectiveness in terms of reduction factor against situation without LEV or residual exposure	LEV and RP are required at certain points in the process (e.g. loading) which operate without total enclosure.
Personal protective equipment (PPE)	-	
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness	Gloves and face-shield are required to minimise dermal exposure where the process is not totally enclosed. Respirator may be required to minimise dermal exposure where the process is not totally enclosed and LEV is not employed.
Other risk management measures related	ed to workers	
		Workers received specific training and instruction in order to ensure minimal contact with the substance.
		Airborne concentrations of acrylonitrile are routinely monitored to ensure compliance with occupational exposure standards.
Risk management measures related to	environmental emissions from in	dustrial sites
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	
Resulting fraction of initially applied amount in waste water released from site	0.0000094 kg/kg	Default release of 6% to waste water Reduction of default by on-site STP by 95%.
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost from the technical process)	Emissions to waste gas at all points in the process are treated by scrubbers or thermal combustion with >99% efficiency.
Resulting fraction of applied amount in waste gas released to environment	0.0005 kg/kg	Default release of 5% to waste gas, taking into account 99% efficiency of combustion or scrubbers
Onsite waste treatment	Effectiveness:>95% removal by STP	An efficient on-site STP is used to remove the any remaining acrylonitrile from the waste water.

Information type	Data field	Explanation
Fraction of initially applied amount sent to external waste treatment. This is the sum of direct losses from processes to waste, and the residues from onsite waste water and waste gas treatment.	Not relevant	No further external waste water treatment.
Municipal or other type of external waste water treatment	Not relevant	No further external waste water treatment.
Effluent (of the waste water treatment plant) discharge rate	2000 m <sup>3</sup> /d	Default: 2.000 m <sup>3</sup> /d
Recovery of sludge for agriculture or horticulture	No	There is no recovery of sludge from acrylonitrile manufacturing plants for agriculture or horticulture

### 9.6.1.6 Waste related measures

### Table 129: Fractions of substance in waste and waste management measures

Information type	Data field	Explanation
Amount of substances in waste resulting from identified uses covered in the exposure scenario	0 kg/y	
Amount of substances in waste resulting from service life of articles	0 kg/y	Not applicable
Type of waste, suitable waste codes	-	Not applicable
Type of external treatment aiming at recycling or recovery of substances	-	Not applicable
Fraction of the initially applied amount of substance recovered.	0 kg/kg	Not applicable
Type of external treatment aiming at final disposal of the waste	-	Not applicable
Fraction of substance released into the environment via air from waste handling	0 kg/kg	Not applicable
Fraction of substance released into the environment via waste water from waste handling	0 kg/kg	Not applicable
Fraction of substance disposed of as secondary waste	0 kg/kg	Not applicable: primary waste only

### 9.6.2 Exposure estimation

### 9.6.2.1 Workers exposure

### 9.6.2.1.1 Acute/Short term exposure

Routes of exposure	PROC	Estimated E Concentration				Explanation / source
		value	unit	Value	unit	of measured data
	PROC 1	0.343 (without LEV and RP)	mg/kg bw/d	-	-	No measured data;
Dermal exposure	PROC 2	0.137	mg/kg bw/d	-	-	does not take into account the use of
	PROC 8b	0.686	mg/kg bw/d	-	-	protective equipment
	PROC 9	0.686	mg/kg bw/d	-	-	
	PROC 1	[0.1376] (without LEV and RP)	mg/m <sup>3</sup>			
Inhalation exposure	PROC 2	[0.688]	mg/m <sup>3</sup>	] -	-	No measured data
	PROC 8b	[1.032]	mg/m <sup>3</sup>			
	PROC 9	[3.44]	mg/m <sup>3</sup>	·		

### Table 130: Acute exposure concentrations to workers [ES6]

all values generated with RP and LEV unless otherwise stated in ECETOC TRA

[estimated based on modelled TWA values and applying a factor of 2]

The production of acrylonitrile occurs in a closed system with full containment so there are no defined emissions and the risk of exposure to acrylonitrile by workers will be minimal. The waste gas produced is mainly nitrogen, carbon dioxide, carbon monoxide, propane, propylene, acetonitrile, HCN and low amounts of acrylonitrile. These wastes are typically collected and sent to a combustion plant. Although production takes place in closed systems in a largely continuous process, start-up, shut-down, product recovery and purification steps results in some exposure to acrylonitrile. For example, exposurecould occur during the sampling of the reactor. In this case, suitable local ventilation extraction or respiratory protection is used to minimise inhalation exposure. Appropriate PPE (gloves, overcoat, safety goggles) are also used in order to minimise dermal exposure.

In the EU RAR, monitoring data for six European producers is quoted. Mean personal average monitoring levels at the workplace varied from <0.12-0.49 ppm (0.26-1.06 mg/m<sub>3</sub>), with the range being between <0.1-2.21 ppm. A level of 5.5 ppm was recorded but this was considered to be an exception as the mean for this producer was 0.06 ppm.

### Table 131: Summary of acute exposure concentrations to workers

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data. Estimated values used.
Inhalation exposure (in ppm)	3.44	Estimated values used.

### 9.6.2.1.2 Long-term exposure

### Table 132: Long-term exposure concentrations to workers

Routes of exposure PROC			Estimated Exposure Concentrations		exposure ons	Explanation / source of measured data	
		value	unit	Value	unit	of measured data	
	PROC 1	0.343 (without LEV and RP)	mg/kg bw/d	-	-		
Dermal exposure	PROC 2	0.137	mg/kg bw/d	-	-	No measured data	
	PROC 8b	0.686	mg/kg bw/d	-	-		
	PROC 9	0.686	mg/kg bw/d	-	-		
	PROC 1	0.0688 (without LEV and RP)	mg/m <sup>3</sup>				
Inhalation exposure	PROC 2	0.344	mg/m <sup>3</sup>	-	-	No measured data	
	PROC 8b	0.516	mg/m <sup>3</sup>				
	PROC 9	1.72	mg/m <sup>3</sup>				

### Table 133: Summary of long-term exposure concentration to workers

Routes of exposure	Concentrations	Justification
Dermal exposure (in mg/kg bw/d)	0.686	No measured dermal data. Estimated values used.
Inhalation exposure (in mg/m <sup>3</sup> )	1.72	Worst case estimated value.

### 9.6.2.2 Consumer exposure

There is no direct exposure of consumers to acrylonitrile resulting from this exposure scenario (manufacture). Acrylonitrile is used as a chemical intermediate or is processed by polymerisation; the potential for consumer exposure is considered under these exposure scenarios.

### 9.6.2.2.1 Acute/Short term

#### 9.6.2.3 Indirect exposure of humans via the environment

Indirect exposure of the general public via the environment from consumption of biota or drinking water and exposure to air containing residual acrylonitrile istheoretically possible although considered to be of low risk due to the negligible amounts released to the environment.

	Estimated exconcentration		Measured expo concentrations	osure	Explanation / source of	
	value	unit	value unit		measured data	
Wet fish	0.0197	mg/kg	-	-	No measured data	
Drinking water	0.0139	mg/L	-	-	No measured data	
Meat	1.64 x 10 <sup>-5</sup>	mg/kg	-	-	No measured data	
Milk	1.64 x 10 <sup>-4</sup>	mg/L	-	-	No measured data	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is 3 sites so the local fraction was changed to 0.33 for a total EU tonnage of 750,000 t/a.

### 9.6.2.4 Environmental exposure

#### 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.

For the environmental assessment industrial categories and use types are chosen to best suit the description of the production and uses of acrylonitrile 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 production of acrylonitrile. In initial assessments for production the figure of 750,000 tpa and a local fraction of 0.33 has been used as the maximum tonnage quoted is for three sites across Europe. An additional plant in Eastern Europe is also active but produces substantially less than the average of the other three sites.

