Printing date 20.03.2021 Revision: 20.03.2021

## 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 01-2119471307-38-0046
- 1.2 Relevant identified uses of the substance or mixture and uses advised against
- · Sector of Use

SU3 Industrial uses: Uses of substances as such or in preparations at industrial sites

SU8 Manufacture of bulk, large scale chemicals (including petroleum products)

SU9 Manufacture of fine chemicals

SU10 Formulation [mixing] of preparations and/or re-packaging (excluding alloys)

SU11 Manufacture of rubber products

SU16 Manufacture of computer, electronic and optical products, electrical equipment

SU19 Building and construction work

SU20 Health services

SU24 Scientific research and development

SU 0: Other: 3: Industrial

SU2b Offshore industries

#### 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

#### 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

PROC5 Mixing or blending in batch processes for formulation of preparations and articles (multistage and/or significant contact)

PROC6 Calendering operations

PROC7 Industrial spraying

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

(Contd. on page 2)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 1)

#### · Environmental release category

ERC1 Manufacture of substances

ERC2 Formulation of preparations

ERC3 Formulation in materials

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

ERC8a Wide dispersive indoor use of processing aids in open systems

ERC8c Wide dispersive indoor use resulting in inclusion into or onto a matrix

ERC10a Wide dispersive outdoor use of long-life articles and materials with low release

· Article category AC1 Vehicles

#### Application of the substance / the mixture

API & intermediate synthesis

Purification of Butadiene in refineries

In organic Synthesis & Mfg. of photographic film

Used in Mfg. of DNA oligonucleotides

Substitute for cholrinated solvent

Solvent for Agrochemical synthesis

#### · 1.3 Details of the supplier of the safety data sheet

#### · Manufacturer/Supplier:

KAIRAV CHEMOFARBE INDUSTRIES LTD,

502 Filix, LBS Marg,

Opposite Asian Paints, Bhandup (West), Mumbai-400078

#### · Further information obtainable from:

Tel; +91 22 25968361 / 62

Fax:- +91 22 25958586 www.chemofarbe.com

#### OR Details

Sustainability Support Services (Europe) AB

Ideon Science Park, Scheelevägen 17, Beta 5, 22370 Lund, Sweden

#### · 1.4 Emergency telephone number:

Contact details of European importer

Emergency telephone number: 9820353425

Telephone number of EU importer:

Opening hours:

Other Comments (e.g. language(s) of the phone service): English

IN

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 2)

#### SECTION 2: Hazards identification

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



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

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.

(Contd. on page 4)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 3)

· 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.

· SVHC The substance is not in the list of SVHC substances

#### 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

(Contd. on page 5)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 4)

(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 describedunder 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.

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 advise 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: Direct jet water

(Contd. on page 6)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 5)

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

Can form explosive gas-air mixtures.

During heating or in case of fire poisonous gases are produced.

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

Heating leads to pressure increase entailing danger of bursting and explosion. Immediately cool neighbouring 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.

IN

(Contd. on page 7)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 6)

## 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.

#### · 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. Wash thoroughly after handling. Cyanide poisoning first-aid (antidote) kits containing amyl nitrite ampules (or equivalent) must be available at the work site.

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.

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

Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

#### Storage:

#### Requirements to be met by storerooms and receptacles:

Store container tightly sealed at a cool and dry place with sufficient ventilation.

Pay attention to special rules for the storage of flammable liquids.

Provide solvent resistant, sealed floor.

#### Information about storage in one common storage facility:

Store away from foodstuffs.

Store away from feed.

#### Further information about storage conditions:

Store in cool, dry conditions in well sealed receptacles.

Protect from humidity and water.

Protect from heat and direct sunlight.

· 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 cholrinated solvent

Solvent for Agrochemical synthesis

IN

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 7)

### 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/m<sup>3</sup>

Acute - local effects-Inhalation:

DNEL (Derived No Effect Level)-68 mg/m<sup>3</sup>

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/m<sup>3</sup>

DN(M)ELs for the general population:

Acute - systemic effects-Inhalation:

DNEL (Derived No Effect Level)-220 mg/m<sup>3</sup>

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/m<sup>3</sup>

Long-term - systemic effects-Inhalation:

DNEL (Derived No Effect Level)-4.8 mg/m<sup>3</sup>

Long-term - local effects-Inhalation:

DNEL (Derived No Effect Level)-4.8 mg/m<sup>3</sup>

(Contd. on page 9)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 8)

#### · PNECs

PNEC water

PNEC aqua (freshwater): 10 mg/L PNEC aqua (marine water): 1 mg/L

PNEC agua (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

#### · 8.2 Exposure controls

- · Personal protective equipment:
- Respiratory protection:

In case of unintentional release of substance, exceeding the occupational exposure limit value:

In case of brief exposure or low pollution use a respiratory filter device. In case of intensive or longer exposure use a respiratory protective device that is independent of circulating air.

