

Product name: API-TOF Reference Mass Solution Kit
Part no.: G1969-85001

This product is composed of the following:

Kit Components, Reagents

Box/Module Part number	Box/Module Name	Kit Component Part Number	Kit Component Name	Qty Units	CLP
-	-	5191-4282	2.5 mM Hexakis	2	Yes
-	-	5191-4283	5.0 mM Purine	2	Yes
-	-	5191-4284	100 mM Ammonium Trifluoroacetate	2	Yes

Article SDSs, if maintained, are available on www.agilent.com. We recommend using the article product code when searching. SDSs are only available for a limited set of countries.

Transport Information for the Kit:

Dangerous Goods classification for: **G1969-85001**

ADR/RID	IMDG	IATA
UN1648, ACETONITRILE solution, 3, II	UN1648, ACETONITRILE solution, 3, II	UN1648, Acetonitrile solution, 3, II

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5.0 mM Purine.....	16
2.5 mM Hexakis.....	30

SDSs for each individual Kit component follow this cover sheet.

SAFETY DATA SHEET

100 mM Ammonium Trifluoroacetate

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

1.1 Product identifier

Product name : 100 mM Ammonium Trifluoroacetate
Part no. : 5191-4284

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

Identified uses : Reagents and Standards for Analytical Chemistry Laboratory Use
2.2 ml
Uses advised against : None known.

1.3 Details of the supplier of the safety data sheet

Agilent Technologies LDA UK Ltd.
 5500 Lakeside Cheadle Royal Business Park,
 Cheadle, Cheshire, SK8 3GR
 United Kingdom
 Tel: +44 (0) 345 712 5292
e-mail address of person responsible for this SDS : pdl-msds_author@agilent.com

1.4 Emergency telephone number

Emergency telephone number (with hours of operation) : CHEMTREC®: +44 20 3807 3798

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Product definition : Mixture

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

H225	FLAMMABLE LIQUIDS	Category 2
H302	ACUTE TOXICITY (oral)	Category 4
H312	ACUTE TOXICITY (dermal)	Category 4
H332	ACUTE TOXICITY (inhalation)	Category 4
H319	SERIOUS EYE DAMAGE/EYE IRRITATION	Category 2

The product is classified as hazardous according to UK CLP Regulation SI 2019/720 as amended.

See Section 16 for the full text of the H statements declared above.

See Section 11 for more detailed information on health effects and symptoms.

2.2 Label elements

Hazard pictograms :



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

100 mM Ammonium Trifluoroacetate

SECTION 2: Hazards identification

- Prevention** : P280 - Wear protective gloves and protective clothing. Wear eye or face protection.
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P261 - Avoid breathing vapour.
P270 - Do not eat, drink or smoke when using this product.
- Response** : P304 + P312 - IF INHALED: Call a POISON CENTER or doctor if you feel unwell.
- Storage** : Not applicable.
- Disposal** : P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
- Hazardous ingredients** : acetonitrile
- Supplemental label elements** : Not applicable.
- Annex XVII - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles** : Not applicable.
- Special packaging requirements**
- Containers to be fitted with child-resistant fastenings** : Not applicable.
- Tactile warning of danger** : Not applicable.

2.3 Other hazards

- Product meets the criteria for PBT or vPvB according to Regulation (EC) No. 1907/2006, Annex XIII** : This mixture does not contain any substances that are assessed to be a PBT or a vPvB.
- Other hazards which do not result in classification** : None known.

SECTION 3: Composition/information on ingredients

3.2 Mixtures : Mixture

Product/ingredient name	Identifiers	%	Classification	Type
acetonitrile	EC: 200-835-2 CAS: 75-05-8 Index: 608-001-00-3	≥90	Flam. Liq. 2, H225 Acute Tox. 4, H302 Acute Tox. 4, H312 Acute Tox. 4, H332 Eye Irrit. 2, H319 See Section 16 for the full text of the H statements declared above.	[1] [2]

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment, are PBTs, vPvBs or Substances of equivalent concern, or have been assigned a workplace exposure limit and hence require reporting in this section.

Type

[1] Substance classified with a health or environmental hazard

[2] Substance with a workplace exposure limit

Occupational exposure limits, if available, are listed in Section 8.

SECTION 4: First aid measures

4.1 Description of first aid measures

- Eye contact** : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention.
- Inhalation** : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If necessary, call a poison center or physician. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
- Skin contact** : Wash with plenty of soap and water. Remove contaminated clothing and shoes. Wash contaminated clothing thoroughly with water before removing it, or wear gloves. Continue to rinse for at least 10 minutes. Get medical attention if adverse health effects persist or are severe. If necessary, call a poison center or physician. Wash clothing before reuse. Clean shoes thoroughly before reuse.
- Ingestion** : Wash out mouth with water. Remove dentures if any. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Stop if the exposed person feels sick as vomiting may be dangerous. Do not induce vomiting unless directed to do so by medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Get medical attention. If necessary, call a poison center or physician. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.
- Protection of first-aiders** : No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Wash contaminated clothing thoroughly with water before removing it, or wear gloves.

4.2 Most important symptoms and effects, both acute and delayed

Over-exposure signs/symptoms

- Eye contact** : Adverse symptoms may include the following:
pain or irritation
watering
redness
- Inhalation** : No specific data.
- Skin contact** : No specific data.
- Ingestion** : No specific data.

4.3 Indication of any immediate medical attention and special treatment needed

- Notes to physician** : In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
- Specific treatments** : No specific treatment.

SECTION 5: Firefighting measures

5.1 Extinguishing media

- Suitable extinguishing media** : Use dry chemical, CO₂, water spray (fog) or foam.
- Unsuitable extinguishing media** : Do not use water jet.

100 mM Ammonium Trifluoroacetate

SECTION 5: Firefighting measures

5.2 Special hazards arising from the substance or mixture

- Hazards from the substance or mixture** : Highly flammable liquid and vapour. Runoff to sewer may create fire or explosion hazard. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.
- Hazardous combustion products** : Decomposition products may include the following materials:
 carbon dioxide
 carbon monoxide
 nitrogen oxides
 cyanides

5.3 Advice for firefighters

- Special protective actions for fire-fighters** : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.
- Special protective equipment for fire-fighters** : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode. Clothing for fire-fighters (including helmets, protective boots and gloves) conforming to British standard BS EN 469 will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

- For non-emergency personnel** : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilt material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapour or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
- For emergency responders** : If specialised clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

6.2 Environmental precautions

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

6.3 Methods and material for containment and cleaning up

- Methods for cleaning up** : Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Dilute with water and mop up if water-soluble. Alternatively, or if water-insoluble, absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.

6.4 Reference to other sections

- : See Section 1 for emergency contact information.
 See Section 8 for information on appropriate personal protective equipment.
 See Section 13 for additional waste treatment information.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

- Protective measures** : Put on appropriate personal protective equipment (see Section 8). Avoid breathing vapour or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Avoid contact with eyes, skin and clothing. Do not ingest. Empty containers retain product residue and can be hazardous. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Do not reuse container. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment.

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SECTION 7: Handling and storage

Advice on general occupational hygiene : Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

7.2 Conditions for safe storage, including any incompatibilities

Storage : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10) and food and drink. Eliminate all ignition sources. Separate from oxidising materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabelled containers. Use appropriate containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.

Seveso Directive - Reporting thresholds

Danger criteria

Category	Notification and MAPP threshold	Safety report threshold
P5c	5000 tonnes	50000 tonnes

7.3 Specific end use(s)

Recommendations : Industrial applications, Professional applications.

Industrial sector specific solutions : Not available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limits

Product/ingredient name	Exposure limit values
acetonitrile	EH40/2005 WELs (United Kingdom (UK), 1/2020) STEL 15 minutes: 102 mg/m ³ . STEL 15 minutes: 60 ppm. TWA 8 hours: 40 ppm. TWA 8 hours: 68 mg/m ³ .

Biological exposure indices

No exposure indices known.