It is proposed that the use of ERC 1 to estimate emissions to the environment will result in an unrealistic assessment for acrylonitrile. This is because the default emissions fractions in ERC 1 represent a worst case and does not take into account the efficiency of the waste water treatment or scrubber systems. Release of Acrylonitrile to the environment, particularly from production plants, is strictly controlled by local and national pollution control. Specific process technology is required to limit and control release at each site. An average efficiency for all sites is not known. Based on the conservative standard risk assessment model, the maximum release to waste water before processing must

### Acrylonitrile

## SAFETY DATA SHEET

not exceed 7.9 kg/d in a standard waste water treatment plant limited to 2000 m3per day. This is equivalent to a sewage influent of 3.5 mg/L. The table below shows the parameters entered into the EUSES model:

Atmospheric releases are treated either by atmospheric scrubbers or by combustion. An average efficiency of the atmospheric treatment for all sites is not known. Based on the conservative standard risk assessment model, atmospheric releases must not exceed 0.005% of the total tonnage (removal by 99.9% compared to the default release). These risk management measure have been incorporated into the EUSES model in order to gain accurate estimations for the various environmental compartments.

### Acrylonitrile

## SAFETY DATA SHEET

### Table 135: Input Parameters [ES6]

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	53.06	g/mol	-
Vapour Pressure	11500	Pa	-
Water Solubility	73000	mg/L	-
Octanol/water partition coefficient	0.25	logKow	-
Biodegradability	Ready biodegradable	-	-
Life Cycle Step	Use	-	-
Tonnage	750000	Tonnes	-
Environmental Release Class	ERC1	-	-
Fraction of Tonnage for Region	0.33	-	
STP	On-site STP	-	
Emission events per year	300	Days	20
Release to Air	0.005 (takes into account 99.9% efficiency of scrubber systems)	%	5
Release to Water	7.86 kg/d	%	5
Dilution factor applied for PEC derivation	-	-	10 (2,000 m <sup>3</sup> /d)
% fraction degraded in STP	95	%	86
% fraction released to water after STP	4.3	%	12.1
% fraction released to air after STP	0.65	%	1.83
% fraction released to sludge after STP	0.0475	%	0.133

### 9.6.2.4.2 Exposure concentration in sewage treatment plants (STP)

The use of ERC 1 default (worst case) values to estimate the environmental emissions of acrylonitrile is considered to be unrealistic for this exposure scenarios, given the enclosed nature of the process and the RMMs used to minimise emissions. Wastes are either incinerated or treated by for example gas scrubbing of emissions followed by release of scrubber washes to wastewater, thus significantly reducing environmental emissions. EUSES has therefore been used to generate a more accurate estimation taking into account risk management measures such as atmospheric scrubbers and efficient on-site STP Product name: Acrylonitrile eSDS EU Version #: 2.0 Issue date: 25-03-2019. Revision date: 25-03-2019. 97 / 131

Compartments	Estimated exconcentration		Measured expo concentrations	sure	Explanation / source of measured data
	value	unit	value	unit	
Sewage (STP effluent)	0.169	mg/L	_	_	
Sewage sludge	4.73	mg/kg	_	_	

### Table 136: Concentrations in sewage using the EUSES exposure model

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of sites across Europe is 3 sites so the local fraction was changed to 0.33 for a total EU tonnage of 750,000 t/a. The following values will be used for the risk assessment and risk characterisation in Section 10.6:

### Table 137: Predicted Exposure Concentrations (PEC) in sewage

	Value	Justification
Concentration in sewage (PECstp)(in mg/l)	0.169	Estimated data. No measured values.
Concentration in sewage sludge (in mg/kg d.w.)	4.73	Worst case sewage sludge concentration.

### 9.6.2.4.3 Exposure concentration in aquatic pelagic compartment

Waste water is treated via an on-site STP which degrades the remaining material by 95% (see section 4.1.3). As a result, the release to waste water is lowerthan predicted using the default emissions. EUSES exposure model was used toobtain a better approximation for the predicted exposure concentration.

Table 138: Local concentrations in water determined using the EUSES exposure model	Table	138:	Local	concentrations	in	water	determined	using	the	EUSES	exposure	model
--	-------	------	-------	----------------	----	-------	------------	-------	-----	-------	----------	-------

Compartments	Estimated exposure concentrat		Measured local exposure concentrations		Explanation / source of measured data	
	value	unit	value	unit		
Freshwater	0.0169	mg/L	-		No measured data	
Marine water	0.00169	mg/L	-		No measured data	
Intermittent releases to water	NA		-		No measured data	

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of major production sites across Europe is 3 sites so the local release fraction was changed to 0.33 for a total EU tonnage of 750,000 t/a. One other plant is in operation but produces substantially lower volumes than the average of the other three.

The following values will be used for the risk assessment and risk characterisation in Section 10.6:

Compartments	Local concentration	PEC aquatic (local+regional)	Justification
Freshwater (in mg/l)	0.0169	0.0169	PEC for regional contributions negligible.
Marine water (in mg/l)	0.00169	0.00169	Default dilution of 10.
Intermittent releases to water (in mg/l)	NA		

Table 139: Predicted Exposure Concentrations (PEC) in aquatic compartment

### 9.6.2.4.4 Exposure concentration in sediments

The use of ERC 1 default (worst case) values to estimate the environmental emissions of acrylonitrile is considered to be unrealistic for this exposure scenarios, given the enclosed nature of the process and the RMMs used to minimise emissions. Wastes are either incinerated or treated by for example gas scrubbing of emissions followed by release of scrubber washes to wastewater, thus significantly reducing environmental emissions. An accurate value for the concentration in sediment was generated using EUSES.

Table 140: Predicted exposure concentration in sediments using EUSES

Compartments	Estimated exposure concentrat		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Freshwater sediments	0.0185	mg/kg	-	-	No measured data are available
Marine water sediments	0.00185	mg/kg	-	-	No measured data are available

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of major production sites across Europe is 3 sites so the local release fraction was changed to 0.33 for a total EU tonnage of 750,000 t/a. One other plant is in operation but produces substantially lower volumes than the average of the other three.

The following values will be used for the risk assessment and risk characterisation in Section 10.6:

Table	141:	Predicted	Exposure	Concentrations	(PEC)	in	sediments	[ES6]	

Compartments	PEC sediment (local+regional)	Justification
Freshwater sediment (in mg/kg d.w)	s 0.0185	No measured values available. Predicted exposure concentration in sediment.
Marine water sedimen (in mg/kg d.w.)	nts 0.00185	Assumed 10-fold reduction factor.

### 9.6.2.4.5 Exposure concentrations in soil and groundwater

Acrylonitrile can potentially be released during production and be deposited onto/into the soil from the atmosphere and aqueous compartments, however RMMs in place mean that any exposure will be very limited. Information from industry also indicates that industrial sludge from Acrylonitrile production and processing plants is not spread onto land and is normally incinerated with other wastes. Therefore the only potential route of exposure to soil is (indirectly) via the atmosphere. However, gaseous emissions are kept to a minimum by the use of waste gas combustion and though the use of scrubbers. The predicted exposure concentrations for soil have been calculated using the EUSES exposure model. The results are given in the table below:

Compartments	Estimated exposure concentrations		Measured exposure concentra		Explanation / source of measured data
	value	unit	value	unit	
Agricultural soil averaged	8.14 x 10 <sup>-4</sup>	mg/kg	-	-	No measured data
Grassland averaged	0.0011	mg/kg	-	-	No measured data
Groundwater	0.0222	mg/L	-	-	No measured data

 Table 142: Local concentrations in soil

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of major production sites across Europe is 3 sites so the local release fraction was changed to 0.33 for a total EU tonnage of 750,000 t/a. One other plant is in operation but produces substantially lower volumes than the average of the other three.

The following values will be used for the risk assessment and risk characterisation in Section 10.6:

Table 143: Predicted Exposure Concentrations (PEC) in soil and groundwater

	Local concentration	PEC soil/groundwater (local+regional)	Justification
Agricultural soil averaged (mg/kg ww)	8.14 x 10 <sup>-4</sup>	8.15 x 10 <sup>-4</sup>	
Grassland averaged (mg/kg ww)	0.0011	0.0011	Estimated values using EUSES. No measured data available.
Groundwater(mg/l)	-	0.0222	

### 9.6.2.4.6 Atmospheric compartment

Acrylonitrile is highly volatile and therefore the atmospheric compartment is the major compartment of distribution. Releases are reduced by the use of oxidisers/combustion of released gases or the scrubbing of gaseous and volatile waste before discharging to the atmosphere. The predicted exposure concentration (PEC) has been estimated using the EUSES exposure model.