· Protection of hands:



## Protective gloves

Chemical resistant gloves

Check the permeability before using the gloves again.

Preventive skin protection by use of skin-protecting agents is recommended.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

- · Material of gloves Use gloves of neoprene, butyl rubber or povethylene.
- · 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:



Tightly sealed goggles

If vapours or aerosols arise which may injure the eyes, wearing of a full mask is recommended.

Body protection:

**Boots** 

Protective work clothing

(Contd. on page 10)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

Impervious protective clothing

(Contd. of page 9)

9.1 Information on basic physical and General Information	d chemical properties
Appearance: Form: Colour: Odour:	Liquid Colourless Faint
Change in condition  Melting point/Melting range:  Boiling point/Boiling range:	-45.7 ℃(1013 hPa) 81.3 ℃ (1013hPa)
Flash point:	closed cup: 12.8 deg C open cup: 5 to 6 deg C
Flammability (solid, gaseous):	3.0 % (lower limit) and 16.0 % (upper limit) a room temperature-Highly Flammable Liquid
Ignition temperature:	524 ℃ 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 ℃:	98.64 hPa
Density: Relative density at20 ℃	0.79 g/cm³
Solubility in / Miscibility with water at 25 °C:	1,000,000 mg/L
Partition coefficient (n-octanol/water	) <b>at 25</b> 0.34 log POW
Viscosity:	
Dynamic at 20 ℃:	0.35 mPas
9.2 Other information	Surface tension-29.04 dynes/cm at 20 deg C Dissociation constant-pKa estimated to be 4.30

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 10)

## 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 °C. This mixture will react with water, steam or acids producing toxic and flammable vapors.

- · 10.4 Conditions to avoid Flames and heat sources.
- · 10.5 Incompatible materials:

Incompatible with strong oxidizers. The product is incompatible with oleum, chlorosulphonic acid, perchlorates, nitric acid Band sulfur trioxide.

· 10.6 Hazardous decomposition products:

When heated to decomposition emits highly toxic fumes of cyanides.

Additional information: Sensitive to heat and light.

## SECTION 11: Toxicological information

- · 11.1 Information on toxicological effects
- · Acute toxicity

Harmful if swallowed, in contact with skin or if inhaled.

Oral	LD50	617mg/Kg (mouse)
		<2000mg/kg (rat)
Dermal	LD50	980 mg/kg (rabbit)
		3587 ppm (mouse)

- Primary irritant effect:
- · Skin corrosion/irritation

Rabbit

Method - Equivalent or similar to OECD guideline 404

SCORING SYSTEM: Draize method

Result- not irritating

· Serious eye damage/irritation

Causes serious eye irritation.

Rabbit (New Zealand White)

Maximum mean total score (MMTS): 31 - 61 of max. 46 (mean) (Time point: 24 hours post-dose) (not fully reversible within: 21 days)

Method-Equivalent or similar to OECD Guideline 405

Result-Irritating

Respiratory or skin sensitisation

Guinea pig (Hartley) male/female

Method-OECD Guideline 406 (Skin Sensitisation)

Buehler test

Induction: epicutaneous, occlusive

(Contd. on page 12)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 11)

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);

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-Not sensitising

#### 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

(Contd. on page 13)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 12)

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.

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.)