Recommended monitoring procedures : Reference should be made to monitoring standards, such as the following: British Standard BS EN 689 (Workplace atmospheres - Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy) British Standard BS EN 14042 (Workplace atmospheres - Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents) British Standard BS EN 482 (Workplace atmospheres - General requirements for the performance of procedures for the measurement of chemical agents) Reference to national guidance documents for methods for the determination of hazardous substances will also be required.

DNELs/DMELs

Product/ingredient name	Result

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SECTION 8: Exposure controls/personal protection

acetonitrile	DNEL - General population - Long term - Oral	0.4 mg/kg bw/day
	DNEL - General population - Short term - Oral	0.6 mg/kg bw/day
	DNEL - General population - Long term - Dermal	1.2 mg/kg bw/day
	DNEL - General population - Long term - Inhalation	2.4 mg/m ³

PNECs

Not available.

8.2 Exposure controls

Appropriate engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapour or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Individual protection measures

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: chemical splash goggles.

Skin protection

Hand protection : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

Body protection : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves. Refer to British Standard BS EN 1149 for further information on material and design requirements and test methods.

Other skin protection : Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory protection : Based on the hazard and potential for exposure, select a respirator that meets the appropriate standard or certification. Respirators must be used according to a respiratory protection program to ensure proper fitting, training, and other important aspects of use.

Environmental exposure controls : Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

SECTION 9: Physical and chemical properties

The conditions of measurement of all properties are at standard temperature and pressure unless otherwise indicated.

9.1 Information on basic physical and chemical properties**Appearance**

Physical state	: Liquid.
Colour	: Not available.
Odour	: Not available.
Odour threshold	: Not available.
Melting point/freezing point	: -41.9°C
Initial boiling point and boiling range	: 81.7°C
Flammability	: Not applicable.
Lower and upper explosion limit/flammability limit	: Not available.
Flash point	: Closed cup: 5.85°C
Auto-ignition temperature	: 524°C [Based on solvent.]
Decomposition temperature	: Not available.
pH	: Not available.
Viscosity	: Dynamic (room temperature): Not available. Kinematic (room temperature): Not available. Kinematic (40°C): Not available.

Solubility	: <table border="1"> <thead> <tr> <th>Media</th> <th>Result</th> </tr> </thead> <tbody> <tr> <td>methanol</td> <td>Soluble</td> </tr> <tr> <td>acetone</td> <td>Soluble</td> </tr> <tr> <td>water</td> <td>Soluble</td> </tr> </tbody> </table>	Media	Result	methanol	Soluble	acetone	Soluble	water	Soluble
Media	Result								
methanol	Soluble								
acetone	Soluble								
water	Soluble								

Partition coefficient: n-octanol/water	: Not applicable.
Vapour pressure	: 9.5 kPa (70.88853 mm Hg) [Based on solvent.]
Relative density	: Not available.
Vapour density	: Not available.

Particle characteristics

Median particle size	: Not applicable.
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9.2 Other information**9.2.1 Information with regard to physical hazard classes**

Explosive properties	: Not available.
Oxidising properties	: Not available.

9.2.2 Other safety characteristics

Miscible with water	: Yes.
Evaporation rate	: Not available.
Physical/chemical properties comments	: Not available.

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SECTION 10: Stability and reactivity

- 10.1 Reactivity** : No specific test data related to reactivity available for this product or its ingredients.
- 10.2 Chemical stability** : The product is stable.
- 10.3 Possibility of hazardous reactions** : Under normal conditions of storage and use, hazardous reactions will not occur.
- 10.4 Conditions to avoid** : Avoid all possible sources of ignition (spark or flame). Do not pressurise, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.
- 10.5 Incompatible materials** : Reactive or incompatible with the following materials:
oxidising materials
- 10.6 Hazardous decomposition products** : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Product/ingredient name	Result	
acetonitrile	Rat - Oral - LD50	2460 mg/kg
	Rat - Inhalation - LC50 Vapour	17100 ppm [4 hours]

Conclusion/Summary [Product] : Not available.

Acute toxicity estimates

Product/ingredient name	Oral (mg/kg)	Dermal (mg/kg)	Inhalation (gases) (ppm)	Inhalation (vapours) (mg/l)	Inhalation (dusts and mists) (mg/l)
100 mM Ammonium Trifluoroacetate	555.6	1222.2	N/A	12.2	N/A
acetonitrile	500	1100	N/A	11	N/A

Skin corrosion/irritation

Conclusion/Summary [Product] : Not available.

Serious eye damage/eye irritation

Product/ingredient name	Result	
acetonitrile	Rabbit - Eyes - Moderate irritant	Duration of treatment/ exposure: 24 hours Amount/concentration applied: 100 uL

Conclusion/Summary [Product] : Not available.

Respiratory corrosion/irritation

Conclusion/Summary [Product] : May cause respiratory irritation.

Ingredient name	Conclusion/Summary
acetonitrile	May cause respiratory irritation.

Respiratory or skin sensitization

Skin

100 mM Ammonium Trifluoroacetate

SECTION 11: Toxicological information

Conclusion/Summary : Not available.
[Product]

Respiratory

Conclusion/Summary : Not available.
[Product]

Germ cell mutagenicity

Conclusion/Summary : Not available.
[Product]

Carcinogenicity

Conclusion/Summary : Not available.
[Product]

Reproductive toxicity

Conclusion/Summary : Not available.
[Product]

Specific target organ toxicity (single exposure)

Not available.

Specific target organ toxicity (repeated exposure)

Not available.

Aspiration hazard

Not available.

Information on likely routes of exposure : Routes of entry anticipated: Oral, Dermal, Inhalation, Eyes.

Potential acute health effects

Eye contact : Causes serious eye irritation.
Inhalation : Harmful if inhaled.
Skin contact : Harmful in contact with skin.
Ingestion : Harmful if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact : Adverse symptoms may include the following:
pain or irritation
watering
redness
Inhalation : No specific data.
Skin contact : No specific data.
Ingestion : No specific data.

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Short term exposure

Potential immediate effects : Not available.
Potential delayed effects : Not available.

Long term exposure

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SECTION 11: Toxicological information

Potential immediate effects : Not available.

Potential delayed effects : Not available.

Potential chronic health effects

Conclusion/Summary [Product] : Not available.

General : No known significant effects or critical hazards.

Carcinogenicity : No known significant effects or critical hazards.

Mutagenicity : No known significant effects or critical hazards.

Reproductive toxicity : No known significant effects or critical hazards.

Other information : Adverse symptoms may include the following: May cause headache, weakness, dizziness, shortness of breath, cyanosis, rapid heart beat, unconsciousness and possible death.

SECTION 12: Ecological information

12.1 Toxicity

Product/ingredient name	Result		
acetonitrile	Acute - LC50 - Fresh water	-	-
	Daphnia - Water flea - <i>Daphnia magna</i> Age: <24 hours 3600 mg/l [48 hours] Mortality	-	-
	Acute - IC50 - Fresh water	-	-
	Aquatic plants - Duckweed - <i>Lemna minor</i> 3685 mg/l [96 hours] Population	-	-
	Chronic - NOEC - Fresh water	-	-
	Daphnia - Water flea - <i>Daphnia magna</i> Age: <24 hours 160 mg/l [21 days] Reproduction	-	-
	Chronic - NOEC - Fresh water	-	-
	Aquatic plants - Duckweed - <i>Lemna minor</i> 1000 mg/l [96 hours] Population	-	-
	Acute - LC50 - Fresh water	-	-
	Fish - Fathead minnow - <i>Pimephales promelas</i> Weight: 1.5 g 1000 mg/l [96 hours] Mortality	-	-

Conclusion/Summary [Product] : Not available.

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SECTION 12: Ecological information**12.2 Persistence and degradability****Product/ingredient name****Result**

acetonitrile OECD [Ready Biodegradability - CO₂ in Sealed Vessels (Headspace Test)] 70% [21 days] - Readily -

Conclusion/Summary [Product] : Not available.

