Safety data sheet

COMMISSION REGULATION (EU) No 2015/830 of 1 June 2015 amending Annex II of Regulation (EU) No 453/2010 **Rev -06**

Printing date 25/08/2020 Revision: 24/08/2020

SECTION 1: Identification of the substance/mixture and of the company/ undertaking

· **Trade name: Acetonitrile**
· **CAS Number:**
75-05-8
· **EC number:**
200-835-2
· **Index number:**
608-001-00-3
· **Registration number** 01-2119471307-38-0036
· **1.2 Relevant identified uses of the substance or mixture and uses advised against**
· **Sector of Use**
SU8 Manufacture of bulk, large scale chemicals (including petroleum products)
SU9 Manufacture of fine chemicals
SU 0: Other: 3: Industrial
· **Product category**
PC19 Intermediate
PC20 Products such as ph-regulators, flocculants, precipitants, neutralisation agents
PC21 Laboratory chemicals
PC29 Pharmaceuticals PC30
Photo-chemicals
PC35 Washing and cleaning products (including solvent based products) PC40
Extraction agents
PC0 Other
· **Process category**
PROC1 Use in closed process, no likelihood of exposure
PROC2 Use in closed, continuous process with occasional controlled exposure
PROC3 Use in closed batch process (synthesis or formulation)
PROC4 Use in batch and other process (synthesis) where opportunity for exposure arises PROC8a Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities
PROC8b Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC9 Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
PROC15 Use as laboratory reagent
· **Environmental release category** ERC1
Manufacture of substances ERC2
Formulation of preparations
ERC4 Industrial use of processing aids in processes and products, not becoming part of articles
ERC6a Industrial use resulting in manufacture of another substance (use of intermediates) ERC6b Industrial use of reactive processing aids
ERC7 Industrial use of substances in closed systems
· **Application of the substance / the mixture**
Acetonitrile is used as a chemical intermediate in pesticide manufacture.
Used as a solvent for polymers, spinning fibers, and casting and molding plastics.
Used as a catalyst and ingredient in transition metal complex catalysts, in the photographic

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industry, and for
the extraction and refining of copper and by-product ammonium sulfate.
Used for dyeing textiles and in coating compositions.
Used as a stabilizer for chlorinated solvents in the presence of aluminum.
Used in the manufacture of perfumes and as a reagent in a wide variety of compounds.
Used as a solvent for extraction of hydrocarbons, for separation of fatty acids from vegetable oils, and as a specialty solvent.
Acetonitrile is used only in industrial situations or by professional workers as a solvent or intermediate.

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

· **1.3 Details of the supplier of the safety data sheet**
· **Manufacturer/Supplier:**
Alkyl Amines Chemicals Ltd
401-407 , Nirman Vyapar Kendra, Plot No-10
Sect-17, Vashi, Navi Mumbai
India - 400703

· **Further information obtainable from:**
Emergency Contact no- Kurkumbh: +91 2117 235175 / 235222 Mobile no - +919423002721
Patalganga : +91 2192 261305 / 261329 Mob e no - +919881973507
Emergency Contact No for US only- +1 703 527 3887 / 800 424 9300
e-mail Address of the competent Person responsible for Safety Data Sheet: rsattigeri@alkylamines.com
Information Dept: R&D

OR Details
Global Product Compliance (Europe) AB,
Ideon Science Park, Scheelevägen 17,
Beta 5, 22370 Lund,
Sweden

· **1.4 Emergency telephone number:**
As mentioned above:
Other Comments (e.g. language(s) of the phone service): English

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SECTION 2: Hazards identification

· **2.1 Classification of the substance or mixture**
· **Classification according to Regulation (EC) No 1272/2008**

flame

Flam. Liq. 2 H225 Highly flammable liquid and vapour.

Acute Tox. 4 H302 Harmful if swallowed.
Acute Tox. 4 H312 Harmful in contact with skin.
Acute Tox. 4 H332 Harmful if inhaled.
Eye Irrit. 2 H319 Causes serious eye irritation.

· **2.2 Label elements**
· **Labelling according to Regulation (EC) No 1272/2008**
The substance is classified and labelled according to the CLP regulation.
· **Hazard pictograms**

GHS02 GHS07

· **Signal word** *Danger*
· **Hazard statements**
H225 Highly flammable liquid and vapour.
H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.
H319 Causes serious eye irritation.
· **Precautionary statements**
P233: Keep container tightly closed.
P240: Ground and bond container and receiving equipment.
P242: Use non-sparking tools.
P243: Take actions to prevent static discharges.
P261: Avoid breathing dust/fume/gas/mist/vapours/spray.
P264: Wash ... thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.
P271: Use only outdoors or in a well-ventilated area.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P301: IF SWALLOWED:
P330: Rinse mouth.
P304: IF INHALED:

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P340: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P337: If eye irritation persists:
P313: Get medical advice/attention.
P312: Call a POISON CENTER/doctor/.../if you feel unwell.
P363: Wash contaminated clothing before reuse.
P370: In case of fire:
P378: Use ...[water fog, foam, dry chemical or carbon dioxide]... for extinction.

P210	*Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.*
P241	*Use explosion-proof electrical/ventilating/lighting/equipment.*
P303+P361+P353	*IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.*
P305+P351+P338	*IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.*
P403+P235	*Store in a well-ventilated place. Keep cool.*
P501	*Dispose of contents/container in accordance with local/regional/national/ international regulations.*

· ***2.3 Other hazards***
· ***Results of PBT and vPvB assessment***
· ***PBT:*** *Not applicable.*
· ***vPvB:*** *Not applicable.*

SECTION 3: Composition/information on ingredients

· ***3.1 Chemical characterisation: Substances***
· ***CAS No. Description***
75-05-8 Acetonitrile
· ***Identification number(s)***
· ***EC number:*** *200-835-2*
· ***Index number:*** *608-001-00-3*
· ***Additional information:***
Molecular Formula : C2H3N
Molecular Weight : 41.05 g/mol
Composition : 99 % min.
Synonyms: Ethanenitrile, Methyl cyanide, HSDB 42, CYANOMETHANE
· ***SVHC*** *The substance is not in the list of SVHC substances*

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SECTION 4: First aid measures

· **4.1 Description of first aid measures**

· **General information:**

Immediately remove any clothing soiled by the product.

Symptoms of poisoning may occur even after several hours; therefore, medical observation is suggested for at least 48 hours after the accident.

· **After inhalation:**

If inhaled, remove to fresh air. Keep person warm and at rest. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Resuscitate using a mouth-to-mask with one-way valve or with Ambu Bag. Get medical attention immediately. If symptoms of cyanide poisoning are evident, administer amylnitrate by inhalation for 15-30 seconds every minute. Immediately inject 10 ml of a 3% solution of sodium nitrate intravenously over a period of 1 to 4 minutes.

· **After skin contact:** *Immediately wash exposed skin with soap and water. Remove contaminated clothing and shoes. Wash clothing before reuse. Contaminated leather, particularly footwear, must be discarded. Note that contaminated clothing may be a fire hazard. Get medical attention immediately.*

· **After eye contact:**

Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Get medical attention immediately.

· *After swallowing:*

Get immediate medical attention. Do not wait for symptoms to develop. Do not induce vomiting. If not breathing, ensure clear airway and institute cardiopulmonary resuscitation (CPR). Avoid mouth to mouth resuscitation. Use mouth to mask ventilation with one way valve to exhaust victim's exhaled air away from rescuer. If breathing is difficult, ensure clear airway and give oxygen. If symptomatic, treat as described under Inhalation. If swallowed, rinse mouth with water (only if the person is conscious). Never give anything by mouth to an unconscious person.

