

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

Table of contents

Kit Component Name	Page
100 mM Ammonium Trifluoroacetate.....	2
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 Deutschland GmbH
 Hewlett-Packard-Str. 8
 76337 Waldbronn
 Germany
 0800 603 1000

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®: +353 1 901 4670

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 Regulation (EC) 1272/2008 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**
- 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	Specific Conc. Limits, M-factors and ATEs	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.	ATE [Oral] = 500 mg/kg ATE [Dermal] = 1100 mg/kg ATE [Inhalation (vapours)] = 11 mg/l	[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.

100 mM Ammonium Trifluoroacetate

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 precautions 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 European standard 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

100 mM Ammonium Trifluoroacetate

SECTION 7: Handling and storage

(ventilating, lighting and material handling) equipment.

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	<p>NAOSH (Ireland, 4/2024) Absorbed through skin. Notes: EU derived Occupational Exposure Limit Values</p> <p>OELV 8 hours: 40 ppm. OELV 8 hours: 70 mg/m³. OELV 15 minutes: 4 mg/m³. OELV 15 minutes: 1.8 ppm.</p> <p>EU OEL (Europe, 1/2022) Absorbed through skin.</p> <p>TWA 8 hours: 40 ppm. TWA 8 hours: 70 mg/m³.</p>

Biological exposure indices

No exposure indices known.

Recommended monitoring procedures

: Reference should be made to monitoring standards, such as the following: European Standard EN 689 (Workplace atmospheres - Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy) European Standard EN 14042 (Workplace atmospheres - Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents) European Standard 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

100 mM Ammonium Trifluoroacetate

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 European Standard 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.

100 mM Ammonium Trifluoroacetate

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
- Boiling point or 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.
- Relative 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.

100 mM Ammonium Trifluoroacetate

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 Rat - Inhalation - LC50 Vapour	2460 mg/kg 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

100 mM Ammonium Trifluoroacetate

SECTION 11: Toxicological information**Skin**

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

Potential immediate effects : Not available.

100 mM Ammonium Trifluoroacetate

SECTION 11: Toxicological information

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.

11.2 Information on other hazards

11.2.1 Endocrine disrupting properties

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.

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	3600 mg/l [48 hours]
	Acute - IC50 - Fresh water	3685 mg/l [96 hours]
	Chronic - NOEC - Fresh water	160 mg/l [21 days]
	Chronic - NOEC - Fresh water	1000 mg/l [96 hours]
	Acute - LC50 - Fresh water	1000 mg/l [96 hours]

Conclusion/Summary [Product] : Not available.

12.2 Persistence and degradability

Product/ingredient name	Result
acetonitrile	- 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.

100 mM Ammonium Trifluoroacetate

SECTION 12: Ecological information

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

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.

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 or ID 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 

100 mM Ammonium Trifluoroacetate

SECTION 14: Transport information

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.

SECTION 15: Regulatory information

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

EU Regulation (EC) No. 1907/2006 (REACH)

Annex XIV - List of substances subject to authorisation

Annex XIV

Substances of very high concern

None of the components are 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.

Other EU regulations

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

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

Ozone depleting substances (EU 2024/590)

Not listed.

Prior Informed Consent (PIC) (649/2012/EU)

Not listed.

Persistent Organic Pollutants

Not listed.

Seveso Directive

100 mM Ammonium Trifluoroacetate

SECTION 15: Regulatory information

This product is controlled under the Seveso Directive.

Danger criteria

Category

P5c

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

Australia	: Not determined.
Canada	: Not determined.
China	: Not determined.
Eurasian Economic Union	: Russian Federation inventory: All components are listed or exempted.
Japan	: Japan inventory (CSCL): Not determined. Japan inventory (ISHL): All components are listed or exempted.
New Zealand	: All components are listed or exempted.
Philippines	: All components are listed or exempted.
Republic of Korea	: Not determined.
Taiwan	: All components are listed or exempted.
Thailand	: Not determined.
Turkey	: Not determined.
United States	: Not determined.
Viet Nam	: All components are listed or exempted.

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

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
- B = Bioaccumulative
- BCF = Bioconcentration Factor
- CLP = Classification, Labelling and Packaging Regulation [Regulation (EC) No. 1272/2008]
- DMEL = Derived Minimal Effect Level
- DNEL = Derived No Effect Level
- EUH statement = CLP-specific Hazard statement
- IATA = International Air Transport Association

100 mM Ammonium Trifluoroacetate

SECTION 16: Other information

IMDG = International Maritime Dangerous Goods
 IMO = International Maritime Organization
 M = Mobile
 N/A = Not available
 P = Persistent
 PBT = Persistent, Bioaccumulative and Toxic
 PMT = Persistent, Mobile 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
 T = Toxic
 vB = Very Bioaccumulative
 vM = Very Mobile
 vP = Very Persistent
 vPvB = Very Persistent and Very Bioaccumulative
 vPvM = Very Persistent and Very Mobile

Procedure used to derive the classification according to Regulation (EC) No. 1272/2008 [CLP/GHS]

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

Full text of abbreviated H statements

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

Full text of classifications [CLP/GHS]

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

Disclaimer: The information contained in this document is based on Agilent’s state of knowledge at the time of preparation. No warranty as to its accurateness, completeness or suitability for a particular purpose is expressed or implied.