Product/ingredient name	Aquatic half-life	Photolysis	Biodegradability
acetonitrile	-	-	Readily

12.3 Bioaccumulative potential

Product/ingredient name	LogP _{ow}	BCF	Potential
acetonitrile	-0.34	3	Low

12.4 Mobility in soil**Soil/water partition coefficient**

Product/ingredient name	logK _{oc}	K _{oc}
acetonitrile	0.42	2.62657

Results of PMT and vPvM assessment

Product/ingredient name	PMT	P	M	T	vPvM	vP	vM
acetonitrile	No	N/A	Yes	No	N/A	N/A	Yes

Mobility : Not available.

Conclusion/Summary : The product does not meet the criteria to be considered as a PMT or vPvM.

12.5 Results of PBT and vPvB assessment**Regulation (EC) No. 1907/2006 [REACH]**

Product/ingredient name	PBT	P	B	T	vPvB	vP	vB
acetonitrile	No	N/A	No	No	No	N/A	No

Regulation (EC) No. 1272/2008 [CLP]

Product/ingredient name	PBT	P	B	T	vPvB	vP	vB
acetonitrile	No	N/A	No	No	No	N/A	No

Conclusion/Summary Regulation (EC) No. 1272/2008 [CLP] : The product does not meet the criteria to be considered as a PBT or vPvB.

12.6 Endocrine disrupting properties

Not available.

Conclusion/Summary [Product] : The product does not meet the criteria to be considered as having endocrine disrupting properties according to the criteria set out in either Regulation (EC) No. 1907/2006 or Regulation (EC) No 1272/2008.

12.7 Other adverse effects

No known significant effects or critical hazards.

100 mM Ammonium Trifluoroacetate

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Methods of disposal : Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. The generation of waste should be avoided or minimised wherever possible. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction.




Hazardous waste : The classification of the product may meet the criteria for a hazardous waste.

Packaging

Methods of disposal : The generation of waste should be avoided or minimised wherever possible. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible.

Special precautions : This material and its container must be disposed of in a safe way. Care should be taken when handling emptied containers that have not been cleaned or rinsed out. Empty containers or liners may retain some product residues. Vapour from product residues may create a highly flammable or explosive atmosphere inside the container. Do not cut, weld or grind used containers unless they have been cleaned thoroughly internally. Avoid dispersal of spilt material and runoff and contact with soil, waterways, drains and sewers.

SECTION 14: Transport information

	ADR/RID	IMDG	IATA
14.1 UN number	UN1648	UN1648	UN1648
14.2 UN proper shipping name	ACETONITRILE solution	ACETONITRILE solution	Acetonitrile solution
14.3 Transport hazard class(es)	3 	3 	3 
14.4 Packing group	II	II	II
14.5 Environmental hazards	No.	No.	No.

Additional information

Remarks: Excepted Quantity

ADR/RID : **Hazard identification number** 33
Limited quantity 1 L
Tunnel code (D/E)

IMDG : **Emergency schedules** F-E, S-D

IATA : **Quantity limitation** Passenger and Cargo Aircraft: 5 L. Packaging instructions: 353. Cargo Aircraft Only: 60 L. Packaging instructions: 364. Limited Quantities - Passenger Aircraft: 1 L. Packaging instructions: Y341.

14.6 Special precautions for user : **Transport within user's premises:** always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

14.7 Transport in bulk according to IMO instruments : Not available.

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SECTION 15: Regulatory information

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

UK (GB)/REACH

Annex XIV - List of substances subject to authorisation

Annex XIV

None of the components are listed.

Substances of very high concern

None of the components are listed.

Ozone depleting substances

Not listed.

Prior Informed Consent (PIC)

Not listed.

Persistent Organic Pollutants

Not listed.

Annex XVII - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles

None of the components are listed / The components are not impacted by a restriction

Labelling : Not applicable.

Seveso Directive

This product is controlled under the Seveso Directive.

Danger criteria

Category

P5c

EU regulations

Industrial emissions (integrated pollution prevention and control) - Air : Listed

Industrial emissions (integrated pollution prevention and control) - Water : Listed

15.2 Chemical safety assessment : This product contains substances for which Chemical Safety Assessments might still be required.

International regulations

Chemical Weapon Convention List Schedules I, II & III Chemicals

Not listed.

Montreal Protocol

Not listed.

Stockholm Convention on Persistent Organic Pollutants

Not listed.

Rotterdam Convention on Prior Informed Consent (PIC)

Not listed.

UNECE Aarhus Protocol on POPs and Heavy Metals

Not listed.

Inventory list

100 mM Ammonium Trifluoroacetate

SECTION 15: Regulatory information

United States : Not determined.

SECTION 16: Other information

Indicates information that has changed from previously issued version.

- Abbreviations and acronyms** :
- ADN = European Provisions concerning the International Carriage of Dangerous Goods by Inland Waterway
 - ADR = The European Agreement concerning the International Carriage of Dangerous Goods by Road
 - ATE = Acute Toxicity Estimate
 - GB CLP = UK CLP (EC No 1272/2008) on the Classification, Labelling and Packaging of Substances and Mixtures as amended by (EU Exit) Regulations 2019 No. 720 and amendments
 - DMEL = Derived Minimal Effect Level
 - DNEL = Derived No Effect Level
 - EUH statement = GB CLP-specific Hazard statement
 - IATA = International Air Transport Association
 - IMDG = International Maritime Dangerous Goods
 - IMO = International Maritime Organization
 - N/A = Not available
 - PBT = Persistent, Bioaccumulative and Toxic
 - PNEC = Predicted No Effect Concentration
 - RID = The Regulations concerning the International Carriage of Dangerous Goods by Rail
 - RRN = REACH Registration Number
 - SGG = Segregation Group
 - vPvB = Very Persistent and Very Bioaccumulative

Procedure used to derive the classification

Classification	Justification
Flam. Liq. 2, H225	On basis of test data
Acute Tox. 4, H302	Calculation method
Acute Tox. 4, H312	Calculation method
Acute Tox. 4, H332	Calculation method
Eye Irrit. 2, H319	Calculation method

Full text of abbreviated H statements

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

Full text of classifications

Acute Tox. 4	ACUTE TOXICITY - Category 4
Eye Irrit. 2	SERIOUS EYE DAMAGE/EYE IRRITATION - Category 2
Flam. Liq. 2	FLAMMABLE LIQUIDS - Category 2

Date of issue/ Date of revision : 09/12/2025

Date of previous issue : 18/06/2025

Version : 1.1

Notice to reader

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SAFETY DATA SHEET

5.0 mM Purine

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

1.1 Product identifier

Product name : 5.0 mM Purine
Part no. : 5191-4283

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

Identified uses : Reagents and Standards for Analytical Chemistry Laboratory Use
 2.2 ml
Uses advised against : None known.

1.3 Details of the supplier of the safety data sheet

Agilent Technologies LDA UK Ltd.
 5500 Lakeside Cheadle Royal Business Park,
 Cheadle, Cheshire, SK8 3GR
 United Kingdom
 Tel: +44 (0) 345 712 5292
e-mail address of person responsible for this SDS : pdl-msds_author@agilent.com

1.4 Emergency telephone number

Emergency telephone number (with hours of operation) : CHEMTREC®: +44 20 3807 3798

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Product definition : Mixture

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

H225	FLAMMABLE LIQUIDS	Category 2
H302	ACUTE TOXICITY (oral)	Category 4
H312	ACUTE TOXICITY (dermal)	Category 4
H332	ACUTE TOXICITY (inhalation)	Category 4
H319	SERIOUS EYE DAMAGE/EYE IRRITATION	Category 2

The product is classified as hazardous according to UK CLP Regulation SI 2019/720 as amended.

See Section 16 for the full text of the H statements declared above.

See Section 11 for more detailed information on health effects and symptoms.

2.2 Label elements

Hazard pictograms :



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

5.0 mM Purine

SECTION 2: Hazards identification

Prevention	: P280 - Wear protective gloves and protective clothing. Wear eye or face protection. P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P261 - Avoid breathing vapour. P270 - Do not eat, drink or smoke when using this product.
Response	: P304 + P312 - IF INHALED: Call a POISON CENTER or doctor if you feel unwell.
Storage	: Not applicable.
Disposal	: P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
Hazardous ingredients	: acetonitrile
Supplemental label elements	: Not applicable.
Annex XVII - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles	: Not applicable.
Special packaging requirements	
Containers to be fitted with child-resistant fastenings	: Not applicable.
Tactile warning of danger	: Not applicable.