Product name: Acrylonitrile eSDS EU Version #: 2.0 Issue date: 25-03-2019. Revision date: 25-03-2019. 100 / 131

	Estimated exp concentrations		Measured lo exposure concentration		Explanation / source of measured data
	value	unit	value	unit	
During emission	0.104	mg/m <sup>3</sup>	0.2	mg/m <sup>3</sup>	Maximum limit allowed to be released into the environment detailed in BREF document.
annual average	0.0857	mg/m <sup>3</sup>	-	-	No measured data
Annual total deposition	0.123	mg/m <sup>2</sup> /d	-	-	No measured data

### Table 144: Local concentrations in air

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95,lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of major production sites across Europe is 3 sites so the local release fraction was changed to 0.33 for a total EU tonnage of 750,000 t/a. One other plant is in operation but produces substantially lower volumes than the average of the other three.

### Table 145: Predicted Exposure Concentration (PEC) in air [ES6]

	Local concentration	PEC air (local+regional)	Justification
During emission (mg/m <sup>3</sup> )	0.104	-	Worst case concentration determined by EUSES.
annual average (mg/m <sup>3</sup> )	0.0857	0.0857	Worst case concentration determined by EUSES.
Annual deposition (mg/m <sup>2</sup> /d)	0.123	-	Worst case release determined by EUSES.

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

Exposure of aquatic species to low levels of acrylonitrile in the aquatic environment is possible. The predicted concentrations relevant for the food chain have been generated using the EUSES exposure model using the measured data for water and atmospheric releases.

	Predicted exposure concentrations		Measured local exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Concentration in food of fish eating predator	9.86 x $10^{-3}$ (freshwater) 9.85 x $10^{-4}$ (marine water)	mg/kg	-	-	No measured data
Concentration in food of fish eating top-predator (marine)	0.0002	mg/kg	-	-	No measured data
Concentration in earthworm	9.0 x 10 <sup>-3</sup>	mg/kg	-	-	No measured data

### Table 146: Local concentration relevant for secondary poisoning [ES6]

## Acrylonitrile

## SAFETY DATA SHEET

\*estimated using EUSES assuming that from the STP the fraction that goes to water is 0.043, amount degraded is 0.95, lost to air is 0.0065 and to sludge is 0.000475. The sewage sludge concentration was set to 0 mg/kg in order to allow for the fact that the sludge is incinerated or landfilled. The number of major production sites across Europe is 3 sites so the local release fraction was changed to 0.33 for a total EU tonnage of 750,000 t/a. One other plant is in operation but produces substantially lower volumes than the average of theother three.

### **10** RISK CHARACTERISATION

### 10.1 Use as a monomer in the production of acrylic and modacrylic textile fibres [ES1]

### 10.1.1 Human health

### 10.1.1.1 Workers

Worker exposures assuming appropriate RMMs are below the levels of the acute and chronic DNELs, indicating and acceptable risk for workers potentially exposed to acrylonitrile under this exposure scenarios. Exposures are therefore considered to be adequately controlled and further RMMs are not required.

	Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	-	NA: See qualitative risk characterisation
systemic effects	Inhalation	1.08 mg/m <sup>3</sup>	Neurotoxicity	-	NA: See qualitative risk characterisation
	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
Acute - local effects	Inhalation	1.08 mg/m <sup>3</sup>	Respiratory irritation	$10 \text{ mg/m}^3$	0.108
	Combined				NA
Long-term -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	1.4 mg/kg bw/d	0.49
systemic effects	Inhalation	$1.08 \text{ mg/m}^3$	Neurotoxicity	2.7 $mg/m^3$	0.40
cricets	Combined				0.89
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	$1.08 \text{ mg/m}^3$	Respiratory irritation	$1.8 \text{ mg/m}^3$	0.6

Table 147: Quantitative risk characterisation for workers [ES1]

### Table 148: Qualitative risk characterisation for workers [ES1]

	Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Acute - systemic effects	Dermal	0.686 mg/kg bw/d	Neurotoxicity	Based on the known effects of skin irritation and sensitisation and the Risk Management Measures expected in its handling, the local Dermal DNEL for vapour exposure is regarded as adequately protective for systemic effects. Direct contact with the liquid should be

	Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
				avoided. The modelled exposure concentration is an overestimate as it does not take into account the use of gloves, which are required for the safe handling of this substance.
	Inhalation	1.08 mg/m <sup>3</sup>	Neurotoxicity	Worker monitoring studies clearly indicate that local effects are critical for short-term exposures, therefore the local short-term inhalation DNEL is considered to be adequately protective of short-term systemic effects.
	Combined routes			-
Acute - local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	1.08 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.
	Dermal	0.686 mg/kg bw/d	Neurotoxicity	NA: quantitative risk characterization is performed.
Long-term - systemic effects	Inhalation	1.08 mg/m <sup>3</sup>	Neurotoxicity	NA: quantitative risk characterization is performed.
	Combined			NA: quantitative risk characterization is performed.
Long-term – local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	1.08 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.

### 10.1.1.2 Consumers

The potential for the direct exposure of consumers to acrylonitrile resulting from the production of acrylic fibres were considered in the EU RAR. The acrylonitrile monomer is present in the manufactured fibres only at very low levels (<0.1 ppm) and is essentially bound within the fibre. Modelled exposures to acrylonitrile resulting from contact with clothing (dermal) and carpets (inhalation) were found to be very low even when based on a number of worst-case assumption. Exposure levels are well below the DNEL values, therefore it can be concluded that the risks are acceptable.

	Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute – local effects	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
	Inhalation	-	Respiratory irritation	3.3 mg/m <sup>3</sup>	There is no exposure of the general population on a short term basis to acrylonitrile.
	Dermal	-	Neurotoxicity	-	NA: See qualitative risk characterisation
A	Inhalation	-	Neurotoxicity	-	NA: See qualitative risk characterisation
Acute – systemic effects	Oral	-	Neurotoxicity	-	There is no exposure of the general population on a short term basis to acrylonitrile.
	Combined routes				NA
	Dermal	0.000000018 mg/kg bw/d	Carcinogenicity	0.009 mg/kg bw/d	0.0000002
Long-term -	Inhalation	$0.00023 \text{ mg/m}^3$	Carcinogenicity	0.1 mg/m <sup>3</sup>	0.0023
systemic effects	Oral	Not relevant to			
	Combined routes		0.0023002		
Long-term – local effects	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
	Inhalation	0.00023 mg/m <sup>3</sup>	Respiratory irritation	$0.06 \text{ mg/m}^3$	0.0038

### Table 149: Quantitative risk characterisation for consumers

### Table 150: Qualitative risk characterisation for consumers

	Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Acute - local	Dermal	-	Irritation / sensitisation	There are no situations where the general population will be directly exposed via the dermal route to acrylonitrile
effects	Inhalation	-	Respiratory irritation	NA: quantitative risk characterization is performed.
Acute -	Dermal	-	Neurotoxicity	There are no situations where the general population will be directly exposed via the dermal route to acrylonitrile
systemic effects	Inhalation	-	Neurotoxicity	There is no direct exposure of the general population on a short term basis to acrylonitrile.

	Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
	Oral	-	Neurotoxicity	There is no direct exposure of the general population on a short term basis to acrylonitrile.
	Combined routes			NA
	Dermal	0.000000018 mg/kg bw/d	Carcinogenicity	NA: quantitative risk characterization is performed.
Long-term -	Inhalation	0.00023 mg/m <sup>3</sup>	Carcinogenicity	NA: quantitative risk characterization is performed.
systemic effects	Oral	0.00003 mg/kg bw/d	Carcinogenicity	NA: quantitative risk characterization is performed.
	Combined routes			NA: quantitative risk characterization is performed.
Long-term –	Dermal	-	Irritation / sensitisation	
local effects	Inhalation	0.00023 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.