· **4.2 Most important symptoms and effects, both acute and delayed**

· *Most important symptoms and effects, both acute and delayed*

Extreme irritation of mucous membranes

After swallowing: Nausea,Vomiting,Dizziness,Headache,Spasms,Unconsciousness,Apnoea

· **Information for doctor:**

Upon absorption and metabolism acetonitrile immediately begins a slow release of cyanide, which can continue for several hours. The toxic effects and associated clinical signs of cyanide poisoning may therefore be delayed. 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.

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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.

· ***4.3 Indication of any immediate medical attention and special treatment needed***
1.Always have a cyanide antidote kit on hand when working with cyanide compounds. Get medical advice to use. The combination of sodium thiosulfate and hydroxycobalamin has been used as an effective antidote.
2.Symptomatic treatment (decontamination, vital functions)

SECTION 5: Firefighting measures

· ***5.1 Extinguishing media***
· ***Suitable extinguishing agents:***
In case of fire, use water fog, foam, dry chemical or carbon dioxide extinguisher or spray.
· ***For safety reasons unsuitable extinguishing agents:*** *Water with full jet*
· ***5.2 Special hazards arising from the substance or mixture***
Decomposition products may include the following materials: carbon oxides (CO, CO2), nitrogen oxides (NO, NO2 etc.), Hydrogen cyanide (HCN).
Unusual fire/explosion hazards: Highly flammable liquid and vapour. Vapour may cause flash fire. Vapours may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.
· ***5.3 Advice for firefighters***
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.
· ***Protective equipment:***
Fire-fighters should wear positive pressure self-contained breathing apparatus (SCBA) and full turnout gear.
· ***Additional information***

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Heating leads to pressure increase entailing danger of bursting and explosion. Immediately cool Neighboring packages and containers with sprayed water and, if possible, remove them out of the danger zone Dispose of fire debris and contaminated fire fighting water in accordance with official regulations. Collect contaminated fire fighting water separately. It must not enter the sewage system.

SECTION 6: Accidental release measures

· **6.1 Personal precautions, protective equipment and emergency procedures**
Immediately contact emergency personnel. Eliminate all ignition sources. Do not touch or walk through spilt material. Keep unnecessary personnel away. Follow all fire-fighting procedures. Use suitable protective equipment.

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

· **6.3 Methods and material for containment and cleaning up:**
Ensure adequate ventilation.
Place spilt material in an appropriate container for disposal. Avoid contact of spilt material with soil and prevent runoff entering surface waterways.

· **6.4 Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

SECTION 7: Handling and storage

· **7.1 Precautions for safe handling**
Do not get in eyes, on skin or on clothing. Keep container closed. Use only with adequate ventilation. Keep away from heat, sparks and flame. Wash thoroughly after handling. Cyanide poisoning first-aid (antidote) kits containing amyl nitrite ampules(or equivalent) must be available at the work site.

· **Information about fire - and explosion protection:**
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. Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
Keep respiratory protective device available.
No welding.
Work on containers and pipelines is permitted only after thorough purging and inerting.

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· **7.2 Conditions for safe storage, including any incompatibilities**
· **Storage:**
· **Requirements to be met by storerooms and receptacles:**
Store under shade at ambient temperature (<45^{0}C) & dry conditions in well-sealed containers. Store in a segregated and approved area.
· **Information about storage in one common storage facility:**
Avoid all possible sources of ignition (spark or flame).
· **Further information about storage conditions:**
Keep container tightly closed and sealed until ready for use.
· **Storage class:** *3 Flammable Liquids*
· **7.3 Specific end use(s)**
API & intermediate synthesis
Purification of Butadiene in refineries
In organic Synthesis & Mfg. of photographic film
Used in Mfg. of DNA oligonucleotides Substitute for chlorinated solvent. Solvent for Agrochemical synthesis

SECTION 8: Exposure controls/personal protection

· **Additional information about design of technical facilities:**
Use adequate ventilation to keep airborne concentrations low. Use explosion-proof ventilation equipment. An eyewash facility and a safety shower shall be provided at suitable places.

· **8.1 Control parameters**

· **Ingredients with limit values that require monitoring at the workplace:**	
75-05-8 acetonitrile	
	EH40-OES (United Kingdom (UK), 2001).
STEL	102 mg/m3 15 minute(s).
STEL	60 ppm 15 minute(s).
TWA	68 mg/m3 8 hour(s).
TWA	40 ppm 8 hour(s).
	EH40-WEL (United Kingdom (UK), 1/2005).
STEL	102 mg/m3 15 minute(s).
STEL	60 ppm 15 minute(s).
TWA	68 mg/m3 8 hour(s).
TWA	40 ppm 8 hour(s).

· **DNELs**
DN(M)ELs for worker:
Acute - systemic effects-Inhalation:
DNEL (Derived No Effect Level)-68 mg/m³

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Acute - local effects-Inhalation:
DNEL (Derived No Effect Level)-68 mg/m³
Long-term - systemic effects-Dermal:
DNEL (Derived No Effect Level)-32.2 mg/kg bw/day
Long-term - systemic effects-Inhalation:
DNEL (Derived No Effect Level)-68 mg/m³
DN(M)ELs for the general population:
Acute - systemic effects-Inhalation:
DNEL (Derived No Effect Level)-220 mg/m³
Acute - systemic effects-Oral
DNEL (Derived No Effect Level)-0.6 mg/kg bw/day
Acute - local effects-Inhalation:
DNEL (Derived No Effect Level)-22 mg/m³
Long-term - systemic effects-Inhalation:
DNEL (Derived No Effect Level)-4.8 mg/m³
Long-term - local effects-Inhalation:
DNEL (Derived No Effect Level)-4.8 mg/m³

· ***PNECs***
PNEC water
PNEC aqua (freshwater): 10 mg/L
PNEC aqua (marine water): 1 mg/L
PNEC aqua (intermittent releases): 10 mg/L
PNEC sediment
PNEC sediment (freshwater): 7.53 mg/kg sediment dw
PNEC soil
PNEC soil: 2.41 mg/kg soil dw
PNEC sewage treatment plant
PNEC STP: 32 mg/L
PNEC oral(secondary poisoning)-No potential for bioaccumulation

· ***Additional information:***
Control Measures: Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapours below their respective occupational exposure limits.

· ***8.2 Exposure controls***
· ***Personal protective equipment:***
· ***General protective and hygienic measures:***
The usual precautionary measures are to be adhered to when handling chemicals.
Wash hands after handling compounds and before eating, smoking and using the lavatory and at the end of the day. Skin and body Do not get on skin or clothing. Wear suitable protective clothing.
· ***Respiratory protection:***
Use with adequate ventilation. Do not breathe vapour or mist. If operating conditions cause high vapour concentrations or the TLV is exceeded, use supplied-air respirator.