2.3 Other hazards

Product meets the criteria for PBT or vPvB according to Regulation (EC) No. 1907/2006, Annex XIII	: This mixture does not contain any substances that are assessed to be a PBT or a vPvB.
Other hazards which do not result in classification	: None known.

SECTION 3: Composition/information on ingredients

3.2 Mixtures : Mixture

Product/ingredient name	Identifiers	%	Classification	Type
acetonitrile	EC: 200-835-2 CAS: 75-05-8 Index: 608-001-00-3	≥90	Flam. Liq. 2, H225 Acute Tox. 4, H302 Acute Tox. 4, H312 Acute Tox. 4, H332 Eye Irrit. 2, H319 See Section 16 for the full text of the H statements declared above.	[1] [2]

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment, are PBTs, vPvBs or Substances of equivalent concern, or have been assigned a workplace exposure limit and hence require reporting in this section.

Type

[1] Substance classified with a health or environmental hazard

[2] Substance with a workplace exposure limit

Occupational exposure limits, if available, are listed in Section 8.

5.0 mM Purine

SECTION 4: First aid measures**4.1 Description of first aid measures**

- Eye contact** : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention.
- Inhalation** : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If necessary, call a poison center or physician. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
- Skin contact** : Wash with plenty of soap and water. Remove contaminated clothing and shoes. Wash contaminated clothing thoroughly with water before removing it, or wear gloves. Continue to rinse for at least 10 minutes. Get medical attention if adverse health effects persist or are severe. If necessary, call a poison center or physician. Wash clothing before reuse. Clean shoes thoroughly before reuse.
- Ingestion** : Wash out mouth with water. Remove dentures if any. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Stop if the exposed person feels sick as vomiting may be dangerous. Do not induce vomiting unless directed to do so by medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Get medical attention. If necessary, call a poison center or physician. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.
- Protection of first-aiders** : No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Wash contaminated clothing thoroughly with water before removing it, or wear gloves.

4.2 Most important symptoms and effects, both acute and delayed**Over-exposure signs/symptoms**

- Eye contact** : Adverse symptoms may include the following:
pain or irritation
watering
redness
- Inhalation** : No specific data.
- Skin contact** : No specific data.
- Ingestion** : No specific data.

4.3 Indication of any immediate medical attention and special treatment needed

- Notes to physician** : In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
- Specific treatments** : No specific treatment.

SECTION 5: Firefighting measures**5.1 Extinguishing media**

- Suitable extinguishing media** : Use dry chemical, CO₂, water spray (fog) or foam.
- Unsuitable extinguishing media** : Do not use water jet.

5.0 mM Purine

SECTION 5: Firefighting measures

5.2 Special hazards arising from the substance or mixture

- Hazards from the substance or mixture** : Highly flammable liquid and vapour. Runoff to sewer may create fire or explosion hazard. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.
- Hazardous combustion products** : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide
nitrogen oxides
cyanides

5.3 Advice for firefighters

- Special protective actions for fire-fighters** : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.
- Special protective equipment for fire-fighters** : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode. Clothing for fire-fighters (including helmets, protective boots and gloves) conforming to British standard BS EN 469 will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

- For non-emergency personnel** : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilt material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapour or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
- For emergency responders** : If specialised clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

6.2 Environmental precautions

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

6.3 Methods and material for containment and cleaning up

- Methods for cleaning up** : Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Dilute with water and mop up if water-soluble. Alternatively, or if water-insoluble, absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.

6.4 Reference to other sections

- : See Section 1 for emergency contact information.
See Section 8 for information on appropriate personal protective equipment.
See Section 13 for additional waste treatment information.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

- Protective measures** : Put on appropriate personal protective equipment (see Section 8). Avoid breathing vapour or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Avoid contact with eyes, skin and clothing. Do not ingest. Empty containers retain product residue and can be hazardous. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Do not reuse container. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment.

5.0 mM Purine

SECTION 7: Handling and storage

Advice on general occupational hygiene : Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

7.2 Conditions for safe storage, including any incompatibilities

Storage : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10) and food and drink. Eliminate all ignition sources. Separate from oxidising materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabelled containers. Use appropriate containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.

Seveso Directive - Reporting thresholds

Danger criteria

Category	Notification and MAPP threshold	Safety report threshold
P5c	5000 tonnes	50000 tonnes

7.3 Specific end use(s)

Recommendations : Industrial applications, Professional applications.

Industrial sector specific solutions : Not available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limits

Product/ingredient name	Exposure limit values
acetonitrile	EH40/2005 WELs (United Kingdom (UK), 1/2020) STEL 15 minutes: 102 mg/m ³ . STEL 15 minutes: 60 ppm. TWA 8 hours: 40 ppm. TWA 8 hours: 68 mg/m ³ .

Biological exposure indices

No exposure indices known.

Recommended monitoring procedures : Reference should be made to monitoring standards, such as the following: British Standard BS EN 689 (Workplace atmospheres - Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy) British Standard BS EN 14042 (Workplace atmospheres - Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents) British Standard BS EN 482 (Workplace atmospheres - General requirements for the performance of procedures for the measurement of chemical agents) Reference to national guidance documents for methods for the determination of hazardous substances will also be required.

DNELs/DMELs

Product/ingredient name	Result

5.0 mM Purine

SECTION 8: Exposure controls/personal protection

acetonitrile	DNEL - General population - Long term - Oral	0.4 mg/kg bw/day
	DNEL - General population - Short term - Oral	0.6 mg/kg bw/day
	DNEL - General population - Long term - Dermal	1.2 mg/kg bw/day
	DNEL - General population - Long term - Inhalation	2.4 mg/m ³

PNECs

Not available.

8.2 Exposure controls

Appropriate engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapour or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Individual protection measures

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: chemical splash goggles.

Skin protection

Hand protection : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

Body protection : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves. Refer to British Standard BS EN 1149 for further information on material and design requirements and test methods.

Other skin protection : Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory protection : Based on the hazard and potential for exposure, select a respirator that meets the appropriate standard or certification. Respirators must be used according to a respiratory protection program to ensure proper fitting, training, and other important aspects of use.

Environmental exposure controls : Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

5.0 mM Purine

SECTION 9: Physical and chemical properties

The conditions of measurement of all properties are at standard temperature and pressure unless otherwise indicated.

9.1 Information on basic physical and chemical properties**Appearance**

Physical state	: Liquid.
Colour	: Not available.
Odour	: Not available.
Odour threshold	: Not available.
Melting point/freezing point	: -41.9°C
Initial boiling point and boiling range	: 81.7°C
Flammability	: Not applicable.
Lower and upper explosion limit/flammability limit	: Not available.
Flash point	: Closed cup: 5.85°C
Auto-ignition temperature	: 524°C [Based on solvent.]
Decomposition temperature	: Not available.
pH	: Not available.
Viscosity	: Dynamic (room temperature): Not available. Kinematic (room temperature): Not available. Kinematic (40°C): Not available.

Solubility	: <table border="1"> <thead> <tr> <th>Media</th> <th>Result</th> </tr> </thead> <tbody> <tr> <td>water</td> <td>Soluble</td> </tr> <tr> <td>methanol</td> <td>Soluble</td> </tr> <tr> <td>acetone</td> <td>Soluble</td> </tr> </tbody> </table>	Media	Result	water	Soluble	methanol	Soluble	acetone	Soluble
Media	Result								
water	Soluble								
methanol	Soluble								
acetone	Soluble								

Partition coefficient: n-octanol/water	: Not applicable.
Vapour pressure	: 9.5 kPa (70.88853 mm Hg) [Based on solvent.]
Relative density	: Not available.
Vapour density	: Not available.