### Table 152: Qualitative risk characterisation for humans exposed via the environment

Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Dermal- systemic (acute or long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	NA: quantitative risk characterisation is performed.
Oral- systemic (long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Combined routes			NA

# 10.1.2 Environment

### 10.1.2.1 Aquatic compartment (including sediment and secondary poisoning)

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Freshwater	0.0169 mg/l	0.017 mg/l	0.99	RCR<1. Acceptable risk management measures.
Marine water	0.00169 mg/l	0.0017 mg/l	0.099	RCR<1. Acceptable risk management measures.
Sediment	0.0185 mg/kg	0.0188 mg/kg	0.98	RCR<1. Acceptable risk management measures.
Aquatic freshwater food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment
Aquatic marine water food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

Table 153: Risk characterisation for the aquatic compartment

# 10.1.2.2 Terrestrial compartment (including secondary poisoning)

#### Table 154: Risk characterisation for the terrestrial compartment

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Agricultural soil	5.13 x 10 <sup>-4</sup> mg/kg	0.00268 mg/kg	0.19	RCR<1. Acceptable risk management measures.
Grassland	6.92 x 10 <sup>-4</sup> mg/kg	0.00268 mg/kg	0.258	RCR<1. Acceptable risk management measures.
Terrestrial food chain	-	-	-	Limited release of acrylonitrile, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

### 10.1.2.3 Atmospheric compartment

No relevant PNEC is derived; risk characterisation is not performed.

#### 10.1.2.4 Microbiological activity in sewage treatment systems

Compartments	PEC	PNEC	PEC/PNEC	Discussion
STP	0.169 mg/l	5 mg/l	0.0338	RCR<1. Acceptable risk management measures.

10.2 Production of acrylonitrile-butadiene-styrene (ABS) and styrene-acrylonitrile (SAN) plastics [ES2]

### 10.2.1 Human health

Worker exposures assuming appropriate RMMs are below the levels of the acute and chronic DNELs, indicating and acceptable risk for workers potentially exposed to acrylonitrile under this exposure scenarios. Exposures are therefore considered to be adequately controlled and further RMMs are not required.

	Route	ES2- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	-	NA: See qualitative risk characterisation
systemic effects	Inhalation	3.44 mg/m <sup>3</sup>	Neurotoxicity	-	NA: See qualitative risk characterisation
	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
Acute - local effects	Inhalation	3.44 mg/m <sup>3</sup>	Respiratory irritation	$10 \text{ mg/m}^3$	0.344
	Combined				NA
Long-term -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	1.4 mg/kg bw/d	0.49
systemic effects	Inhalation	$1.72 mg/m^3$	Neurotoxicity	2.7 $mg/m^3$	0.24
	Combined		_	_	0.61
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	$1.72 mg/m^3$	Respiratory irritation	$1.8 \text{ mg/m}^3$	0.96

#### Table 155: Quantitative risk characterisation for workers [ES2]

	Route	ES 2- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Acute - systemic effects	Dermal	0.686 mg/kg bw/d	Neurotoxicity	Based on the known effects of skin irritation and sensitisation and the Risk Management Measures expected in its handling, the local Dermal DNEL for vapour exposure is regarded as adequately protective for systemic effects. Direct contact with the liquid should be avoided. The modelled exposure concentration is an overestimate as it does not take into account the use of gloves, which are required for the safe handling of this substance.
	Inhalation	3.44 mg/m <sup>3</sup>	Neurotoxicity	Worker monitoring studies clearly indicate that local effects are critical for short-term exposures, therefore the local short-term inhalation DNEL is considered to be adequately protective of short-term systemic effects.
	Combined routes			-
Acute - local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	3.44 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.
	Dermal	0.686 mg/kg bw/d	Neurotoxicity	NA: quantitative risk characterization is performed.
Long-term - systemic effects	Inhalation	1.72 mg/m <sup>3</sup>	Neurotoxicity	NA: quantitative risk characterization is performed.
	Combined			NA: quantitative risk characterization is performed.
Long-term – local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	1.72 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.

# Table 156: Qualitative risk characterisation for workers [ES2]

# 10.2.1.1 Consumers

The potential for the direct exposure of consumers to acrylonitrile resulting from the use of ABS/SAN plastics in food contact materials was considered in the EU RAR. The acrylonitrile monomer is present in manufactured articles only at very low levels and limited migration is seen. Modelled exposures to acrylonitrile resulting from food contact were found to be low and below the DNEL values, therefore it can be concluded that the risks are acceptable.

	Route	ES2- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
Acute – local effects	Inhalation	-	Respiratory irritation	3.3 mg/m <sup>3</sup>	There is no exposure of the general population on a short term basis to acrylonitrile.
	Dermal		Naumatawiaitu		NA: See qualitative risk
	Dermai	-	Neurotoxicity	-	characterisation
Acute –	Inhalation	-	Neurotoxicity	-	NA: See qualitative risk characterisation
systemic effects	Oral	-	Neurotoxicity -		There is no exposure of the general population on a short term basis to acrylonitrile.
	Combined routes			NA	
	Dermal	Not relevant for	this exposure scen	nario	
	Inhalation	Not relevant for	this exposure scen		
Long-term - systemic effects	Oral	0.00003 mg/kg bw/d	Carcinogenicity	0.009 mg/kg bw/d	0.003
	Combined routes			-	NA
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	0.00023 mg/m <sup>3</sup>	Respiratory irritation	0.06 mg/m <sup>3</sup>	0.0038

Table 157: Quantitative risk characterisation for consumers [ES2]

	Route	ES 2- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation	
Acute -	Dermal	-	Irritation / sensitisation	There are no situations where the general population will be directly exposed via the dermal route to acrylonitrile	
local effects	Inhalation	-	Respiratory irritation	NA: quantitative risk characterization is performed.	
	Dermal	-	Neurotoxicity	There are no situations where the general population will be directly exposed via the dermal route to acrylonitrile	
Acute - systemic	Inhalation	-	Neurotoxicity	There is no direct exposure of the general population on a short term basis to acrylonitrile.	
effects	Oral	-	Neurotoxicity	There is no direct exposure of the general population on a short term basis to acrylonitrile.	
	Combined routes			NA	
	Dermal	Not relevant for	this exposure scer	nario	
T	Inhalation	Not relevant for this exposure scenario			
Long-term - systemic effects	Oral	0.00003 mg/kg bw/d	Carcinogenicity	NA: quantitative risk characterization is performed.	
	Combined routes			NA: quantitative risk characterization is performed.	
Long-term –	Dermal	-	Irritation / sensitisation	NA: quantitative risk characterization is performed.	
local effects	Inhalation	-	Respiratory irritation	Not relevant for this exposure scenario	

### Table 158: Qualitative risk characterisation for consumers

#### 10.2.1.2 Indirect exposure of humans via the environment

The EU RAR concludes that indirect exposure of consumers through the environment (food, drinking water, air) for all uses combined is minimal due to the limited releases of acrylonitrile and its biodegradability. Predicted exposures are well below the DNEL values, therefore exposures are considered to be acceptable.