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· ***Protection of hands:***

Protective gloves

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

· ***Material of gloves*** *Use gloves of neoprene, butyl rubber or polyethylene.*

· ***Penetration time of glove material***
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

· ***Eye protection:*** *Avoid contact with eyes. Chemical splash goggles.*

· ***Body protection:***
Boots
Impervious protective clothing

SECTION 9: Physical and chemical properties

· ***9.1 Information on basic physical and chemical properties***	
· ***General Information***	
Appearance:	*Liquid*
· ***Form:***	*Liquid*
· ***Colour:***	*Colourless*
· ***Odour:***	*Faint*
· ***Odour threshold:***	*70.0 mg/m³*
· ***pH-value:***	*Not applicable*
· ***Change in condition***	
Melting point/Melting range:	*-45.7 °C (1013 hPa)*
Boiling point/Boiling range:	*81.6 °C (at 101325 Pa)*
· ***Flash point:***	*closed cup: 12.8 deg C* *open cup: 5 to 6 deg C*
· ***Flammability (solid, gaseous):***	*Not applicable*

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· **Ignition temperature:**	524 °C
· **Danger of explosion:**	Product is not explosive. However, formation of explosive air/vapour mixtures is possible
· **Explosion limits:**	
Lower:	3.00 Vol %
Upper:	16 Vol %
· **Oxidising properties**	No
· **Vapour pressure at 20 °C:**	98.64 hPa
· **Density:**	
Relative density at 20 °C	0.79 g/cm³
Vapour density	1.42 (Air=1)
Evaporation rate	5.79 (Butyl Acetate=1)
· **Solubility in / Miscibility with water at 25 °C:**	1,000,000 mg/L
· **Partition coefficient (n-octanol/water) at 25 °C:**	0.34 log POW
· **Viscosity:**	
Dynamic at 20 °C:	0.35 mPas
Kinematic:	Not applicable
· **9.2 Other information**	- Surface tension-29.04 mN/m at 20 deg C - Dissociation constant-pKa estimated to be around 30 - Specific Gravity: 0.78745 at 15 °C/4 °C - Refraction Index: 1.33934 at 30 °C/D - Ionization Potential (eV): 12.20

SECTION 10: Stability and reactivity

· **10.1 Reactivity** No further relevant information available.
· **10.2 Chemical stability** Highly reactive substance.
· **10.3 Possibility of hazardous reactions**
Exothermic reaction with sulfuric acid at 53 º C. This mixture will react with water, steam or acids producing toxic and flammable vapors.
· **10.4 Conditions to avoid**
Avoid all possible sources of ignition (spark or flame). Take precautionary measures against static discharges.
· **10.5 Incompatible materials:**
Incompatible with acids, bases, nitrating agents, nitrogen-fluorine compounds, oxidizers, perchlorates, sulphites.

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· ***10.6 Hazardous decomposition products:***
Decomposition products may include the following materials: carbon oxides (CO, CO2), nitrogen oxides (NO, NO2 etc.), Hydrogen cyanide (HCN).
· ***Additional information:***
Hazardous polymerizationn: Under normal conditions of storage and use, hazardous polymerization will not occur.

SECTION 11: Toxicological information

· ***11.1 Information on toxicological effects***
· ***Acute toxicity***
Harmful if swallowed, in contact with skin or if inhaled.

· **LD/LC50 values relevant for classification:**		
Oral	*LD50*	*617 mg/kg (mouse) (OECD guideline 401)*
		<2000mg/kg (rat)
Dermal	*LD50*	*> 2000 mg/kg (rabbit) (OECD guideline 402)*
Inhalative	*LC50*	*3587 ppm (mouse) (OECD guideline 403)*

· ***Primary irritant effect:***
· ***Skin corrosion/irritation***
In a guideline (OECD 404 equivalent) and GLP study, Acetonitrile (HPLC Grade) was found to be non-irritating to the skin of rabbits (4 -hour exposure). All scores at each observation interval were 0.0 for each animal. No other signs of ill health or test article-related effects were observed during the study. Based on the results of this study, Acetonitrile (HPLC Grade) is non-irritating to the skin of rabbits.
· ***Serious eye damage/irritation***
Causes serious eye irritation.
In a guideline (OECD 405 equivalent) and GLP study, Acetonitrile (HPLC Grade) was found to be severely irritating to the eyes of rabbits, with a maximum group average ocular Draize irritation score of 46.0 occurring at 24 hours post dose. Considerable ocular irritation was observed in all animals, including easily discernable corneal opacity, slight iris injection, diffuse beefy red conjunctivae, obvious swelling, partial lid eversion, and considerable discharge. Some ocular irritation was present in 4 of 6 animals at study termination 21 Days after dosing. No other signs of ill health or toxicity were observed during the study.
· ***Respiratory or skin sensitisation***
Guinea pig (Hartley) male/female
Method-OECD Guideline 406 (Skin Sensitisation)
Buehler test
Induction: epicutaneous, occlusive
Challenge: epicutaneous, occlusive
Result-
No. with positive reactions:
1st reading: 3 out of 20 (test group); 24 h after chall.; dose: Undiluted acetonitrile
2nd reading: 1 out of 20 (test group);

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48 h after chall.; dose: Undiluted Acetonitrile
1st reading: 2 out of 10 (negative control); 24 h after chall.; dose: Undiluted Acetonitrile
2nd reading: 2 out of 10 (negative control); 48 h after chall.; dose: Undiluted Acetonitrile
1st reading: 1 out of 10 (distilled water); 24 h after chall.; dose: undiluted
2nd reading: 2 out of 10 (distilled water); 48 h after chall.; dose: undiluted
1st reading: 10 out of 10 (positive control); 24 h after chall.; dose: 1%
2nd reading: 10 out of 10 (positive control); 48 h after chall.; dose: 1%
1st reading: 3 out of 5 (naive positive control); 24 h after chall.; dose: 1%
2nd reading: 0 out of 5 (naive positive control); 48 h after chall.; dose: 1%
Result- Acetonitrile was found to be non-irritating and non-sensitizing to guinea pig skin.

· ***Subacute to chronic toxicity:***
Respiratory sensitization-Repeated inhalation exposures of experimental animals to acetonitrile has not indicated the potential to cause respiratory sensitization.

· ***Additional toxicological information:***
Acute toxicity: other routes
Acute intraperitoneal toxicity-Rat (Wistar or Nelson rats) female-
LD50: 0.85 - 7.96 mL/kg bw (female) (undiluted)
LD50: 3.89 - 5.62 g/kg bw (female) (in saline)
Acute intravenous toxicity-Rat (Wistar or Nelson rats) female-
LD50: 1.68 mL/kg bw (male)
LD50: 1.68 mL/kg bw (female)
Acute subcutaneous toxicity-mouse
LDLo: 600 - 700 mg/kg bw

· ***Toxicokinetics, metabolism and distribution***
1.Species-rat (Sprague-Dawley) male
oral: gavage
Exposure regime: Single dose
Doses/conc.: LD50 dose (2460 mg/kg) of acetonitrile administered.
Results-metabolism: Cytochrome c oxidase activity and GSH levels of brain, liver and kidney of rats were not remarkably affected 1 hour after administration of an oral LD50 dose of acetonitrile, although cyanide levels were increased in these tissues.
2.Species-mouse (ICR) male
Route-intravenous
Exposure regime: Single dose
Doses/conc.: 684 uCi/kg, equivalent to 60uMol/kg
Results-
Distribution: Whole body autoradiography indicated that radioactivity was widely distributed throughout the body, with high levels in liver, kidney, and gastrointestinal tissues.
Excretion: The half-life of elimination of 2-14C-acetonitrile from blood and most tissues ranged from 5.52 hr in the liver to 8.45 hr in the blood.
3.in vitro study
Route-human cadaver skin
Coverage (dermal absorption study): occlusive
Exposure regime: PERMEABILITY COEFFICIENT: until steady state was achieved
DETERMINATION OF SHORT-TERM ABSORPTION RATE: 10 and 60 MINUTES
Exposure area of 0.64 cm2.

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Doses/conc.: PERMEABILITY COEFFICIENT
Result-
0.2 % at 8 hours (Based on the slope at steady-state, the permeability coefficient was calculated to be 1.82 x 10-4 cm/h.)
≤0.7 % at 60 minutes (Following a 60-minute exposure to a finite application, the short-term penetration rate was calculated to be 66.0 µg equiv/cm2/h.)
% at 10 minutes (Following a 10-minute exposure to a finite application the short-term penetration rate was calculated to be 375.6 µg equiv/cm2/h.)