 $\leq$  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  $\mu$ g 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 sensitizina

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

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)

(Contd. on page 14)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 13)

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)

Result-NOAEC (toxicity): 200 ppm (nominal) (male/female) (highest level tested)

Neoplastic effects: no effects

Mutagenecity-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 viivo Genotoxicitv-

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

(Contd. on page 15)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 14)

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 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 No data available
- · 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:

Short term toxicity fish

1. Species-Pimephales promelas

Type of water-freshwater flow-through

Guideline not specified

Value-LC50 (96 h): 1640 mg/L

2. Species-Oryzias latipes

Type of water-freshwater semi-static

OECD Guideline 203 (Fish, Acute Toxicity Test)

Value-LC50 (96 h): > 100 mg/L test mat. (nominal)

Long term toxicity Fish-

Species-Oryzias latipes

Type of water-flow-through freshwater

Value-NOEC (21 d): 102 mg/L test mat. (nominal) based on: mortality, toxicological

symptoms, body weight, body length.

Short-term toxicity to aquatic invertebrates

1. Species-Daphnia magna

Type of water-freshwater static

Value-LC50 (48 h): 3600 mg/L

2. Species-Artemia salina

Type of water-static saltwater

Value-LC50 (24 h): 641 mg/L

LC50 (24 h): 521 mg/L

LC50 (24 h): 400 mg/L

Long-term toxicity to aquatic invertebrates

Daphnia magna freshwater static

Value-

NOEC (21 d): 160 mg/L based on: reproduction

(Contd. on page 16)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 15)

NOEC (21 d): 640 mg/L based on: mortality LOEC (21 d): 320 mg/L based on: reproduction LOEC (21 d): > 1300 mg/L based on: mortality

Algae and aquatic plants-

1.Phaeodactylum tricornutum (algae)

Type of water-saltwater static

Value-EC50 (72 h): 3560 mg/L test mat. (nominal) based on: yield EC50 (72 h): 9696 mg/L test mat. (nominal) based on growth rate

NOEC (72 h): 400 mg/L test mat. (nominal) based on growth rate and yield

2. Species-Microcystis aeruginosa (algae)

Type of water-freshwater static

Value-TT (8 d): 520 mg/L based on: biomass 3.Lemna minor (aquatic plants) freshwater Value-IC50 (96 h): 3663 mg/L (nominal)

NOEC (96 h): 1000 mg/L (nominal) based on: Chlorophyll a concentration

NOEC (96 h): 1000 mg/L (nominal) based on: growth rate

#### · 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.

#### · 12.3 Bioaccumulative potential

BCF: 0.3 - 0.4

Result-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 LogKow

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

(Contd. on page 17)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 16)

• 12.6 Other adverse effects No further relevant information available.

## SECTION 13: Disposal considerations

- · 13.1 Waste treatment methods
- · Recommendation

Disposal Consideration / Waste information: 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:
- Recommended cleansing agents: Water, if necessary together with cleansing agents.

SECTION 14: Transport information		
· 14.1 UN-Number · ADR, IMDG, IATA	1648	
<ul> <li>14.2 UN proper shipping name</li> <li>ADR</li> <li>IMDG, IATA</li> </ul>	1648 ACETONITRILE ACETONITRILE	
· 14.3 Transport hazard class(es) · ADR, IMDG, IATA		
Class Label	3 Flammable liquids. 3	
· 14.4 Packing group · ADR, IMDG, IATA	II	
· 14.5 Environmental hazards: · Marine pollutant:	No	
<ul> <li>14.6 Special precautions for user</li> <li>Danger code (Kemler):</li> <li>EMS Number:</li> </ul>	<i>Warning: Flammable liquids.</i> 33 <i>F-E</i> ,S-D	
<ul> <li>14.7 Transport in bulk according to An II of Marpol and the IBC Code</li> </ul>	<b>nex</b> Not applicable.	

(Contd. on page 18)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 17)

· Transport/Additional information:

· ADR

Limited quantities (LQ)
 Transport category
 Tunnel restriction code

· UN "Model Regulation": UN1648, ACETONITRILE, 3, 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

Please refer section 2





GHS02 GHS07

· Signal word

Danger

Danger

· Hazard statements

Please refer section 2

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

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

(Contd. on page 19)

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 18)

- · 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:

A Chemical Safety Assessment has been carried out.

#### **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.
- · 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

Data is from ECHA registered dossier;

https://echa.europa.eu/registration-dossier/-/registered-dossier/15440

\* 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.

(Contd. on page 20)

Page 20/20

## Safety data sheet COMMISSION REGULATION (EU) No 2015/830 of 1 June 2015 amending Annex II of Regulation (EU) No 453/2010

Printing date 20.03.2021 Revision: 20.03.2021

Trade name: acetonitrile

(Contd. of page 19)

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

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