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 Deutschland GmbH
 Hewlett-Packard-Str. 8
 76337 Waldbronn
 Germany
 0800 603 1000
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®: +353 1 901 4670

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 Regulation (EC) 1272/2008 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**
- 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	Specific Conc. Limits, M-factors and ATEs	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.	ATE [Oral] = 500 mg/kg ATE [Dermal] = 1100 mg/kg ATE [Inhalation (vapours)] = 11 mg/l	[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 precautions 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 European standard 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

5.0 mM Purine

SECTION 7: Handling and storage

(ventilating, lighting and material handling) equipment.

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	<p>NAOSH (Ireland, 4/2024) Absorbed through skin. Notes: EU derived Occupational Exposure Limit Values OELV 8 hours: 40 ppm. OELV 8 hours: 70 mg/m³. OELV 15 minutes: 4 mg/m³. OELV 15 minutes: 1.8 ppm.</p> <p>EU OEL (Europe, 1/2022) Absorbed through skin. TWA 8 hours: 40 ppm. TWA 8 hours: 70 mg/m³.</p>

Biological exposure indices

No exposure indices known.

Recommended monitoring procedures

: Reference should be made to monitoring standards, such as the following: European Standard EN 689 (Workplace atmospheres - Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy) European Standard EN 14042 (Workplace atmospheres - Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents) European Standard 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 European Standard 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
- Boiling point or 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
	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.
- Relative 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.

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

5.0 mM Purine

SECTION 11: Toxicological information

Skin

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

Potential immediate effects : Not available.

5.0 mM Purine

SECTION 11: Toxicological information

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.

11.2 Information on other hazards

11.2.1 Endocrine disrupting properties

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.

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	3600 mg/l [48 hours]
	Acute - IC50 - Fresh water	3685 mg/l [96 hours]
	Chronic - NOEC - Fresh water	160 mg/l [21 days]
	Chronic - NOEC - Fresh water	1000 mg/l [96 hours]
	Acute - LC50 - Fresh water	1000 mg/l [96 hours]

Conclusion/Summary [Product] : Not available.

12.2 Persistence and degradability

Product/ingredient name	Result
acetonitrile	- 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.

5.0 mM Purine

SECTION 12: Ecological information

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

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.

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 or ID 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 

5.0 mM Purine

SECTION 14: Transport information

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.

SECTION 15: Regulatory information

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

EU Regulation (EC) No. 1907/2006 (REACH)

Annex XIV - List of substances subject to authorisation

Annex XIV

Substances of very high concern

None of the components are 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.

Other EU regulations

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

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

Ozone depleting substances (EU 2024/590)

Not listed.

Prior Informed Consent (PIC) (649/2012/EU)

Not listed.

Persistent Organic Pollutants

Not listed.

Seveso Directive

5.0 mM Purine

SECTION 15: Regulatory information

This product is controlled under the Seveso Directive.

Danger criteria

Category

P5c

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

Australia	: Not determined.
Canada	: Not determined.
China	: Not determined.
Eurasian Economic Union	: Russian Federation inventory: All components are listed or exempted.
Japan	: Japan inventory (CSCL): Not determined. Japan inventory (ISHL): Not determined.
New Zealand	: Not determined.
Philippines	: Not determined.
Republic of Korea	: All components are listed or exempted.
Taiwan	: All components are listed or exempted.
Thailand	: Not determined.
Turkey	: Not determined.
United States	: Not determined.
Viet Nam	: All components are listed or exempted.

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

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
 B = Bioaccumulative
 BCF = Bioconcentration Factor
 CLP = Classification, Labelling and Packaging Regulation [Regulation (EC) No. 1272/2008]
 DMEL = Derived Minimal Effect Level
 DNEL = Derived No Effect Level
 EUH statement = CLP-specific Hazard statement
 IATA = International Air Transport Association

5.0 mM Purine

SECTION 16: Other information

IMDG = International Maritime Dangerous Goods
 IMO = International Maritime Organization
 M = Mobile
 N/A = Not available
 P = Persistent
 PBT = Persistent, Bioaccumulative and Toxic
 PMT = Persistent, Mobile 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
 T = Toxic
 vB = Very Bioaccumulative
 vM = Very Mobile
 vP = Very Persistent
 vPvB = Very Persistent and Very Bioaccumulative
 vPvM = Very Persistent and Very Mobile

Procedure used to derive the classification according to Regulation (EC) No. 1272/2008 [CLP/GHS]

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

Full text of abbreviated H statements

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

Full text of classifications [CLP/GHS]

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

Disclaimer: The information contained in this document is based on Agilent’s state of knowledge at the time of preparation. No warranty as to its accurateness, completeness or suitability for a particular purpose is expressed or implied.