· ***Sensitisation***
Sensitization
Type: Buehler test
Species: guinea pig
Result: Not sensitizing
Method: OECD Guide-line 406 "skin sensitization"

Type: Patch test
Species: guinea pig
Result: Not sensitizing
Method: OECD Guide-line 406 " skin sensitization"

· ***Repeated dose toxicity***
Repeated dose toxicity: oral
Data waiving-Repeated oral exposure is not expected based on the uses of this substance.
Repeated dose toxicity: inhalation
1. Species-mouse (B6C3F1) male/female-subchronic (inhalation) (whole body) Dose-0, 100, 200, 400, 800, 1600 ppm
Exposure: 13 weeks (6 hours/day, 5 days/week)
Result-
NOAEC: 200 ppm (female) based on: test mat. (Mortality)
NOAEC: 400 ppm (male) based on: test mat. (Mortality)
2. Species-mouse (B6C3F1) male/female-combined repeated dose and carcinogenicity (Inhalation) (Whole body)
Dose-0, 50, 100, 200 ppm (nominal conc.)
Exposure: 103 weeks (6 hours/day, 5 days/week)
Result-NOAEC: 200 ppm (nominal) (male/female) based on: test mat.

· ***CMR effects (carcinogenity, mutagenicity and toxicity for reproduction)***
Carcinogenicity-
Carcinogenicity: inhalation
1. Species-rat (Fischer 344) male/female
Route-whole body
Dose-0, 100, 200, or 400ppm (nominal conc.)
Result-NOAEC (toxicity): 400 ppm (nominal) (male/female) (highest level tested)
Neoplastic effects: no effects
2. Species-Mouse (B6C3F1) male/female
Route-whole body
Dose-0, 50, 100, or 200 ppm (nominal)
Exposure: 103 weeks (6 hours/day, 5 days/week)

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Trade name: Acetonitrile

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Result-NOAEC (toxicity): 200 ppm (nominal) (male/female) (highest level tested)
Neoplastic effects: no effects
Mutagenicity-
In vitro Genotoxicity
1. Method-bacterial reverse mutation assay (e.g. Ames test) (gene mutation)
Species-Salmonella typhimurium strains TA 97, 98, 100, 1535, 1537 (met. act.: with and without)
Doses: 0, 100, 333, 1000, 3333, 10000 ug/plate
Results-Negative (Salmonella typhimurium strains TA 97, 98, 100, 1535, 1537); met. act.: with and without; cytotoxicity: no, but tested up to limit concentrations
2. Method-mammalian cell gene mutation assay (gene mutation)
Chinese hamster Ovary (CHO) (met. act.: with and without)
Doses: Experiment 1 without activation: 11 concentrations ranging from 0.1 - 30 mg/ml
Results-Negative for Chinese hamster Ovary (CHO); met. act.: with and without; cytotoxicity: yes
3. Method-mammalian cell gene mutation assay (gene mutation)
Species-L5178Y mouse lymphoma cells (met. act.: with and without)
Doses: up to 5 ug/ml
Results-Negative (L5178Y mouse lymphoma cells); met. act.: with and without
In vivo Genotoxicity-
Method-EU Method B.12 (Mutagenicity - In Vivo Mammalian Erythrocyte Micronucleus Test)
Micronucleus assay (chromosome aberration)
Species-mouse (NMRI) male/female
Route-intraperitoneal
Dose-100 mg/kg (male); 125 mg/kg (female)
Results-Genotoxicity: negative (male/female); toxicity: yes
Toxicity to reproduction-
Species-Rat (Sprague-Dawley) male/female
Route-inhalation: vapour (whole body)
Dose-0, 150, 300, 600, 1200 ppm (nominal conc.)
Exposure: male: 42 days female: 35-41 days (6 hours daily)
Results-NOEC (P): 600 ppm (male/female) (In the 1200 ppm groups, fertility rate was slightly low , and oestrous cycles changed in some animals. Mortality also occurred.)
Developmental Toxicity-
1. Species-rat (Sprague-Dawley)
Route-oral: gavage
Dose-0, 125, 190, and 275 mg/kg/day
Exposure: Days 6-19 of gestation (Single daily doses)
Result-
NOAEL (maternal toxicity): 190 mg/kg bw/day
NOAEL (embryotoxicity): 190 mg/kg bw/day
NOAEL (teratogenicity): 275 mg/kg bw/day
2. Species-rat (Sprague-Dawley)
Route-inhalation: vapour (whole body)
0, 100, 400, or 1200 ppm (nominal conc.)
Exposure: 6 hours per day on gestation days 6-19

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Result-NOAEC (maternal toxicity): 100 ppm (nominal)
NOAEC (developmental toxicity): ≥1200 ppm (nominal)

· ***Germ cell mutagenicity*** *No data available*
· ***Carcinogenicity*** *No data available*
· ***Reproductive toxicity***
Groups of 10 males and 10 females were exposed to acetonitrile vapor in whole-body inhalation chambers for 6 hours daily for 6 weeks (42 days) for males (from 2 weeks before mating until 2 weeks after the end of the mating period), and for 35 -41 days for females (from 2 weeks before mating until day 19 of pregnancy) at concentrations of 0, 150, 300, 600 or 1200 ppm. In the 1200 ppm group, the fertility rate was slightly lower than controls, and the changes of estrous cycles were found in some animals in the study. Mortality also occurred at the 1200 ppm exposure level. Based on these results the NOECs for systemic toxicity and reproductive toxicity were considered to be 600 ppm in both sexes.
· ***STOT-single exposure*** *No data available*
· ***STOT-repeated exposure*** *No data available*
· ***Aspiration hazard*** *No data available*

SECTION 12: Ecological information

· ***12.1 Toxicity***

· ***Aquatic toxicity:***	
LC50 (72 h) (static)	*400 mg/L (Artemia salina (brine shrimp) Fish)*
LC50 (96 h)	*1640 mg/L (Pimephales promelas (Fish, fresh water))*
NOEC (21 days)	*102 mg/L (Oryzias latipes) (OECD Guideline 204)*
	160 mg/L (Daphnia magna)
NOEC (72 h)	*400 mg/L (Phaeodactylum tricornutum (algae))*

· ***12.2 Persistence and degradability***
Biodegradation in water-
Estimated data-acetonitrile is readily biodegradable
Screening tests-
Result-readily biodegradable
% Degradation of test substance:
65 after 28 d (BOD) (Mean value)
84 after 28 d (TOC removal) (Mean value)
88 after 28 d (GC) (Mean value)
Biodegradation in soil-
A half-life range for acetonitrile in soil of 168 -672 hours (1 -4 weeks) has been estimated from data on aqueous aerobic biodegradation. Further testing for degradation of this substance in soil is not justified on the basis that the substance is readily biodegradable.

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

· ***12.4 Mobility in soil***
Study type: adsorption (soil)
Estimated from the Log Kow
Result-Adsorption coefficient: Koc: 0.3 - 16 (using the octanol-water partition coefficient, log Kow = -0.34.Estimated Koc values for acetonitrile range from 0.3 - 16 and indicate a low potential for adsorption to soils.