Table 159:	Ouantitative	risk	characterisation	for	humans	exposed	via	the	environment
1 abic 137.	Zuannan	1191	character isation	101	manans	caposcu	1 100	unc	ch v h omnene

Route	ES 2- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Dermal- systemic (acute or long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	0.1 mg/m <sup>3</sup>	0.000005
Oral- systemic (long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Combined routes				<1

#### Table 160: Qualitative risk characterisation for humans exposed via the environment

Route	ES 2- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Dermal- systemic (acute or long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	NA: quantitative risk characterisation is performed.
Oral- systemic (long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Combined routes			NA

# 10.2.2 Environment

### 10.2.2.1 Aquatic compartment (including sediment and secondary poisoning)

Table	161:	Risk	characterisation	for	the	aquatic	compartment
-------	------	------	------------------	-----	-----	---------	-------------

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Freshwater	0.0169 mg/l	0.017 mg/l	0.99	RCR<1. Acceptable risk management measures.
Marine water	0.00169 mg/l	0.017 mg/l	0.099	RCR<1. Acceptable risk management measures.
Sediment	0.0185 mg/kg	0.0188 mg/kg	0.98	RCR<1. Acceptable risk management measures.
Aquatic freshwater food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment
Aquatic marine water food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

# 10.2.2.2 Terrestrial compartment (including secondary poisoning)

### Table 162: Risk characterisation for the terrestrial compartment

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Agricultural soil	0.000513 mg/kg	0.00268 mg/kg	0.19	RCR< 1, indicating acceptable risk
Grassland	0.000692 mg/kg	0.00268 mg/kg	0.258	RCR< 1, indicating acceptable risk
Terrestrial food chain	-	-	-	Limited release of acrylonitrile, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

### 10.2.2.3 Atmospheric compartment

No relevant PNEC is derived; risk characterisation is not performed.

### 10.2.2.4 Microbiological activity in sewage treatment systems

#### Table 163: Risk characterisation for the sewage treatment systems

Compartments	PEC	PNEC	PEC/PNEC	Discussion
STP	0.169 mg/l	5 mg/l	0.0338	RCR< 1, indicating acceptable risk

# 10.3 Monomer for production of nitrile rubbers [ES3]

#### 10.3.1 Human health

#### 10.3.1.1 Workers

Worker exposures assuming appropriate RMMs are below the levels of the acute and chronic DNELs, indicating and acceptable risk for workers potentially exposed to acrylonitrile under this exposure scenarios. Exposures are therefore considered to be adequately controlled and further RMMs are not required.

	Route	ES3- exposure concentrations (EC)			Risk characterisation ratio
Acute -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	-	NA: See qualitative risk characterisation
systemic effects	Inhalation	3.44 mg/m <sup>3</sup>	Neurotoxicity	-	NA: See qualitative risk characterisation
	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
Acute - local effects	Inhalation	3.44 mg/m <sup>3</sup>	Respiratory irritation	$10 \text{ mg/m}^3$	0.344
	Combined			NA	
Long-term -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	1.4 mg/kg bw/d	0.49
systemic effects	Inhalation	1.72 mg/m <sup>3</sup> Neurotoxicity		$2.7 \text{ mg/m}^3$	0.24
	Combined			0.73	
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	$1.72 \text{ mg/m}^3$	Respiratory irritation	1.8 mg/m <sup>3</sup>	0.96

Table 164: Quantitative risk characterisation for workers [ES3]

	Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation		
Acute - systemic effects	Dermal	0.686 mg/kg bw/d	Neurotoxicity	Based on the known effects of skin irritation and sensitisation and the Risk Management Measures expected in its handling, the local Dermal DNEL for vapour exposure is regarded as adequately protective for systemic effects. Direct contact with the liquid should be avoided. The modelled exposure concentration is an overestimate as it does not take into account the use of gloves, which are required for the safe handling of this substance.		
	Inhalation	3.44 mg/m <sup>3</sup>	Neurotoxicity	Worker monitoring studies clearly indicate that local effects are critical for short-term exposures, therefore the local short-term inhalation DNEL is considered to be adequately protective of short-term systemic effects.		
	Combined routes			-		
Acute - local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.		
	Inhalation	3.44 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.		
	Dermal	0.686 mg/kg bw/d	Neurotoxicity	NA: quantitative risk characterization is performed.		
Long-term - systemic effects	Inhalation	1.72 mg/m <sup>3</sup>	Neurotoxicity	NA: quantitative risk characterization is performed.		
	Combined			NA: quantitative risk characterization is performed.		
Long-term – local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.		
	Inhalation	1.72 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.		

# Table 165: Qualitative risk characterisation for workers [ES3]

# Acrylonitrile

# SAFETY DATA SHEET

# 10.3.1.2 Consumers

	Route	ES3- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio		
Acute –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation		
local effects	Inhalation	-	Respiratory irritation	3.3 mg/m <sup>3</sup>	NA: See qualitative risk characterisation		
	Dermal	-	Neurotoxicity	-	NA: See qualitative risk characterisation		
Acute –	Inhalation	-	Neurotoxicity	-	NA: See qualitative risk characterisation		
systemic effects	Oral	-	Neurotoxicity	-	NA: See qualitative risk characterisation		
	Combined routes				NA: See qualitative risk characterisation		
	Dermal	Not relevant for this exposure scenario					
T.	Inhalation	Not relevant for	this exposure scer				
Long-term - systemic effects	Oral	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation		
	Combined routes			NA: See qualitative risk characterisation			
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation		
local effects	Inhalation	-	Respiratory irritation	0.06 mg/m <sup>3</sup>	NA: See qualitative risk characterisation		

# Table 166: Quantitative risk characterisation for consumers [ES3]

	Route	ES3- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation					
Acute -	Dermal	-	Irritation / sensitisation						
local effects	Inhalation	-	Respiratory irritation	Nitrile rubber is used to manufacture a large					
	Dermal	-	Neurotoxicity	number of articles including those which could potentially result in consumer					
Acute -	Inhalation	-	Neurotoxicity	exposure, such as protective gloves and flooring. However unreacted acrylonitrile is					
systemic effects	Oral	-	Neurotoxicity	only present in the manufactured polymer at trace amounts (if at all) and is considered to					
	Combined routes			be bound within the polymer. Consumer exposure to acrylonitrile resulting from the use of nitrile rubber articles is therefore					
	Dermal	-	Carcinogenicity	considered to be negligible and will be less than the very low exposures to residual					
Long-term -	Inhalation	-	Carcinogenicity	acrylonitrile monomer calculated above for					
systemic effects	Oral	-	Carcinogenicity	inhalation and dermal exposure to acrylic fibres and oral exposure to residual					
	Combined routes			acrylonitrile monomer calculated above for oral exposure resulting from the use of ABS plastics for food packaging.					
Long-term –	Dermal	-	Irritation / sensitisation						
local effects	Inhalation	-	Respiratory irritation						

### Table 167: Qualitative risk characterisation for consumers [ES3]

# 10.3.1.3 Indirect exposure of humans via the environment

The EU RAR concludes that indirect exposure of consumers through the environment (food, drinking water, air) for all uses combined is minimal due to the limited releases of acrylonitrile and its biodegradability. Predicted exposures are well below the DNEL values, therefore exposures are considered to be acceptable.

Route	ES3- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Dermal- systemic (acute or long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	0.1 mg/m <sup>3</sup>	0.000005
Oral- systemic (long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Combined routes				<1

Table	169:	Qualitative	risk	characterisation	for	humans	exposed	via	the	environment
-------	------	-------------	------	------------------	-----	--------	---------	-----	-----	-------------

Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Dermal- systemic (acute or long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	NA: quantitative risk characterisation is performed.
Oral- systemic (long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Combined routes			NA

#### 10.3.2 Environment

### 10.3.2.1 Aquatic compartment (including sediment and secondary poisoning)

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Freshwater	0.0169 mg/L	0.017 mg/L	0.99	RCR<1 Acceptable risk management measures
Marine water	0.0169 mg/L	0.017 mg/L	0.099	RCR<1 Acceptable risk management measures
Sediment	0.0185 mg/kg	0.0188 mg/kg	0.98	RCR<1. Acceptable risk management measures.
Aquatic freshwater food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment
Aquatic marine water food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

Table 170: Risk characterisation for the aquatic compartment

# 10.3.2.2 Terrestrial compartment (including secondary poisoning)

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Agricultural soil	1.93 x 10 <sup>-4</sup> mg/kg	0.00268 mg/kg	0.072	RCR <1: indicating acceptable risk
Grassland	2.6 x 10 <sup>-4</sup> mg/kg	0.00268 mg/kg	0.097	RCR <1: indicating acceptable risk
Terrestrial food chain	-	-	-	Limited release of acrylonitrile, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

Table 171: Risk characterisation for the terrestrial compartment

# 10.3.2.3 Atmospheric compartment

No relevant PNEC is derived; risk characterisation is not performed.