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 Deutschland GmbH
 Hewlett-Packard-Str. 8
 76337 Waldbronn
 Germany
 0800 603 1000
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®: +353 1 901 4670

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 Regulation (EC) 1272/2008 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	
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	Specific Conc. Limits, M-factors and ATEs	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.	ATE [Oral] = 500 mg/kg ATE [Dermal] = 1100 mg/kg ATE [Inhalation (vapours)] = 11 mg/l	[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 precautions 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 European standard 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

2.5 mM Hexakis

SECTION 7: Handling and storage

(ventilating, lighting and material handling) equipment.

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	<p>NAOSH (Ireland, 4/2024) Absorbed through skin. Notes: EU derived Occupational Exposure Limit Values</p> <p>OELV 8 hours: 40 ppm. OELV 8 hours: 70 mg/m³. OELV 15 minutes: 4 mg/m³. OELV 15 minutes: 1.8 ppm.</p> <p>EU OEL (Europe, 1/2022) Absorbed through skin.</p> <p>TWA 8 hours: 40 ppm. TWA 8 hours: 70 mg/m³.</p>

Biological exposure indices

No exposure indices known.

Recommended monitoring procedures

: Reference should be made to monitoring standards, such as the following: European Standard EN 689 (Workplace atmospheres - Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy) European Standard EN 14042 (Workplace atmospheres - Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents) European Standard 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

2.5 mM Hexakis

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 European Standard 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.

2.5 mM Hexakis

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								
Boiling point or 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.								
Relative 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.

2.5 mM Hexakis

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)
2.5 mM Hexakis	500.0	1100.0	N/A	11.0	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

2.5 mM Hexakis

SECTION 11: Toxicological information

Skin

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

Potential immediate effects : Not available.

2.5 mM Hexakis

SECTION 11: Toxicological information

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.

11.2 Information on other hazards

11.2.1 Endocrine disrupting properties

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.

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	3600 mg/l [48 hours]
	Acute - IC50 - Fresh water	3685 mg/l [96 hours]
	Chronic - NOEC - Fresh water	160 mg/l [21 days]
	Chronic - NOEC - Fresh water	1000 mg/l [96 hours]
	Acute - LC50 - Fresh water	1000 mg/l [96 hours]

Conclusion/Summary [Product] : Not available.

12.2 Persistence and degradability

Product/ingredient name	Result
acetonitrile	- 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.

2.5 mM Hexakis

SECTION 12: Ecological information

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

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.

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 or ID 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 

2.5 mM Hexakis

SECTION 14: Transport information

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.

SECTION 15: Regulatory information

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

EU Regulation (EC) No. 1907/2006 (REACH)

Annex XIV - List of substances subject to authorisation

Annex XIV

Substances of very high concern

None of the components are 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.

Other EU regulations

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

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

Ozone depleting substances (EU 2024/590)

Not listed.

Prior Informed Consent (PIC) (649/2012/EU)

Not listed.

Persistent Organic Pollutants

Not listed.

Seveso Directive

2.5 mM Hexakis

SECTION 15: Regulatory information

This product is controlled under the Seveso Directive.

Danger criteria

Category

P5c

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

Australia	: Not determined.
Canada	: Not determined.
China	: Not determined.
Eurasian Economic Union	: Russian Federation inventory: All components are listed or exempted.
Japan	: Japan inventory (CSCL): Not determined. Japan inventory (ISHL): Not determined.
New Zealand	: Not determined.
Philippines	: Not determined.
Republic of Korea	: Not determined.
Taiwan	: All components are listed or exempted.
Thailand	: Not determined.
Turkey	: Not determined.
United States	: Not determined.
Viet Nam	: Not determined.

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

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
 B = Bioaccumulative
 BCF = Bioconcentration Factor
 CLP = Classification, Labelling and Packaging Regulation [Regulation (EC) No. 1272/2008]
 DMEL = Derived Minimal Effect Level
 DNEL = Derived No Effect Level
 EUH statement = CLP-specific Hazard statement
 IATA = International Air Transport Association

2.5 mM Hexakis

SECTION 16: Other information

IMDG = International Maritime Dangerous Goods
 IMO = International Maritime Organization
 M = Mobile
 N/A = Not available
 P = Persistent
 PBT = Persistent, Bioaccumulative and Toxic
 PMT = Persistent, Mobile 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
 T = Toxic
 vB = Very Bioaccumulative
 vM = Very Mobile
 vP = Very Persistent
 vPvB = Very Persistent and Very Bioaccumulative
 vPvM = Very Persistent and Very Mobile

Procedure used to derive the classification according to Regulation (EC) No. 1272/2008 [CLP/GHS]

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

Full text of abbreviated H statements

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

Full text of classifications [CLP/GHS]

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

Disclaimer: The information contained in this document is based on Agilent’s state of knowledge at the time of preparation. No warranty as to its accurateness, completeness or suitability for a particular purpose is expressed or implied.