· ***12.5 Results of PBT and vPvB assessment***
· ***PBT:*** *Not PBT*
· ***vPvB:*** *Not vPvB*
· ***12.6 Other adverse effects*** *No further relevant information available.*

SECTION 13: Disposal considerations

· ***13.1 Waste treatment methods***
· ***Recommendation :*** *Avoid contact of spilt material and runoff with soil and surface waterways. Consult an environmental professional to determine if local, regional or national regulations would classify spilled or contaminated materials as hazardous waste. Use only approved transporters, recyclers, treatment, storage or disposal facilities. Comply with all local, regional, and national laws pertaining to waste management.*
· ***Uncleaned packaging: Recommendation:*** *Disposal must be made according to official regulations. It is strongly recommended to disfigure the drum/container before disposal.*
· ***Recommended cleansing agents:*** *Water, if necessary together with cleansing agents. Decontamination of drums shall be done by repetitive washing with water.*

SECTION 14: Transport information

· ***14.1 UN-Number***	
· ***ADR, IMDG, IATA***	*UN1648*
· ***14.2 UN proper shipping name***	
· ***ADR***	*1648 ACETONITRILE*
· ***IMDG***	*ACETONITRILE*
· ***IATA***	*Acetonitrile*

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Trade name: Acetonitrile

· **14.3 Transport hazard class(es)**	
· **ADR**	
	
· **Class**	3 Flammable liquids.
· **Label**	3
· **IMDG**	
	
· **Class**	3 Flammable liquids.
· **Label**	3
· **IATA**	
	
· **Class**	3 Flammable liquids.
· **Label**	3
· **14.4 Packing group**	
· **ADR, IMDG, IATA**	II
· **14.5 Environmental hazards:**	
· **Marine pollutant:**	No
· **14.6 Special precautions for user**	Warning: Flammable liquids.
· **Danger code (Kemler):**	336
· **EMS Number:**	F-E,S-D
· **Stowage Category**	B
· **Stowage Code**	SW2 Clear of living quarters.
· **14.7 Transport in bulk according to Annex II of Marpol and the IBC Code**	Not applicable.
· **Transport/Additional information:**	
· **ADR**	
· **Limited quantities (LQ)**	1L
· **Excepted quantities (EQ)**	Code: E2 Maximum net quantity per inner packaging: 3

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·	*Maximum net quantity per outer packaging: 500 ml*
· **Transport category**	*2*
· **Tunnel restriction code**	*D/E*
· **IMDG**	
· **Limited quantities (LQ)**	*1L*
· **Excepted quantities (EQ)**	*Code: E2* *Maximum net quantity per inner packaging: 30 ml* *Maximum net quantity per outer packaging: 500 ml*
· **UN "Model Regulation":**	*UN 1648 ACETONITRILE, 3 (6.1), II*

SECTION 15: Regulatory information

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

· **Labelling according to Regulation (EC) No 1272/2008**

The substance is classified and labelled according to the CLP regulation.

· **Hazard pictograms**

GHS02 GHS07

· **Signal word** *Danger*

· **Hazard statements**

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

· **Precautionary statements**

P233: Keep container tightly closed.
P240: Ground and bond container and receiving equipment.
P242: Use non-sparking tools.
P243: Take actions to prevent static discharges.
P261: Avoid breathing dust/fume/gas/mist/vapours/spray.
P264: Wash ... thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.
P271: Use only outdoors or in a well-ventilated area.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P301: IF SWALLOWED:
P330: Rinse mouth.

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P304: IF INHALED:
P340: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P337: If eye irritation persists:
P313: Get medical advice/attention.
P312: Call a POISON CENTER/doctor/.../if you feel unwell.
P322: Specific measures (see ... on this label).
P363: Wash contaminated clothing before reuse.
P370: In case of fire:
P378: Use ...[water fog, foam, dry chemical or carbon dioxide]... for extinction.

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P241	Use explosion-proof electrical/ventilating/lighting/equipment.
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P321	Specific treatment (see on this label).
P501	Dispose of contents/container in accordance with local/regional/national/ international regulations.

· **Chemical safety assessment** The CSR has been completed

· **National regulations:**

· **Other regulations, limitations and prohibitive regulations**
User to follow national laws and regulations.
· **Substances of very high concern (SVHC) according to REACH, Article 57**
The substance is not listed as SVHC.

· **15.2 Chemical safety assessment:**
Please refer to Annex I for risk management measures and exposure scenario.

SECTION 16: Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

· **Department issuing MSDS:** Product safety department.
· **Contact:**
Emergency Contact no- Kurkumbh: +91 2117 235175 / 235222 Mob e no - +919423002721, +919881973507, Patalganga : +91 2192 261305 / 261329 Mob e no - +919423093443
Emergency Contact No for US only- +1 703 527 3887 / 800 424 9300
e-mail Address of the competent Person responsible for Safety Data Sheet: rsattigeri@alkylamines.com

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· ***Abbreviations and acronyms:***
RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
ICAO: International Civil Aviation Organisation
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
IATA: International Air Transport Association
GHS: Globally Harmonised System of Classification and Labelling of Chemicals
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
DNEL: Derived No-Effect Level (REACH)
PNEC: Predicted No-Effect Concentration (REACH)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
PBT: Persistent, Bioaccumulative and Toxic
SVHC: Substances of Very High Concern
vPvB: very Persistent and very Bioaccumulative
Flam. Liq. 2: Flammable liquids, Hazard Category 2
Acute Tox. 4: Acute toxicity, Hazard Category 4
Eye Irrit. 2: Serious eye damage/eye irritation, Hazard Category 2

· ***Sources***
REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.
- Data is from ECHA registered dossier;
https://echa.europa.eu/registration-dossier/-/registered-dossier/15440
- Genium's Handbook of Safety, Health, and Environmental Data for Common Hazardous Substances.

· **** Data compared to the previous version altered.***
Section 1: Identification of substance and company
Section 3: Composition /Information on Ingredients
Section 4: First-aid measures
Section 5: Fire-fighting measures
Section 6: Accidental Release measures
Section 7: Handling and storage.
Section 8: Exposure Controls/Personal protection.
Section 9: Physical and Chemical properties.
Section 10: Stability and Reactivity.
Section 11: Toxicological Information.
Section 12: Ecological Information.
Section 13 - Disposal Considerations
Section 15 - Regulatory Information
Section 16: Other information

ES FOR COMMUNICATION

Substance Name: acetonitrile

EC Number: 200-835-2

CAS Number: 75-05-8

Registration Number: 01-2119471307-38-0036

Date of Generation:12/06/2014

Date of Revision: 26/09/2019

Rev No - 01

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EXPOSURE ASSESSMENT

The need to carry out an environmental exposure assessment and risk characterisation for acetonitrile has been assessed under the terms of the ECHA document "Guidance on information requirements and chemical safety assessment" Part B, draft chapter B.8 which deals with the scope of the exposure assessment.

This guidance chapter sets out the criteria for which a classification of "no hazard" may be derived for the purposes of REACH and relates the classification to the need to carry out the exposure assessment. It is considered that acetonitrile meets all the criteria thus allowing a classification of "no hazard" for the environment to be derived and, as such, it is determined that no risk characterisation for the environment is required. Details of the relevant properties of acetonitrile which determine the lack of any hazard are listed below. The risk of exposure of man via inhalation is dealt with separately in the human/worker exposure assessment sections.

In order to derive a classification of "no hazard" for the environment the following criteria (which are well below the classification of dangerous in accordance with directive 67/548/EEC and Regulations (EC/1272/2008) should be met:

1. The substance should be readily biodegradable. As demonstrated in section 4.1.2.1.2 acetonitrile may be considered readily biodegradable based on the results of two keys studies and several supporting studies. In the two keys studies degradation in OECD ready biodegradability studies was comfortably above the relevant pass criteria. As such it is considered that this criterion is met.
2. The substance should have a very low potential for bioaccumulation with a log Kow less than 2 and/or a BCF of less than 10. The log Kow for acetonitrile has been determined to be -0.54 which is significantly less than the trigger value considered for the purposes of REACH. In addition to this the estimated BCF for acetonitrile is 2 which is again much less than the value which might indicate a concern.
3. The aquatic toxicity should fulfil both of the following conditions:
    a. Acute EC_{50} or LC_{50} values should be >1000 mg/L. In fish studies the effects on many fish have been investigated with acute LC50s up to 7050 mg/L derived in static studies.