Particle characteristics

Median particle size	: Not applicable.
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9.2 Other information**9.2.1 Information with regard to physical hazard classes**

Explosive properties	: Not available.
Oxidising properties	: Not available.

9.2.2 Other safety characteristics

Miscible with water	: Yes.
Evaporation rate	: Not available.
Physical/chemical properties comments	: Not available.

5.0 mM Purine

SECTION 10: Stability and reactivity

- 10.1 Reactivity** : No specific test data related to reactivity available for this product or its ingredients.
- 10.2 Chemical stability** : The product is stable.
- 10.3 Possibility of hazardous reactions** : Under normal conditions of storage and use, hazardous reactions will not occur.
- 10.4 Conditions to avoid** : Avoid all possible sources of ignition (spark or flame). Do not pressurise, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.
- 10.5 Incompatible materials** : Reactive or incompatible with the following materials:
oxidising materials
- 10.6 Hazardous decomposition products** : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Product/ingredient name	Result	
acetonitrile	Rat - Oral - LD50	2460 mg/kg
	Rat - Inhalation - LC50 Vapour	17100 ppm [4 hours]

Conclusion/Summary [Product] : Not available.

Acute toxicity estimates

Product/ingredient name	Oral (mg/kg)	Dermal (mg/kg)	Inhalation (gases) (ppm)	Inhalation (vapours) (mg/l)	Inhalation (dusts and mists) (mg/l)
5.0 mM Purine	555.6	1222.3	N/A	12.2	N/A
acetonitrile	500	1100	N/A	11	N/A

Skin corrosion/irritation

Conclusion/Summary [Product] : Not available.

Serious eye damage/eye irritation

Product/ingredient name	Result	
acetonitrile	Rabbit - Eyes - Moderate irritant	Duration of treatment/ exposure: 24 hours Amount/concentration applied: 100 uL

Conclusion/Summary [Product] : Not available.

Respiratory corrosion/irritation

Conclusion/Summary [Product] : May cause respiratory irritation.

Ingredient name	Conclusion/Summary
acetonitrile	May cause respiratory irritation.

Respiratory or skin sensitization

Skin

5.0 mM Purine

SECTION 11: Toxicological information

Conclusion/Summary : Not available.
[Product]

Respiratory

Conclusion/Summary : Not available.
[Product]

Germ cell mutagenicity

Conclusion/Summary : Not available.
[Product]

Carcinogenicity

Conclusion/Summary : Not available.
[Product]

Reproductive toxicity

Conclusion/Summary : Not available.
[Product]

Specific target organ toxicity (single exposure)

Not available.

Specific target organ toxicity (repeated exposure)

Not available.

Aspiration hazard

Not available.

Information on likely routes of exposure : Routes of entry anticipated: Oral, Dermal, Inhalation, Eyes.

Potential acute health effects

Eye contact : Causes serious eye irritation.
Inhalation : Harmful if inhaled.
Skin contact : Harmful in contact with skin.
Ingestion : Harmful if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact : Adverse symptoms may include the following:
pain or irritation
watering
redness
Inhalation : No specific data.
Skin contact : No specific data.
Ingestion : No specific data.

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Short term exposure

Potential immediate effects : Not available.
Potential delayed effects : Not available.

Long term exposure

5.0 mM Purine

SECTION 11: Toxicological information

Potential immediate effects : Not available.

Potential delayed effects : Not available.

Potential chronic health effects

Conclusion/Summary [Product] : Not available.

General : No known significant effects or critical hazards.

Carcinogenicity : No known significant effects or critical hazards.

Mutagenicity : No known significant effects or critical hazards.

Reproductive toxicity : No known significant effects or critical hazards.

Other information : Adverse symptoms may include the following: May cause headache, weakness, dizziness, shortness of breath, cyanosis, rapid heart beat, unconsciousness and possible death.

SECTION 12: Ecological information

12.1 Toxicity

Product/ingredient name	Result		
acetonitrile	Acute - LC50 - Fresh water	-	-
	Daphnia - Water flea - <i>Daphnia magna</i> Age: <24 hours 3600 mg/l [48 hours] Mortality		
	Acute - IC50 - Fresh water	-	-
	Aquatic plants - Duckweed - <i>Lemna minor</i> 3685 mg/l [96 hours] Population		
	Chronic - NOEC - Fresh water	-	-
Daphnia - Water flea - <i>Daphnia magna</i> Age: <24 hours 160 mg/l [21 days] Reproduction			
	Chronic - NOEC - Fresh water	-	-
Aquatic plants - Duckweed - <i>Lemna minor</i> 1000 mg/l [96 hours] Population			
	Acute - LC50 - Fresh water	-	-
Fish - Fathead minnow - <i>Pimephales promelas</i> Weight: 1.5 g 1000 mg/l [96 hours] Mortality			

Conclusion/Summary [Product] : Not available.

5.0 mM Purine

SECTION 12: Ecological information**12.2 Persistence and degradability****Product/ingredient name****Result**

acetonitrile OECD [Ready Biodegradability - CO₂ in Sealed Vessels (Headspace Test)] 70% [21 days] - Readily -

Conclusion/Summary [Product] : Not available.

Product/ingredient name	Aquatic half-life	Photolysis	Biodegradability
acetonitrile	-	-	Readily

12.3 Bioaccumulative potential

Product/ingredient name	LogP _{ow}	BCF	Potential
acetonitrile	-0.34	3	Low

12.4 Mobility in soil**Soil/water partition coefficient**

Product/ingredient name	logK _{oc}	K _{oc}
acetonitrile	0.42	2.62657

Results of PMT and vPvM assessment

Product/ingredient name	PMT	P	M	T	vPvM	vP	vM
acetonitrile	No	N/A	Yes	No	N/A	N/A	Yes

Mobility : Not available.

Conclusion/Summary : The product does not meet the criteria to be considered as a PMT or vPvM.

12.5 Results of PBT and vPvB assessment**Regulation (EC) No. 1907/2006 [REACH]**

Product/ingredient name	PBT	P	B	T	vPvB	vP	vB
acetonitrile	No	N/A	No	No	No	N/A	No

Regulation (EC) No. 1272/2008 [CLP]

Product/ingredient name	PBT	P	B	T	vPvB	vP	vB
acetonitrile	No	N/A	No	No	No	N/A	No

Conclusion/Summary : The product does not meet the criteria to be considered as a PBT or vPvB.

Regulation (EC) No. 1272/2008 [CLP]

12.6 Endocrine disrupting properties

Not available.

Conclusion/Summary [Product] : The product does not meet the criteria to be considered as having endocrine disrupting properties according to the criteria set out in either Regulation (EC) No. 1907/2006 or Regulation (EC) No 1272/2008.

12.7 Other adverse effects

No known significant effects or critical hazards.

5.0 mM Purine

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Methods of disposal : Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. The generation of waste should be avoided or minimised wherever possible. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction.




Hazardous waste : The classification of the product may meet the criteria for a hazardous waste.

Packaging

Methods of disposal : The generation of waste should be avoided or minimised wherever possible. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible.

Special precautions : This material and its container must be disposed of in a safe way. Care should be taken when handling emptied containers that have not been cleaned or rinsed out. Empty containers or liners may retain some product residues. Vapour from product residues may create a highly flammable or explosive atmosphere inside the container. Do not cut, weld or grind used containers unless they have been cleaned thoroughly internally. Avoid dispersal of spilt material and runoff and contact with soil, waterways, drains and sewers.

SECTION 14: Transport information

	ADR/RID	IMDG	IATA
14.1 UN number	UN1648	UN1648	UN1648
14.2 UN proper shipping name	ACETONITRILE solution	ACETONITRILE solution	Acetonitrile solution
14.3 Transport hazard class(es)	3 	3 	3 
14.4 Packing group	II	II	II
14.5 Environmental hazards	No.	No.	No.

Additional information

Remarks: Excepted Quantity

ADR/RID : **Hazard identification number** 33
Limited quantity 1 L
Tunnel code (D/E)

IMDG : **Emergency schedules** F-E, S-D

IATA : **Quantity limitation** Passenger and Cargo Aircraft: 5 L. Packaging instructions: 353. Cargo Aircraft Only: 60 L. Packaging instructions: 364. Limited Quantities - Passenger Aircraft: 1 L. Packaging instructions: Y341.