#### 10.3.2.4 Microbiological activity in sewage treatment systems

Compartments	PEC	PNEC	PEC/PNEC	Discussion
STP	0.169 mg/l	5 mg/l	0.0338	RCR<1 Acceptable risk management measures

# 10.4 Intermediate use for manufacture of bulk chemicals, materials and resins [ES4]

#### 10.4.1 Human health

#### 10.4.1.1 Workers

Worker exposures assuming appropriate RMMs are below the levels of the acute and chronic DNELs, indicating and acceptable risk for workers potentially exposed to acrylonitrile under this exposure scenarios. Exposures are therefore considered to be adequately controlled and further RMMs are not required.

Table 172: Quantitative	e risk	characterisation	for	workers	[ES4]	
-------------------------	--------	------------------	-----	---------	-------	--

	Route	ES4- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute -	Dermal	0.686 mg/kg bw/d	Neurotoxicity -		NA: See qualitative risk characterisation
systemic effects	Inhalation	on 3.44 mg/m <sup>3</sup> Neurotoxicity	-	NA: See qualitative risk characterisation	
	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
Acute - local effects	Inhalation	3.44 mg/m <sup>3</sup>	Respiratory irritation	$10 \text{ mg/m}^3$	0.344
	Combined				NA
Long-term -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	1.4 mg/kg bw/d	0.49
systemic effects	Inhalation	1.72 $mg/m^3$	Neurotoxicity	$2.7 \text{ mg/m}^3$	0.24
	Combined				0.73
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	$1.72 \text{ mg/m}^3$	Respiratory irritation	$1.8 \text{ mg/m}^3$	0.96

	Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Acute - systemic	Dermal	0.686 mg/kg bw/d	Neurotoxicity	Based on the known effects of skin irritation and sensitisation and the Risk Management Measures expected in its handling, the local Dermal DNEL for vapour exposure is regarded as adequately protective for systemic effects. Direct contact with the liquid should be avoided. The modelled exposure concentration is an overestimate as it does not take into account the use of gloves, which are required for the safe handling of this substance.
effects	Inhalation	3.44 mg/m <sup>3</sup>	Neurotoxicity	Worker monitoring studies clearly indicate that local effects are critical for short-term exposures, therefore the local short-term inhalation DNEL is considered to be adequately protective of short-term systemic effects.
	Combined routes			-
Acute - local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	3.44 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.
	Dermal	0.686 mg/kg bw/d	Neurotoxicity	NA: quantitative risk characterization is performed.
Long-term - systemic effects	Inhalation	1.72 mg/m <sup>3</sup>	Neurotoxicity	NA: quantitative risk characterization is performed.
	Combined			NA: quantitative risk characterization is performed.
Long-term – local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	1.72 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.

# Table 173: Qualitative risk characterisation for workers [ES4]

# 10.4.1.2 Consumers

Table 174: Quantitative risk characterisation for consumers [ES4]

	Route	ES4- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	-	Respiratory irritation	3.3 mg/m <sup>3</sup>	NA: See qualitative risk characterisation
	Dermal	-	Neurotoxicity	-	NA: See qualitative risk characterisation
Acute –	Inhalation -	-	Neurotoxicity	-	NA: See qualitative risk characterisation
systemic effects	Oral	-	Neurotoxicity	-	NA: See qualitative risk characterisation
	Combined routes				NA: See qualitative risk characterisation
	Dermal	Not relevant for	this exposure scer		
T (	Inhalation	Not relevant for	this exposure scer	nario	
Long-term - systemic effects	Oral	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
	Combined routes				NA: See qualitative risk characterisation
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	-	Respiratory irritation	$0.06 \text{ mg/m}^3$	NA: See qualitative risk characterisation

	Route	ES4- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Acute -	Dermal	-	Irritation / sensitisation	
local effects	Inhalation	-	Respiratory irritation	
	Dermal	-	Neurotoxicity	
Acute -	Inhalation	-	Neurotoxicity	
systemic effects	Oral	-	Neurotoxicity	
	Combined routes			There will be no direct consumer exposure to acrylonitrile resulting from this use as an
	Dermal	-	Carcinogenicity	industrial intermediate.
Long-term -	Inhalation	-	Carcinogenicity	
systemic effects	Oral	-	Carcinogenicity	
	Combined routes			
Long-term –	Dermal	-	Irritation / sensitisation	
local effects	Inhalation	-	Respiratory irritation	

### Table 175: Qualitative risk characterisation for consumers [ES4]

# 10.4.1.3 Indirect exposure of humans via the environment

The EU RAR concludes that indirect exposure of consumers through the environment (food, drinking water, air) for all uses combined is minimal due to the limited releases of acrylonitrile and its biodegradability. Predicted exposures are well below the DNEL values, therefore exposures are considered to be acceptable.

<b>Table 176:</b>	Quantitative	risk	characterisation	for	humans	exposed	via	the	environment	ES4	1
-------------------	--------------	------	------------------	-----	--------	---------	-----	-----	-------------	-----	---

Route	ES4- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Dermal- systemic (acute or long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	$0.1 \text{ mg/m}^3$	0.000005
Oral- systemic (long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Combined routes				<1

Table 177: Qualitative risk characterisation for humans exposed via the environment [ES4]

Route	ES4- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Dermal- systemic (acute or long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	NA: quantitative risk characterisation is performed.
Oral- systemic (long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Combined routes			NA

#### 10.4.2 Environment

### 10.4.2.1 Aquatic compartment (including sediment and secondary poisoning)

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Freshwater	0.0169 mg/l	0.017 mg/l	0.99	RCR<1 Acceptable risk management measures
Marine water	0.00169 mg/l	0.017 mg/l	0.099	RCR<1 Acceptable risk management measures
Sediment	0.0185 mg/kg	0.0188 mg/kg	0.98	RCR<1. Acceptable risk management measures.
Aquatic freshwater food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment
Aquatic marine water food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

 Table 178: Risk characterisation for the aquatic compartment [ES4]

# 10.4.2.2 Terrestrial compartment (including secondary poisoning)

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Agricultural soil	4.93 x 10 <sup>-4</sup> mg/kg	0.00268 mg/kg	0.184	RCR<1 Acceptable risk management measures
Grassland	6.65 x 10 <sup>-4</sup> mg/kg	0.00268 mg/kg	0.248	RCR<1 Acceptable risk management measures
Terrestrial food chain	-	-	-	Limited release of acrylonitrile, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

Table 179: Risk characterisation for the terrestrial compartment [ES4	Table
---	-------

# 10.4.2.3 Atmospheric compartment

No relevant PNEC is derived; risk characterisation is not performed.

10.4.2.4	Microbiological	activity i	in sewage	treatment	systems	IES41
10000	1, Her obrorogreat	activity i	in sevenae	u cucuiteite	Sy Seemis	

Compartments	PEC	PNEC	PEC/PNEC	Discussion
STP	0.169 mg/l	5 mg/l	0.0388	RCR<1 Acceptable risk management measures

### 10.5 Exposure Scenario 5: Laboratory Reagent

#### 10.5.1 Human health

#### 10.5.1.1 Workers

Worker exposures assuming appropriate RMMs are below the levels of the acute and chronic DNELs, indicating and acceptablerisk for workers potentially exposed to acrylonitrile under this exposure scenarios. Exposures are therefore considered to be adequately controlled and further RMMs are not required.