       Acute toxicity studies in Daphnia derived EC_{50} values of up to 10,000 mg/L which indicates no potential for toxicity. In addition to the daphnia studies an acute study was carried out for the very sensitive marine brine shrimp (the results of this study would be considered to be outside the scope of the REACH classification due to the marine nature of this sensitive organism) with mean LC_{50} values in the region of 500 mg/L. Acute algal studies yielded EC50 values greater than 1000 mg/L in all cases with EC_{50} values up to 9696 mg/L derived.

       In a further demonstration of the general lack of toxicity of acetonitrile in the aquatic compartment an 18 hour EC50 was derived for a sediment dwelling organism (the amphipod *Hyalella*). The derived value was 6530 mg/L. Again this demonstrates the lack of potential for toxicity.

    b. Chronic/long terms NOECs should be greater than 10mg/L. Chronic studies for acetonitrile in fish are greater than 100 mg/L. Long term studies using Daphnia derived NOEC values greater than 160 mg/L in all cases. The 48 and 72 hours NOEC values for freshwater and marine algae are 520 and 400 mg/L respectively.

It is considered that acetonitrile comfortably meets the above criteria for the aquatic compartment and no toxicity risk for aquatic organism is indicated.

In addition to these criteria no risk to the terrestrial environment is indicated for acetonitrile based on the studies presented in section 7.2 and there is no evidence for endocrine activity.

Given the above parameters it can be concluded that acetonitrile poses no risk to the environment and as such a classification of "no hazard" may be derived based in the REACH criteria. In addition to this it can be concluded based on the relevant guidance document that there is no need to assess the oral exposure of man via the environment. As such no exposure assessment or risk characterisation is presented or required for risk to the environment or risk to man via the environment.

1. Exposure scenario 1 – Industrial use or manufacture of acetonitrile

1.1. Exposure scenario

Acetonitrile is a coproduct in the manufacture of acrylonitrile by catalytic ammoxidation of propylene.

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

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

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

Environmental Release Category:
ERC1: Manufacture of substances.
ERC2: Formulation of preparations.
ERC4: Industrial use of processing aids in processes and products, not becoming part of articles.
ERC 6a: Industrial use resulting in manufacture of another substance (use of intermediates).
ERC 6b: Industrial use of reactive processing aids.
ERC 7: Industrial use of substances in closed systems.

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

Acetonitrile is manufactured and processed at industrial sites in closed continuous processes with either no likelihood of exposure or with only occasional opportunity for exposure in contolled conditions e.g. during maintenance, sampling or discharge of the material. It is also used in industrial processes which are either closed, continuous processes, or closed batch processes and in batch synthesis where some opportunity for exposure may arise.

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

There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required outdoors, except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. The bulk transfer of Acetonitrile, following manufacture is conducted outside at dedicated facilities using a closed system processes with a vapour return to closed vessels e.g. from external terminal tanks via road or rail tankers, barges or ships to large scale bulk storage vessels.

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

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

Acetonitrile alone.

Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures and use eye goggles, protective gloves/gauntlets (for example butyl rubber gloves), boots and clothing with long sleeves and long legs, in order to minimise exposure.

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

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

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	>1000 tonnes/y	Tonnage produced per year
Emission days per site	365 d/y	Worst case

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

Table: Characteristics of the substance

Information type	Data field	Explanation
Physical state	Liquid	See section 1.3
For solids: Categorisation of dust grades	Not applicable	
Concentration of substance in preparation	99.9%	
Concentration after dilution for use (if relevant)	Not applicable	
Risk management measures related to the design of product		Acetonitrile is manufactured and processed at industrial sites in closed continuous processes with either no likelihood of exposure or with only occasional opportunity for exposure in contolled conditions e.g. during maintenance, sampling or discharge of the material. It is also used in industrial processes which are either a closed, continuous process, or closed batch processes and in batch synthesis where some opportunity for exposure may arise. Exposure to acetonitrile is likely during charging, sampling or discharge of the material. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves), boots and clothing with long sleeves and long legs, in order to minimise exposure.

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

Table: Operational conditions related to respiration and skin contact

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

1.1.5. Other operational conditions of use

Table : 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 kg/kg	The loss of the test substance as a gas is not likely due to the physical chemical properties of the substance.
Fraction of applied amount lost from process/use to waste water	0 kg/kg	Loss of the test substance to waste water is not likely as acetonitrile will be transferred to a closed vessel.
Fraction of applied amount lost from process/use to waste	0 kg/kg	Loss of acetonitrile to waste is not likely as acetonitrile will be transferred to a closed vessel.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

1.1.6. Risk management measures

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

There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. The bulk production of acetonitrile is transported to an external terminal (tankers, barges, ships, large scale bulk storage vessels) for filling into vessels via a closed system with a vapour return. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves), boots and clothing with long sleeves and long legs, in order to minimise exposure.

Table: Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to

Information type	Data field	Explanation
		cope with the worst case scenario.
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) may be required for indoor industrial use.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves
Other risk management measures related to workers		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the production, handling, sampling and transfer of materials are well-trained.
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Not relevant since not classified as dangerous for the environment. In addition acetonitrile is readily biodegradable and would be efficiently removed in the municipal SP system.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	-	Not relevant since not classified as dangerous for the environment
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Not required: no release of substance to waste gas.
Resulting fraction of applied amount in waste gas released to environment	-	Not relevant since not classified as dangerous for the environment.
Onsite waste treatment	Effectiveness (fraction after on-site treatment compared to the fraction entered into waste treatment.	Waste management: incineration and biological waste water treatment on site.
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 since not classified as dangerous for the environment
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. Environmental emissions (air or water) are not predicted.
Effluent (of the waste water treatment plant) discharge rate	-	Not relevant since not classified as dangerous for the environment.
Recovery of sludge for agriculture or horticulture	Yes/no	No

1.1.7. Waste related measures

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such waste related measures are not required.

1.2. Exposure estimation

1.2.1. Worker exposure

Acetonitrile is manufactured and processed at industrial sites in closed continuous processes with either no likelihood of exposure or with only occasional opportunity for exposure in contolled conditions e.g. during maintenance, sampling or discharge of the material. It is also used in industrial processes which are either a closed, continuous process, or closed batch processes and in batch synthesis where some opportunity for exposure may arise.

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

There is potential exposure to acetonitrile during the transfer of the substance. However transfer of the substance is conducted at dedicated facilities using a closed-system with vapour return. Some bulk transfers may occur at facilities which are industrial or professional but not specifically dedicated to Acetonitrile alone however the use of closed systems with vapour return is a requirement because of the flammability risk.

Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. The bulk production of acetonitrile is transported to an external terminal (tankers, barges, ships, large scale bulk storage vessels) for use in industrial processes. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves), boots and clothing with long sleeves and long legs, in order to minimise exposure.

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

Table: Exposure concentrations to workers

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

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

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

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

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

1.2.2. Consumer exposure

Consumers are not directly exposed to the manufacture of acetonitrile.

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

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

1.2.4. Environmental exposure

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such no exposure estimation for the environment is required.

2. Exposure scenario 2 – Pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile

2.1. Exposure scenario

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

As with ES1 exposure to workers has been determined using ECETOC TRA.