14.6 Special precautions for user : **Transport within user's premises:** always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

14.7 Transport in bulk according to IMO instruments : Not available.

5.0 mM Purine

SECTION 15: Regulatory information

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

UK (GB)/REACH

Annex XIV - List of substances subject to authorisation

Annex XIV

None of the components are listed.

Substances of very high concern

None of the components are listed.

Ozone depleting substances

Not listed.

Prior Informed Consent (PIC)

Not listed.

Persistent Organic Pollutants

Not listed.

Annex XVII - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles

None of the components are listed / The components are not impacted by a restriction

Labelling : Not applicable.

Seveso Directive

This product is controlled under the Seveso Directive.

Danger criteria

Category

P5c

EU regulations

Industrial emissions (integrated pollution prevention and control) - Air : Listed

Industrial emissions (integrated pollution prevention and control) - Water : Listed

15.2 Chemical safety assessment : This product contains substances for which Chemical Safety Assessments might still be required.

International regulations

Chemical Weapon Convention List Schedules I, II & III Chemicals

Not listed.

Montreal Protocol

Not listed.

Stockholm Convention on Persistent Organic Pollutants

Not listed.

Rotterdam Convention on Prior Informed Consent (PIC)

Not listed.

UNECE Aarhus Protocol on POPs and Heavy Metals

Not listed.

Inventory list

5.0 mM Purine

SECTION 15: Regulatory information

United States : Not determined.

SECTION 16: Other information

Indicates information that has changed from previously issued version.

- Abbreviations and acronyms** :
- ADN = European Provisions concerning the International Carriage of Dangerous Goods by Inland Waterway
 - ADR = The European Agreement concerning the International Carriage of Dangerous Goods by Road
 - ATE = Acute Toxicity Estimate
 - GB CLP = UK CLP (EC No 1272/2008) on the Classification, Labelling and Packaging of Substances and Mixtures as amended by (EU Exit) Regulations 2019 No. 720 and amendments
 - DMEL = Derived Minimal Effect Level
 - DNEL = Derived No Effect Level
 - EUH statement = GB CLP-specific Hazard statement
 - IATA = International Air Transport Association
 - IMDG = International Maritime Dangerous Goods
 - IMO = International Maritime Organization
 - N/A = Not available
 - PBT = Persistent, Bioaccumulative and Toxic
 - PNEC = Predicted No Effect Concentration
 - RID = The Regulations concerning the International Carriage of Dangerous Goods by Rail
 - RRN = REACH Registration Number
 - SGG = Segregation Group
 - vPvB = Very Persistent and Very Bioaccumulative

Procedure used to derive the classification

Classification	Justification
Flam. Liq. 2, H225	On basis of test data
Acute Tox. 4, H302	Calculation method
Acute Tox. 4, H312	Calculation method
Acute Tox. 4, H332	Calculation method
Eye Irrit. 2, H319	Calculation method

Full text of abbreviated H statements

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

Full text of classifications

Acute Tox. 4	ACUTE TOXICITY - Category 4
Eye Irrit. 2	SERIOUS EYE DAMAGE/EYE IRRITATION - Category 2
Flam. Liq. 2	FLAMMABLE LIQUIDS - Category 2

Date of issue/ Date of revision : 09/12/2025

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Notice to reader

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SAFETY DATA SHEET

2.5 mM Hexakis

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

1.1 Product identifier

Product name : 2.5 mM Hexakis
Part no. : 5191-4282

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

Identified uses : Reagents and Standards for Analytical Chemistry Laboratory Use
2.2 ml
Uses advised against : None known.

1.3 Details of the supplier of the safety data sheet

Agilent Technologies LDA UK Ltd.
 5500 Lakeside Cheadle Royal Business Park,
 Cheadle, Cheshire, SK8 3GR
 United Kingdom
 Tel: +44 (0) 345 712 5292
e-mail address of person responsible for this SDS : pdl-msds_author@agilent.com

1.4 Emergency telephone number

Emergency telephone number (with hours of operation) : CHEMTREC®: +44 20 3807 3798

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Product definition : Mixture

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

H225	FLAMMABLE LIQUIDS	Category 2
H302	ACUTE TOXICITY (oral)	Category 4
H312	ACUTE TOXICITY (dermal)	Category 4
H332	ACUTE TOXICITY (inhalation)	Category 4
H319	SERIOUS EYE DAMAGE/EYE IRRITATION	Category 2

The product is classified as hazardous according to UK CLP Regulation SI 2019/720 as amended.

See Section 16 for the full text of the H statements declared above.

See Section 11 for more detailed information on health effects and symptoms.

2.2 Label elements

Hazard pictograms :



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

2.5 mM Hexakis

SECTION 2: Hazards identification

- Prevention** : P280 - Wear protective gloves and protective clothing. Wear eye or face protection.
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P261 - Avoid breathing vapour.
P270 - Do not eat, drink or smoke when using this product.
- Response** : P304 + P312 - IF INHALED: Call a POISON CENTER or doctor if you feel unwell.
- Storage** : Not applicable.
- Disposal** : P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
- Hazardous ingredients** : acetonitrile
- Supplemental label elements** : Not applicable.
- Annex XVII - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles** : Not applicable.
- Special packaging requirements**
- Containers to be fitted with child-resistant fastenings** : Not applicable.
- Tactile warning of danger** : Not applicable.

2.3 Other hazards

- Product meets the criteria for PBT or vPvB according to Regulation (EC) No. 1907/2006, Annex XIII** : This mixture does not contain any substances that are assessed to be a PBT or a vPvB.
- Other hazards which do not result in classification** : None known.

SECTION 3: Composition/information on ingredients

3.2 Mixtures : Mixture

Product/ingredient name	Identifiers	%	Classification	Type
acetonitrile	EC: 200-835-2 CAS: 75-05-8 Index: 608-001-00-3	≥90	Flam. Liq. 2, H225 Acute Tox. 4, H302 Acute Tox. 4, H312 Acute Tox. 4, H332 Eye Irrit. 2, H319 See Section 16 for the full text of the H statements declared above.	[1] [2]

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment, are PBTs, vPvBs or Substances of equivalent concern, or have been assigned a workplace exposure limit and hence require reporting in this section.

Type

[1] Substance classified with a health or environmental hazard

[2] Substance with a workplace exposure limit

Occupational exposure limits, if available, are listed in Section 8.

2.5 mM Hexakis

SECTION 4: First aid measures**4.1 Description of first aid measures**

- Eye contact** : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention.
- Inhalation** : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If necessary, call a poison center or physician. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
- Skin contact** : Wash with plenty of soap and water. Remove contaminated clothing and shoes. Wash contaminated clothing thoroughly with water before removing it, or wear gloves. Continue to rinse for at least 10 minutes. Get medical attention if adverse health effects persist or are severe. If necessary, call a poison center or physician. Wash clothing before reuse. Clean shoes thoroughly before reuse.
- Ingestion** : Wash out mouth with water. Remove dentures if any. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Stop if the exposed person feels sick as vomiting may be dangerous. Do not induce vomiting unless directed to do so by medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Get medical attention. If necessary, call a poison center or physician. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.
- Protection of first-aiders** : No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Wash contaminated clothing thoroughly with water before removing it, or wear gloves.

4.2 Most important symptoms and effects, both acute and delayed**Over-exposure signs/symptoms**

- Eye contact** : Adverse symptoms may include the following:
pain or irritation
watering
redness
- Inhalation** : No specific data.
- Skin contact** : No specific data.
- Ingestion** : No specific data.

4.3 Indication of any immediate medical attention and special treatment needed

- Notes to physician** : In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
- Specific treatments** : No specific treatment.

SECTION 5: Firefighting measures**5.1 Extinguishing media**

- Suitable extinguishing media** : Use dry chemical, CO₂, water spray (fog) or foam.
- Unsuitable extinguishing media** : Do not use water jet.