Table	180:	Quantitative	risk	characterisation	for	workers	[ES5]
-------	------	--------------	------	------------------	-----	---------	-------

	Route	ES5- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute -	Dermal	ermal 0.343 mg/kg Neurotoxicity -		-	NA: See qualitative risk characterisation
systemic effects	Inhalation	0.688 mg/m <sup>3</sup>	Neurotoxicity	-	NA: See qualitative risk characterisation
	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
Acute - local effects	Inhalation	0.688 mg/m <sup>3</sup>	Respiratory irritation	$10 \text{ mg/m}^3$	0.0688
	Combined				NA
Long-term -	Dermal	0.343 mg/kg bw/d	Neurotoxicity	1.4 mg/kg bw/d	0.49
systemic effects	Inhalation	0.344 mg/m <sup>3</sup>	Neurotoxicity	2.7 $mg/m^{3}$	0.13
enteets	Combined				0.62
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	0.344 mg/m <sup>3</sup>	Respiratory irritation	1.8 mg/m <sup>3</sup>	0.191

	Route	ES 5- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Acute - systemic	Dermal	0.343 mg/kg bw/d	Neurotoxicity	Based on the known effects of skin irritation and sensitisation and the Risk Management Measures expected in its handling, the local Dermal DNEL for vapour exposure is regarded as adequately protective for systemic effects. Direct contact with the liquid should be avoided. The modelled exposure concentration is an overestimate as it does not take into account the use of gloves, which are required for the safe handling of this substance.
effects	Inhalation	0.688 mg/m <sup>3</sup>	Neurotoxicity	Worker monitoring studies clearly indicate that local effects are critical for short-term exposures, therefore the local short-term inhalation DNEL is considered to be adequately protective of short-term systemic effects.
	Combined routes			_
Acute - local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	0.688 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.
	Dermal	0.343 mg/kg bw/d	Neurotoxicity	NA: quantitative risk characterization is performed.
Long-term - systemic effects	Inhalation	0.344 mg/m <sup>3</sup>	Neurotoxicity	NA: quantitative risk characterization is performed.
	Combined			NA: quantitative risk characterization is performed.
Long-term – local effects	Dermal	0.343 mg/kg bw/d	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	0.344 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.

# Table 181: Qualitative risk characterisation for workers [ES5]

# 10.5.1.2 Consumers

Table 182: Quantitative risk characterisation for consumers [ES5]

	Route	ES5- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	-	Respiratory irritation	3.3 mg/m <sup>3</sup>	NA: See qualitative risk characterisation
	Dermal	-	Neurotoxicity	-	NA: See qualitative risk characterisation
Acute –	Inhalation	-	Neurotoxicity	-	NA: See qualitative risk characterisation
systemic effects	Oral	-	Neurotoxicity	-	NA: See qualitative risk characterisation
	Combined routes				NA: See qualitative risk characterisation
	Dermal	Not relevant for	this exposure scer	nario	
T	Inhalation	Not relevant for	this exposure scer	nario	
Long-term - systemic effects	Oral	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
	Combined routes			NA: See qualitative risk characterisation	
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	-	Respiratory irritation	0.06 mg/m <sup>3</sup>	NA: See qualitative risk characterisation

	Route	ES5- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation				
Acute -	Dermal	-	Irritation / sensitisation					
local effects	Inhalation	-	Respiratory irritation					
	Dermal	-	Neurotoxicity					
Acute -	Inhalation	-	Neurotoxicity					
systemic effects	Oral	-	Neurotoxicity					
	Combined routes			There will be no direct consumer exposure to acrylonitrile resulting from laboratory use				
	Dermal	-	Carcinogenicity					
Long-term -	Inhalation	-	Carcinogenicity					
systemic effects	Oral	-	Carcinogenicity					
	Combined routes							
Long-term –	Dermal	-	Irritation / sensitisation					
local effects	Inhalation	-	Respiratory irritation					

#### Table 183: Qualitative risk characterisation for consumers [ES5]

#### 10.5.1.3 Indirect exposure of humans via the environment

The EU RAR concludes that indirect exposure of consumers through the environment (food, drinking water, air) for all uses combined is minimal due to the limited releases of acrylonitrile and its biodegradability. Predicted exposures are well below the DNEL values, therefore exposures are considered to be acceptable.

<b>Table 184:</b>	Quantitative	risk	characterisation	for	humans	exposed	via	the	environment
-------------------	--------------	------	------------------	-----	--------	---------	-----	-----	-------------

Route	ES3- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Dermal- systemic (acute or long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	$0.1 \text{ mg/m}^3$	0.000005
Oral- systemic (long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Combined routes				<1

Table 185	Qualitative	risk	characterisation	for	humans	exposed	via	the	environment
-----------	-------------	------	------------------	-----	--------	---------	-----	-----	-------------

Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Dermal- systemic (acute or long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	NA: quantitative risk characterisation is performed.
Oral- systemic (long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Combined routes			NA

#### 10.5.2 Environment

# 10.5.2.1 Aquatic compartment (including sediment and secondary poisoning)

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Freshwater	3.69 x 10 <sup>-5</sup> mg/l	0.017 mg/l	0.0022	RCR <1: indicating acceptable risk
Marine water	3.02 x 10 <sup>-6</sup> mg/l	0.017 mg/l	0.000177	RCR <1: indicating acceptable risk
Sediment	4.02 x 10 <sup>-5</sup> mg/kg	0.0188 mg/kg	0.00214	RCR <1: indicating acceptable risk
Aquatic freshwater food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment
Aquatic marine water food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

 Table 186: Risk characterisation for the aquatic compartment

### 10.5.2.2 Terrestrial compartment (including secondary poisoning)

Table	187:	Risk	characterisation	for	the	terrestrial	compartment

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Agricultural soil	4.21 x 10 <sup>-7</sup> mg/kg	0.00268 mg/kg	0.000157	RCR <1: indicating acceptable risk
Grassland	4.22 x 10 <sup>-7</sup> mg/kg	0.00268 mg/kg	0.000157	RCR <1: indicating acceptable risk
Terrestrial food chain	-	-	-	Limited release of acrylonitrile, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

#### 10.5.2.3 Atmospheric compartment

No relevant PNEC is derived; risk characterisation is not performed.

#### 10.5.2.4 Microbiological activity in sewage treatment systems

No release to water from sewage treatment systems. All waste is disposed of via special waste.

# 10.6 Manufacture of acrylonitrile [ES6]

#### 10.6.1 Human health

#### 10.6.1.1 Workers

Worker exposures assuming appropriate RMMs are below the levels of the acute and chronic DNELs, indicating and acceptable risk for workers potentially exposed to acrylonitrile under this exposure scenarios. Exposures are therefore considered to be adequately controlled and further RMMs are not required.

Table	188:	Quantitative	risk	characterisation	for	workers	[ES6]	
-------	------	--------------	------	------------------	-----	---------	-------	--

	Route	ES6- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Acute -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	-	NA: See qualitative risk characterisation
systemic effects	Inhalation	3.44 mg/m <sup>3</sup>	Neurotoxicity	-	NA: See qualitative risk characterisation
	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
Acute - local effects	Inhalation	3.44 mg/m <sup>3</sup>	Respiratory irritation	$10 \text{ mg/m}^3$	0.344
	Combined				NA
Long-term -	Dermal	0.686 mg/kg bw/d	Neurotoxicity	1.4 mg/kg bw/d	0.49
systemic effects	Inhalation	$1.72 \text{ mg/m}^3$	Neurotoxicity	$2.7 \text{ mg/m}^3$	0.24
•••••	Combined				0.73
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation
local effects	Inhalation	1.72 mg/m <sup>3</sup>	Respiratory irritation	1.8 mg/m <sup>3</sup>	0.96

	Route	ES 6- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Acute - systemic	Dermal	0.686 mg/kg bw/d	Neurotoxicity	Based on the known effects of skin irritation and sensitisation and the Risk Management Measures expected in its handling, the local Dermal DNEL for vapour exposure is regarded as adequately protective for systemic effects. Direct contact with the liquid should be avoided. The modelled exposure concentration is an overestimate as it does not take into account the use of gloves, which are required for the safe handling of this substance.
effects	Inhalation 3.44 mg/m <sup>3</sup>		Neurotoxicity	Worker monitoring studies clearly indicate that local effects are critical for short-term exposures, therefore the local short-term inhalation DNEL is considered to be adequately protective of short-term systemic effects.
	Combined routes			-
Acute - local effects	Dermal	-	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	3.44 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.
	Dermal	0.686 mg/kg bw/d	Neurotoxicity	NA: quantitative risk characterization is performed.
Long-term - systemic effects	Inhalation	1.72 mg/m <sup>3</sup>	Neurotoxicity	NA: quantitative risk characterization is performed.
	Combined			NA: quantitative risk characterization is performed.
Long-term – local effects	Dermal	0.686 mg/kg bw/d	Irritation / sensitisation	The substance is a skin irritant and skin sensitizer. Dermal exposure must be minimized through the use of engineering controls and protective equipment.
	Inhalation	1.72 mg/m <sup>3</sup>	Respiratory irritation	NA: quantitative risk characterization is performed.