Sector of Use:
SU9: Manufacture of fine chemicals.

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

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

Environmental Release Category:
ERC1: Manufacture of substances.
ERC4: Industrial use of processing aids in processes and products, not becoming part of articles. ERC6a:
Industrial use resulting in manufacture of another substance (use of intermediates).

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

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

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

There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required outdoors, except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. The bulk transfer of Acetonitrile following delivery is conducted

outside at dedicated facilities using a closed system processes with a vapour return from road or rail tankers, barges or ships to large scale bulk storage vessels.

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

Workers involved in pharmaceutical, fine chemical and active substance production as plant protection and biocidal products, handling, sampling and transfer of intermediate and process materials are well-trained in these procedures and use eye goggles, protective gloves/gauntlets (for example butyl rubber gloves), boots and clothing with long sleeves and long legs, in order to minimise exposure.

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

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

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	>1000 tonnes/y	Tonnage produced per year
Emission days per site	365 d/y	Worst case

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

Table : Characteristics of the substance

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

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

Table: Operational conditions related to respiration and skin contact

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

2.1.5. Other operational conditions of use

Table: 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 kg/kg	The loss of the test substance as a gas is not likely due to the physical chemical properties of the substance.
Fraction of applied amount lost from process/use to waste water	0 kg/kg	Loss of the test substance to waste water is not likely as acetonitrile will be transferred to a closed vessel.
Fraction of applied amount lost from process/use to waste	0 kg/kg	Loss of acetonitrile to waste is not likely as acetonitrile will be transferred to a closed vessel.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

2.1.6. Risk management measures

The pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile are conducted outdoors in industrial scale processing plants in closed and continuous processes. There is some use in batch processing and synthesis indoors, in highly contolled conditions with LEV. Modern laboratories have local exhaust ventilation (LEV) systems and therefore, the potential for worker exposure to acetonitrile is limited. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves), boots and clothing with long sleeves and long legs, in order to minimise exposure. Pumps, dispensers and pipettes are also used to limit volatilisation. If only general ventilation is employed (*i.e.* weighing acetonitrile in scales outside fumehood), use of respiratory protection may be required.

Table: Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.

Information type	Data field	Explanation
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) may be required for activities where exposure arises.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves Respiratory protection
Other risk management measures related to workers		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the production, handling, sampling and transfer of materials are well-trained.
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Not relevant since not classified as dangerous for the environment
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	-	Not relevant since not classified as dangerous for the environment
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Not required: no release of substance to waste gas.
Resulting fraction of applied amount in waste gas released to environment	-	Not relevant since not classified as dangerous for the environment.
Onsite waste treatment	Effectiveness (fraction after on-site treatment compared to the fraction entered into waste treatment.	Waste management: incineration and biological waste water treatment on site.
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 since not classified as dangerous for the environment
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. Environmental emissions (air or water) are not predicted.
Effluent (of the waste water treatment plant) discharge rate	-	Not relevant since not classified as dangerous for the environment.
Recovery of sludge for agriculture or horticulture	Yes/no	No

2.1.7. Waste related measures

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such waste related measures are not required.

2.2. Exposure estimation

2.2.1. Worker exposure

The pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile are performed outdoors in closed batch and continuous processes. Most modern laboratories have local exhaust ventilation (LEV) systems and therefore, the potential for worker exposure to acetonitrile is limited. Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves), boots and clothing with long sleeves and long legs, in order to minimise exposure. If only general ventilation is employed (*i.e.* weighing acetonitrile in scales outside fumehood), use of respiratory protection may be required.

Table : Exposure concentrations to workers

Routes of exposure	Description of activity	PROC	State of material	Estimated Exposure Concentrations		Measured exposure concentrations	
				Value*	unit	Value	unit
Dermal exposure	Manufacturing including sampling	PROC 1	Liquid	0.343	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 2	Liquid	1.37	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 3	Liquid	0.343	mg/kg/day	No measured data	
	Manufacturing including sampling	PROC 4	Liquid	6.86	mg/kg/day	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8a	Liquid	13.71	mg/kg/day	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8b	Liquid	6.86	mg/kg/day	No measured data	
	Use as laboratory reagent	PROC 15	Liquid	0.0343**	mg/kg/day	No measured data	
Inhalation exposure	Manufacturing including sampling	PROC 1	Liquid	0.012	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 2	Liquid	12.0	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 3	Liquid	29.9	mg/m^3	No measured data	
	Manufacturing including sampling	PROC 4	Liquid	24.0	mg/m^3	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8a	Liquid	60.0	mg/m^3	No measured data	
	Transfer of substance, filling, cleaning of equipment	PROC 8b	Liquid	60.0	mg/m^3	No measured data	
	Use as laboratory reagent	PROC 15	Liquid	1.71**	mg/m^3	No measured data	

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

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

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

Measured inhalation exposure data are not available. The pharmaceutical, fine chemical and active substance manufacture uses of acetonitrile are performed outdoors in closed batch and continuous processes. There is potential exposure to acetonitrile during the transfer of the substance. Generally, no respiratory protection is required except for certain critical activities where respiratory protective equipment is used, for example, cleaning tanks or reactors. The bulk delivery of acetonitrile is via barges, ships, road or rail tankers to bulk storage vessels. Workers involved in the production, handling, sampling and transfer of materials are well- trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves), boots and clothing with long sleeves and long legs, in order to minimise exposure.

2.2.2. Consumer exposure

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

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

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

2.2.4. Environmental exposure

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such no exposure estimation for the environment is required.

3. Exposure scenario 3 – Laboratory use of acetonitrile

3.1. Exposure scenario

Acetonitrile is used as a laboratory reagent.

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

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

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

Environmental Release Category:
ERC4: Industrial use of processing aids in processes and products, not becoming part of articles. ERC6a: Industrial use resulting in manufacture of another substance (use of intermediates).
ERC7: Industrial use of substances in closed systems.

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

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

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

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

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	>1000 tonnes/y	Tonnage produced per year
Emission days per site	365 d/y	Worst case

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

Table : Characteristics of the substance

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

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

Table : Operational conditions related to respiration and skin contact

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

3.1.5. Other operational conditions of use

Table: 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 kg/kg	The loss of the test substance as a gas is not likely due to the physical chemical properties of the substance.
Fraction of applied amount lost from process/use to waste water	0 kg/kg	Loss of the test substance to waste water is not likely as acetonitrile will be transferred to a closed vessel.
Fraction of applied amount lost from process/use to waste	0 kg/kg	Loss of acetonitrile to waste is not likely as acetonitrile will be transferred to a closed vessel.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

3.1.6. Risk management measures

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

Table : Risk management measures for professional use

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.
Local exhaust ventilation not required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) may be required for activities where

Information type	Data field	Explanation
		exposure arises.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves
Risk management measures related to environmental emissions from wide dispersive professional use		
Municipal or other type of waste water treatment	Yes/no	Not relevant since not classified as dangerous for the environment.
Effluent (of the waste water treatment plant) discharge rate	m^3/d	Not relevant since not classified as dangerous for the environment.
Other risk management measures		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the handling, sampling and transfer of materials are well-trained.

3.1.7. Waste related measures

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such waste related measures are not required.

3.2. Exposure estimation

3.2.1. Worker exposure

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

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

Table : Exposure concentrations to workers

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

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

protection.

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

Measured inhalation exposure data are not available. No respiratory protection is required. Professional workers involved in handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves) and clothing with long sleeves and long legs, in order to minimise exposure.

3.2.2. Consumer exposure

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

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

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

3.2.4. Environmental exposure

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such no exposure estimation for the environment is required.