2.5 mM Hexakis

SECTION 5: Firefighting measures

5.2 Special hazards arising from the substance or mixture

- Hazards from the substance or mixture** : Highly flammable liquid and vapour. Runoff to sewer may create fire or explosion hazard. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.
- Hazardous combustion products** : Decomposition products may include the following materials:
 carbon dioxide
 carbon monoxide
 nitrogen oxides
 cyanides

5.3 Advice for firefighters

- Special protective actions for fire-fighters** : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.
- Special protective equipment for fire-fighters** : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode. Clothing for fire-fighters (including helmets, protective boots and gloves) conforming to British standard BS EN 469 will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

- For non-emergency personnel** : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilt material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapour or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
- For emergency responders** : If specialised clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

6.2 Environmental precautions

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

6.3 Methods and material for containment and cleaning up

- Methods for cleaning up** : Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Dilute with water and mop up if water-soluble. Alternatively, or if water-insoluble, absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.

6.4 Reference to other sections

- : See Section 1 for emergency contact information.
 See Section 8 for information on appropriate personal protective equipment.
 See Section 13 for additional waste treatment information.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

- Protective measures** : Put on appropriate personal protective equipment (see Section 8). Avoid breathing vapour or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Avoid contact with eyes, skin and clothing. Do not ingest. Empty containers retain product residue and can be hazardous. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Do not reuse container. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment.

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SECTION 7: Handling and storage

Advice on general occupational hygiene : Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

7.2 Conditions for safe storage, including any incompatibilities

Storage : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10) and food and drink. Eliminate all ignition sources. Separate from oxidising materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabelled containers. Use appropriate containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.

Seveso Directive - Reporting thresholds

Danger criteria

Category	Notification and MAPP threshold	Safety report threshold
P5c	5000 tonnes	50000 tonnes

7.3 Specific end use(s)

Recommendations : Industrial applications, Professional applications.

Industrial sector specific solutions : Not available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limits

Product/ingredient name	Exposure limit values
acetonitrile	EH40/2005 WELs (United Kingdom (UK), 1/2020) STEL 15 minutes: 102 mg/m ³ . STEL 15 minutes: 60 ppm. TWA 8 hours: 40 ppm. TWA 8 hours: 68 mg/m ³ .

Biological exposure indices

No exposure indices known.

Recommended monitoring procedures : Reference should be made to monitoring standards, such as the following: British Standard BS EN 689 (Workplace atmospheres - Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy) British Standard BS EN 14042 (Workplace atmospheres - Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents) British Standard BS EN 482 (Workplace atmospheres - General requirements for the performance of procedures for the measurement of chemical agents) Reference to national guidance documents for methods for the determination of hazardous substances will also be required.

DNELs/DMELs

Product/ingredient name	Result

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SECTION 8: Exposure controls/personal protection

acetonitrile	DNEL - General population - Long term - Oral	0.4 mg/kg bw/day
	DNEL - General population - Short term - Oral	0.6 mg/kg bw/day
	DNEL - General population - Long term - Dermal	1.2 mg/kg bw/day
	DNEL - General population - Long term - Inhalation	2.4 mg/m ³

PNECs

Not available.

8.2 Exposure controls

Appropriate engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapour or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Individual protection measures

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: chemical splash goggles.

Skin protection

Hand protection : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

Body protection : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves. Refer to British Standard BS EN 1149 for further information on material and design requirements and test methods.

Other skin protection : Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory protection : Based on the hazard and potential for exposure, select a respirator that meets the appropriate standard or certification. Respirators must be used according to a respiratory protection program to ensure proper fitting, training, and other important aspects of use.

Environmental exposure controls : Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

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SECTION 9: Physical and chemical properties

The conditions of measurement of all properties are at standard temperature and pressure unless otherwise indicated.

9.1 Information on basic physical and chemical properties

Appearance

- Physical state** : Liquid.
- Colour** : Not available.
- Odour** : Not available.
- Odour threshold** : Not available.
- Melting point/freezing point** : -41.9°C
- Initial boiling point and boiling range** : 81.7°C
- Flammability** : Not applicable.
- Lower and upper explosion limit/flammability limit** : Not available.
- Flash point** : Closed cup: 5.85°C
- Auto-ignition temperature** : 524°C [Based on solvent.]
- Decomposition temperature** : Not available.
- pH** : Not available.
- Viscosity** : Dynamic (room temperature): Not available.
Kinematic (room temperature): Not available.
Kinematic (40°C): Not available.

Solubility	Media	Result
	methanol	Soluble
	acetone	Soluble
	water	Soluble

- Partition coefficient: n-octanol/water** : Not applicable.
- Vapour pressure** : 9.5 kPa (70.88853 mm Hg) [Based on solvent.]
- Relative density** : Not available.
- Vapour density** : Not available.

Particle characteristics

- Median particle size** : Not applicable.

9.2 Other information

9.2.1 Information with regard to physical hazard classes

- Explosive properties** : Not available.
- Oxidising properties** : Not available.

9.2.2 Other safety characteristics

- Miscible with water** : Yes.
- Evaporation rate** : Not available.
- Physical/chemical properties comments** : Not available.

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SECTION 10: Stability and reactivity

- 10.1 Reactivity** : No specific test data related to reactivity available for this product or its ingredients.
- 10.2 Chemical stability** : The product is stable.
- 10.3 Possibility of hazardous reactions** : Under normal conditions of storage and use, hazardous reactions will not occur.
- 10.4 Conditions to avoid** : Avoid all possible sources of ignition (spark or flame). Do not pressurise, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.
- 10.5 Incompatible materials** : Reactive or incompatible with the following materials:
oxidising materials
- 10.6 Hazardous decomposition products** : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Product/ingredient name	Result	
acetonitrile	Rat - Oral - LD50	2460 mg/kg
	Rat - Inhalation - LC50 Vapour	17100 ppm [4 hours]

Conclusion/Summary : Not available.

[Product]

Acute toxicity estimates

Product/ingredient name	Oral (mg/kg)	Dermal (mg/kg)	Inhalation (gases) (ppm)	Inhalation (vapours) (mg/l)	Inhalation (dusts and mists) (mg/l)
2.5 mM Hexakis acetonitrile	500.0 500	1100.0 1100	N/A N/A	11.0 11	N/A N/A

Skin corrosion/irritation

Conclusion/Summary : Not available.

[Product]

Serious eye damage/eye irritation

Product/ingredient name	Result	
acetonitrile	Rabbit - Eyes - Moderate irritant	Duration of treatment/ exposure: 24 hours Amount/concentration applied: 100 uL

Conclusion/Summary : Not available.

[Product]

Respiratory corrosion/irritation

Conclusion/Summary : May cause respiratory irritation.

[Product]

Ingredient name	Conclusion/Summary
acetonitrile	May cause respiratory irritation.

Respiratory or skin sensitization

Skin

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SECTION 11: Toxicological information

Conclusion/Summary [Product] : Not available.

Respiratory

Conclusion/Summary [Product] : Not available.

Germ cell mutagenicity

Conclusion/Summary [Product] : Not available.

Carcinogenicity

Conclusion/Summary [Product] : Not available.

Reproductive toxicity

Conclusion/Summary [Product] : Not available.

Specific target organ toxicity (single exposure)

Not available.

Specific target organ toxicity (repeated exposure)

Not available.

Aspiration hazard

Not available.

Information on likely routes of exposure : Routes of entry anticipated: Oral, Dermal, Inhalation, Eyes.

Potential acute health effects

Eye contact : Causes serious eye irritation.
Inhalation : Harmful if inhaled.
Skin contact : Harmful in contact with skin.
Ingestion : Harmful if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact : Adverse symptoms may include the following:
pain or irritation
watering
redness
Inhalation : No specific data.
Skin contact : No specific data.
Ingestion : No specific data.

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Short term exposure

Potential immediate effects : Not available.
Potential delayed effects : Not available.

Long term exposure

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SECTION 11: Toxicological information

Potential immediate effects : Not available.

Potential delayed effects : Not available.