# Table 189: Qualitative risk characterisation for workers [ES6]

# 10.6.1.2 Consumers

 Table 190: Quantitative risk characterisation for consumers [ES6]

	Route	ES6- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio			
Acute –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation			
local effects	Inhalation	-	Respiratory irritation	3.3 mg/m <sup>3</sup>	NA: See qualitative risk characterisation			
	Dermal	-	Neurotoxicity	-	NA: See qualitative risk characterisation			
Acute –	Inhalation	-	Neurotoxicity	-	NA: See qualitative risk characterisation			
systemic effects	Oral	-	Neurotoxicity	-	NA: See qualitative risk characterisation			
	Combined routes				NA: See qualitative risk characterisation			
	Dermal	Not relevant for this exposure scenario						
T (	Inhalation	Not relevant for this exposure scenario						
Long-term - systemic effects	Oral	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation			
	Combined routes				NA: See qualitative risk characterisation			
Long-term –	Dermal	-	Irritation / sensitisation	-	NA: See qualitative risk characterisation			
local effects	Inhalation	-	Respiratory irritation	0.06 mg/m <sup>3</sup>	NA: See qualitative risk characterisation			

	Route	ES6- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Acute -	Dermal	-	Irritation / sensitisation	
local effects	Inhalation	-	Respiratory irritation	
	Dermal	-	Neurotoxicity	
Acute -	Inhalation	-	Neurotoxicity	
systemic effects	Oral	-	Neurotoxicity	
	Combined routes			There will be no direct consumer exposure to acrylonitrile resulting from manufacture
	Dermal	-	Carcinogenicity	
Long-term -	Inhalation	-	Carcinogenicity	
systemic effects	Oral	-	Carcinogenicity	
	Combined routes			
Long-term –	Dermal	-	Irritation / sensitisation	
local effects	Inhalation	-	Respiratory irritation	

### Table 191: Qualitative risk characterisation for consumers [ES6]

#### 10.6.1.3 Indirect exposure of humans via the environment

The EU RAR concludes that indirect exposure of consumers through the environment (food, drinking water, air) for all uses combined is minimal due to the limited releases of acrylonitrile and its biodegradability. Predicted exposures are well below the DNEL values, therefore exposures are considered to be acceptable.

Table 192:	Quantitative	risk	characterisation	for	humans	exposed	via	the	environment
------------	--------------	------	------------------	-----	--------	---------	-----	-----	-------------

Route	ES6- exposure concentrations (EC)	Leading toxic end point / Critical effect	DN(M)EL	Risk characterisation ratio
Dermal- systemic (acute or long term)	-	Carcinogenicity	0.009 mg/kg bw/d	NA: See qualitative risk characterisation
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	$0.1 \text{ mg/m}^3$	0.000005
Oral- systemic (long term)	-	Carcinogenicity	0.068 mg/kg bw/d	NA: See qualitative risk characterisation
Combined routes				<1

Route	ES 1- exposure concentrations (EC)	Leading toxic end point / Critical effect	Qualitative risk characterisation
Dermal- systemic (acute or long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Inhalation- systemic (long term)	0.0000005 mg/m <sup>3</sup>	Carcinogenicity	NA: quantitative risk characterisation is performed.
Oral- systemic (long term)	-	Carcinogenicity	Indirect exposure of the general public will be negligible
Combined routes			NA

### 10.6.2 Environment

# 10.6.2.1 Aquatic compartment (including sediment and secondary poisoning)

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Freshwater	0.0169 mg/l	0.017 mg/l	0.99	RCR <1: indicating acceptable risk
Marine water	0.00169 mg/l	0.017 mg/l	0.099	RCR <1: indicating acceptable risk
Sediment	0.0185 mg/kg	0.0188 mg/kg	0.98	RCR<1. Acceptable risk management measures.
Aquatic freshwater food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment
Aquatic marine water food chain	-	-	-	Limited release of acrylonitrile in waste water, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

Table 194: Risk characterisation for the aquatic compartment

# 10.6.2.2 Terrestrial compartment (including secondary poisoning)

Table 1	195:	Risk	characterisation	for	the	terrestrial	compartment
---------	------	------	------------------	-----	-----	-------------	-------------

Compartments	PEC	PNEC	PEC/PNEC	Discussion
Agricultural soil	8.15 x 10 <sup>-4</sup>	0.00268 mg/kg	0.304	RCR <1: indicating acceptable risk
Grassland	0.0011	0.00268 mg/kg	0.410	RCR <1: indicating acceptable risk
Terrestrial food chain	-	-	-	Limited release of acrylonitrile, degradation in the environment and a lack of bioaccumulation indicates that the risk will be acceptable for this compartment

#### 10.6.2.3 Atmospheric compartment

No relevant PNEC is derived; risk characterisation is not performed.

# 10.6.2.4 Microbiological activity in sewage treatment systems

Compartments	PEC	PNEC	PEC/PNEC	Discussion
STP	0.169 mg/l	5 mg/l	0.0338	RCR <1: indicating acceptable risk

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

#### 10.7.1 Human health (combined for all exposure routes)

#### Table 196: Identification of relevant combination of exposure scenarios

Exposure scenarios	<b>Combination</b> 1	Combination 2	Combination 2	Combination 3		
ES 1						
ES 2						
ES 3				1. 4 1		
ES 4	No relevant com	vinations of exposure scenarios are predicted				
ES 5						
ES 6						

The potential combined exposure to acrylonitrile of workers participating in different tasks needs to be considered, as the total (combined) exposures may potentially exceed the relevant DNEL value. However the uses of acrylonitrile covered by this Chemical Safety Report are typically performed at different sites; the substance is manufactured at dedicated sites and is subsequently transported to other sites for use as an intermediate or in polymer manufacture. Workers are therefore not exposed to acrylonitrile as result of any combination of scenarios. In any case, worker exposure modelling has assumed exposure to acrylonitrile over the duration of a full shift for all individual activities described as part of the exposure scenarios. Any (theoretical) exposure to acrylonitrile resulting from a combination of scenarios would therefore not result in the DNEL values being exceeded.

In addition to direct (occupational) exposure, workers may also be exposed indirectly to acrylonitrile via the environment (oral, inhalation) or through the use of acrylonitrile polymers in textiles and food contact materials. However the EU RAR concludes that the potential for the indirect exposure of the general population to acrylonitrile through the environment is very low. It is alsodemonstrated that theoretical worst-case exposures of consumers to acrylonitrile through the use of polymers in textiles or food contact materials are also very low. It is therefore concluded that any additional indirect exposure of workers to acrylonitrile will not add significantly to the overall exposure level.

### 10.7.2 Environment (combined for all emission sources)

Environmental emissions of acrylonitrile from individual sites are shown to result in acceptable risk for all compartments. Emissions of acrylonitrile to all compartments are limited by the use of RMMs because individual plants comply both with local limits on release and with the PNEC values derived in this document. The uses of acrylonitrile covered by this Chemical Safety Report are typically performed at different sites; the substance is manufactured at dedicated sites and is subsequently transported to other sites for use as an intermediate or in polymer manufacture. No relevant combination of local environmental exposure scenarios is therefore identified. Acrylonitrile is not persistent or bioaccumulative, reacts readily with organic matter and is biodegraded under environmental conditions, therefore levels of the substance are not likely to persist in the environment.

#### Table 197: Risk characterisation for combined relevant emission

Relevant combination of exposure scenario	Risk characterisation ratio				
Combination 1					
Combination 2	No relevant combinations of exposure scenarios are predicted				