4. Exposure scenario 4 – Photographic/printing uses of acetonitrile

4.1. Exposure scenario

Acetonitrile is used in photographic/printing applications.

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

Product Categories:
PC30: Photochemicals.

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

Environmental Release Category:
ERC7: Industrial use of substances in closed systems.

Article Category:
AC01: Photographic and reprographic articles.

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

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

The photographic/printing use of acetonitrile is performed indoors with general ventilation. Generally, no respiratory protection is required. Professional workers involved in the handling, sampling and transfer of the substance are well-trained in these procedures and they use eye goggles, protective gloves/gauntlets (for example butyl rubber gloves) and clothing with long sleeves and long legs, in order to minimise exposure.

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

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

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	>1000 tonnes/y	Tonnage produced per year
Emission days per site	365 d/y	Worst case

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

Table : Characteristics of the substance

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

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

Table : Operational conditions related to respiration and skin contact

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

4.1.5. Other operational conditions of use

Table : 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 kg/kg	The loss of the test substance as a gas is not likely due to the physical chemical properties of the substance.
Fraction of applied amount lost from process/use to waste water	0 kg/kg	Loss of the test substance to waste water is not likely as acetonitrile will be transferred to a closed vessel.
Fraction of applied amount lost from process/use to waste	0 kg/kg	Loss of acetonitrile to waste is not likely as acetonitrile will be transferred to a closed vessel.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

4.1.6. Risk management measures

The photographic/printing use of acetonitrile is performed indoors with general ventilation. Most modern professional photographic processing is conducted in closed systems with recycling of processing agents and solvents. Given the flammability risk of Acetonitrile, its use and release in such processes will be highly controlled. Limited opportunity for exposure will occur in these situations.

Normally no LEV ventilation is required. Only general ventilation is used. No respiratory protection is required. Professional workers involved in the handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves) and clothing with long sleeves and long legs, in order to minimise exposure.

Table : Risk management measures for professional use

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of

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

4.1.7. Waste related measures

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such waste related measures are not required.

4.2. Exposure estimation

4.2.1. Worker exposure

The photographic/printing use of acetonitrile is performed indoors with general ventilation. Most modern professional photographic processing is conducted in closed systems with recycling of processing agents and solvents. Given the flammability risk of Acetonitrile its use in such processes will be highly controlled. Limited opportunity for exposure will occur in these situations.

Generally, no respiratory protection is required. Professional workers involved in the handling, sampling and transfer of the substance are well-trained in these procedures and they use of appropriate personal protective equipment, in order to minimise exposure and risks. Dermal contact is therefore minimised by the use of personal protective equipment (butyl rubber gloves, long sleeves and long legs).

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

Table : Exposure concentrations to workers

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

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

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

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

Measured inhalation exposure data are not available. The photographic/printing use of acetonitrile is performed indoors with general ventilation. No respiratory protection is required. Professional workers involved in handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves) and clothing with long sleeves and long legs, in order to minimise exposure.

4.2.2. Consumer exposure

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

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

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

4.2.4. Environmental exposure

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such no exposure estimation for the environment is required.

5. Exposure scenario 5 – Repackaging/dilution (Azeotrope creation) of acetonitrile

5.1. Exposure scenario

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

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

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

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

Environmental Release Category:
ERC2: Formulation of preparations.

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

The use of acetonitrile in repacking/dilution applications take place in a closed batch reactor where opportunity for exposure can arise (*i.e.* taking samples at different points of the process, when transferring or loading the substance to/from reactor, when mixing or blending). For tasks where opportunity for exposure arises, use of personal protection equipment is required. Use of local exhaust ventilation (LEV) may also be employed during these activities.

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

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

Information type	Data field	Explanation
Used amount of substance (as such or in preparation) per worker [workplace] per day	Not known	
Duration of exposure per day at workplace [for one worker]	8 h/day	Shift period detailed in R14.2
Frequency of exposure at workplace [for one worker]	220 days per year.	Default value
Annual amount used per site	>1000 tonnes/y	Tonnage produced per year
Emission days per site	365 d/y	Worst case

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

Table : Characteristics of the substance

Information type	Data field	Explanation
Physical state	Liquid	See section 1.3
For solids: Categorisation of dust grades	Not applicable	
Concentration of substance in preparation	99.9%	
Concentration after dilution for use (if relevant)	Not applicable	

Risk management measures related to the design of product		The use of acetonitrile for repackaging/dilution applications takes place in closed batch or continuous processes where potential exposure to workers arises for some specific tasks (*i.e.* taking samples, transfer of the substance, mixing or blending). For tasks where opportunity for exposure arises, use of personal protection equipment is required. Use of local exhaust ventilation (LEV) may also be employed during these activities.

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

Table : Operational conditions related to respiration and skin contact

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

5.1.5. Other operational conditions of use

Table : 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 kg/kg	The loss of the test substance as a gas is not likely due to the physical chemical properties of the substance.
Fraction of applied amount lost from process/use to waste water	0 kg/kg	Loss of the test substance to waste water is not likely as acetonitrile will be transferred to a closed vessel.
Fraction of applied amount lost from process/use to waste	0 kg/kg	Loss of acetonitrile to waste is not likely as acetonitrile will be transferred to a closed vessel.
Fraction consumed in process/use	n/a	n/a
Fraction of applied amount leaving the site with products	n/a	n/a

5.1.6. Risk management measures

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

Table : Risk management measures for professional site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness in terms of residual exposure	Workers involved in production, handling, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario.
Local exhaust ventilation not required and good work practise required	Effectiveness in terms of residual exposure	Local exhaust ventilation (LEV) may be required for activities where exposure arises.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness Gloves: 90% (dermal)	Protective gloves Respiratory protection
Other risk management measures related to workers		
Training to workers to ensure good practise methods.	Effectiveness in terms of residual exposure	Workers involved in the production, handling, sampling and transfer of materials are well-trained.
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Not relevant since not classified as dangerous for the environment
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	-	Not relevant since not classified as dangerous for the environment
Air emission abatement	Effectiveness (emitted fraction after on-site treatment compared to the fraction lost form the technical process)	Not required: no release of substance to waste gas.
Resulting fraction of applied amount in waste gas released to environment	-	Not relevant since not classified as dangerous for the environment.
Onsite waste treatment	Effectiveness (fraction after on-site treatment compared to the fraction entered into waste treatment.	Waste management: incineration and biological waste water treatment on site.
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 since not classified as dangerous for the environment
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. Environmental emissions (air or water) are not predicted.
Effluent (of the waste water treatment plant) discharge rate	-	Not relevant since not classified as dangerous for the environment.
Recovery of sludge for agriculture or horticulture	Yes/no	No

5.1.7. Waste related measures

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such waste related measures are not required.

5.2. Exposure estimation

5.2.1. Worker exposure

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

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

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

Table : Exposure concentrations to workers

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

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

Measured dermal exposure data are not available. There is possible exposure during transfer and sampling, however the use of eye goggles, protective gloves (for example butyl rubber gloves) and clothing with long sleeves and long legs, in order to minimise exposure the widespread use of protective personal equipment (gloves) minimises dermal exposure of this substance.

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

Workers involved in the production, handling, sampling and transfer of materials are well-trained in these procedures and they use eye goggles, protective gloves (for example butyl rubber gloves), clothing with long sleeves and long legs adn respiratory protection in order to minimise exposure.

5.2.2. Consumer exposure

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

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

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

5.2.4. Environmental exposure

As discussed in the overview of the exposure scenarios in section 9 above acetonitrile is considered to be non-hazardous for the environments based on the REACH characterisation criteria. As such no exposure estimation for the environment is required.