Potential chronic health effects

Conclusion/Summary [Product] : Not available.

General : No known significant effects or critical hazards.

Carcinogenicity : No known significant effects or critical hazards.

Mutagenicity : No known significant effects or critical hazards.

Reproductive toxicity : No known significant effects or critical hazards.

Other information : Adverse symptoms may include the following: May cause headache, weakness, dizziness, shortness of breath, cyanosis, rapid heart beat, unconsciousness and possible death.

SECTION 12: Ecological information

12.1 Toxicity

Product/ingredient name	Result		
acetonitrile	Acute - LC50 - Fresh water	-	-
	Daphnia - Water flea - <i>Daphnia magna</i> Age: <24 hours 3600 mg/l [48 hours] Mortality		
	Acute - IC50 - Fresh water	-	-
	Aquatic plants - Duckweed - <i>Lemna minor</i> 3685 mg/l [96 hours] Population		
	Chronic - NOEC - Fresh water	-	-
	Daphnia - Water flea - <i>Daphnia magna</i> Age: <24 hours 160 mg/l [21 days] Reproduction		
	Chronic - NOEC - Fresh water	-	-
	Aquatic plants - Duckweed - <i>Lemna minor</i> 1000 mg/l [96 hours] Population		
	Acute - LC50 - Fresh water	-	-
	Fish - Fathead minnow - <i>Pimephales promelas</i> Weight: 1.5 g 1000 mg/l [96 hours] Mortality		

Conclusion/Summary [Product] : Not available.

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SECTION 12: Ecological information**12.2 Persistence and degradability****Product/ingredient name****Result**

acetonitrile OECD [Ready Biodegradability - CO₂ in Sealed Vessels (Headspace Test)] 70% [21 days] - Readily -

Conclusion/Summary [Product] : Not available.

Product/ingredient name	Aquatic half-life	Photolysis	Biodegradability
acetonitrile	-	-	Readily

12.3 Bioaccumulative potential

Product/ingredient name	LogP _{ow}	BCF	Potential
acetonitrile	-0.34	3	Low

12.4 Mobility in soil**Soil/water partition coefficient**

Product/ingredient name	logK _{oc}	K _{oc}
acetonitrile	0.42	2.62657

Results of PMT and vPvM assessment

Product/ingredient name	PMT	P	M	T	vPvM	vP	vM
acetonitrile	No	N/A	Yes	No	N/A	N/A	Yes

Mobility : Not available.

Conclusion/Summary : The product does not meet the criteria to be considered as a PMT or vPvM.

12.5 Results of PBT and vPvB assessment**Regulation (EC) No. 1907/2006 [REACH]**

Product/ingredient name	PBT	P	B	T	vPvB	vP	vB
acetonitrile	No	N/A	No	No	No	N/A	No

Regulation (EC) No. 1272/2008 [CLP]

Product/ingredient name	PBT	P	B	T	vPvB	vP	vB
acetonitrile	No	N/A	No	No	No	N/A	No

Conclusion/Summary : The product does not meet the criteria to be considered as a PBT or vPvB.

Regulation (EC) No. 1272/2008 [CLP]

12.6 Endocrine disrupting properties

Not available.

Conclusion/Summary [Product] : The product does not meet the criteria to be considered as having endocrine disrupting properties according to the criteria set out in either Regulation (EC) No. 1907/2006 or Regulation (EC) No 1272/2008.

12.7 Other adverse effects

No known significant effects or critical hazards.

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SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Methods of disposal : Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. The generation of waste should be avoided or minimised wherever possible. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction.




Hazardous waste : The classification of the product may meet the criteria for a hazardous waste.

Packaging

Methods of disposal : The generation of waste should be avoided or minimised wherever possible. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible.

Special precautions : This material and its container must be disposed of in a safe way. Care should be taken when handling emptied containers that have not been cleaned or rinsed out. Empty containers or liners may retain some product residues. Vapour from product residues may create a highly flammable or explosive atmosphere inside the container. Do not cut, weld or grind used containers unless they have been cleaned thoroughly internally. Avoid dispersal of spilt material and runoff and contact with soil, waterways, drains and sewers.

SECTION 14: Transport information

	ADR/RID	IMDG	IATA
14.1 UN number	UN1648	UN1648	UN1648
14.2 UN proper shipping name	ACETONITRILE solution	ACETONITRILE solution	Acetonitrile solution
14.3 Transport hazard class(es)	3 	3 	3 
14.4 Packing group	II	II	II
14.5 Environmental hazards	No.	No.	No.

Additional information

Remarks: Excepted Quantity

ADR/RID : **Hazard identification number** 33
Limited quantity 1 L
Tunnel code (D/E)

IMDG : **Emergency schedules** F-E, S-D

IATA : **Quantity limitation** Passenger and Cargo Aircraft: 5 L. Packaging instructions: 353. Cargo Aircraft Only: 60 L. Packaging instructions: 364. Limited Quantities - Passenger Aircraft: 1 L. Packaging instructions: Y341.

14.6 Special precautions for user : **Transport within user's premises:** always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

14.7 Transport in bulk according to IMO instruments : Not available.

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SECTION 15: Regulatory information

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

UK (GB)/REACH

Annex XIV - List of substances subject to authorisation

Annex XIV

None of the components are listed.

Substances of very high concern

None of the components are listed.

Ozone depleting substances

Not listed.

Prior Informed Consent (PIC)

Not listed.

Persistent Organic Pollutants

Not listed.

Annex XVII - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles

None of the components are listed / The components are not impacted by a restriction

Labelling : Not applicable.

Seveso Directive

This product is controlled under the Seveso Directive.

Danger criteria

Category

P5c

EU regulations

Industrial emissions (integrated pollution prevention and control) - Air : Listed

Industrial emissions (integrated pollution prevention and control) - Water : Listed

15.2 Chemical safety assessment : This product contains substances for which Chemical Safety Assessments might still be required.

International regulations

Chemical Weapon Convention List Schedules I, II & III Chemicals

Not listed.

Montreal Protocol

Not listed.

Stockholm Convention on Persistent Organic Pollutants

Not listed.

Rotterdam Convention on Prior Informed Consent (PIC)

Not listed.

UNECE Aarhus Protocol on POPs and Heavy Metals

Not listed.

Inventory list

2.5 mM Hexakis

SECTION 15: Regulatory information

United States : Not determined.

SECTION 16: Other information

Indicates information that has changed from previously issued version.

Abbreviations and acronyms :

- ADN = European Provisions concerning the International Carriage of Dangerous Goods by Inland Waterway
- ADR = The European Agreement concerning the International Carriage of Dangerous Goods by Road
- ATE = Acute Toxicity Estimate
- GB CLP = UK CLP (EC No 1272/2008) on the Classification, Labelling and Packaging of Substances and Mixtures as amended by (EU Exit) Regulations 2019 No. 720 and amendments
- DMEL = Derived Minimal Effect Level
- DNEL = Derived No Effect Level
- EUH statement = GB CLP-specific Hazard statement
- IATA = International Air Transport Association
- IMDG = International Maritime Dangerous Goods
- IMO = International Maritime Organization
- N/A = Not available
- PBT = Persistent, Bioaccumulative and Toxic
- PNEC = Predicted No Effect Concentration
- RID = The Regulations concerning the International Carriage of Dangerous Goods by Rail
- RRN = REACH Registration Number
- SGG = Segregation Group
- vPvB = Very Persistent and Very Bioaccumulative

Procedure used to derive the classification

Classification	Justification
Flam. Liq. 2, H225	On basis of test data
Acute Tox. 4, H302	Calculation method
Acute Tox. 4, H312	Calculation method
Acute Tox. 4, H332	Calculation method
Eye Irrit. 2, H319	Calculation method

Full text of abbreviated H statements

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

Full text of classifications

Acute Tox. 4	ACUTE TOXICITY - Category 4
Eye Irrit. 2	SERIOUS EYE DAMAGE/EYE IRRITATION - Category 2
Flam. Liq. 2	FLAMMABLE LIQUIDS - Category 2

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Version : 1.1

Notice to reader

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