Conforms to US OSHA Hazard Communication 29CFR1910.1200

SAFETY DATA SHEET

Agilent Technologies

API-TOF Reference Mix

Section 1. Identification

1.1 Product identifier

Product name : API-TOF Reference Mix

Part no. (chemical kit) : G1969-85001

Part no. :

100 mM Ammonium Trifluoroacetate	5191-4284
5.0 mM Purine	5191-4283
2.5 mM Hexakis	5191-4282

Validation date : 5/31/2024

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

Identified uses : Reagents and Standards for Analytical Chemistry Laboratory Use

100 mM Ammonium Trifluoroacetate	2 x 2.2 ml
5.0 mM Purine	2 x 2.2 ml
2.5 mM Hexakis	2 x 2.2 ml

1.3 Details of the supplier of the safety data sheet

Supplier/Manufacturer : Agilent Technologies, Inc.
5301 Stevens Creek Blvd
Santa Clara, CA 95051, USA
800-227-9770

1.4 Emergency telephone number

In case of emergency : CHEMTREC®: 1-800-424-9300

Section 2. Hazards identification

2.1 Classification of the substance or mixture

OSHA/HCS status :

100 mM Ammonium Trifluoroacetate	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
5.0 mM Purine	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
2.5 mM Hexakis	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Classification of the substance or mixture

100 mM Ammonium Trifluoroacetate

H225	FLAMMABLE LIQUIDS - Category 2
H302	ACUTE TOXICITY (oral) - Category 4
H312	ACUTE TOXICITY (dermal) - Category 4
H332	ACUTE TOXICITY (inhalation) - Category 4
H319	EYE IRRITATION - Category 2A

5.0 mM Purine

H225	FLAMMABLE LIQUIDS - Category 2
H302	ACUTE TOXICITY (oral) - Category 4
H312	ACUTE TOXICITY (dermal) - Category 4
H332	ACUTE TOXICITY (inhalation) - Category 4
H319	EYE IRRITATION - Category 2A

2.5 mM Hexakis

H225	FLAMMABLE LIQUIDS - Category 2
H302	ACUTE TOXICITY (oral) - Category 4

Section 2. Hazards identification

H312	ACUTE TOXICITY (dermal) - Category 4
H332	ACUTE TOXICITY (inhalation) - Category 4
H319	EYE IRRITATION - Category 2A

2.2 GHS label elements

Hazard pictograms :

100 mM Ammonium Trifluoroacetate

5.0 mM Purine

2.5 mM Hexakis

Signal word :

100 mM Ammonium Trifluoroacetate	Danger
5.0 mM Purine	Danger
2.5 mM Hexakis	Danger

Hazard statements :

100 mM Ammonium Trifluoroacetate	H225 - Highly flammable liquid and vapor. H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled. H319 - Causes serious eye irritation.
5.0 mM Purine	H225 - Highly flammable liquid and vapor. H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled. H319 - Causes serious eye irritation.
2.5 mM Hexakis	H225 - Highly flammable liquid and vapor. H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled. H319 - Causes serious eye irritation.

Precautionary statements

Prevention :

100 mM Ammonium Trifluoroacetate	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. P241 - Use explosion-proof electrical, ventilating or lighting equipment. P242 - Use non-sparking tools. P243 - Take action to prevent static discharges. P233 - Keep container tightly closed. P261 - Avoid breathing vapor. P270 - Do not eat, drink or smoke when using this product. P264 - Wash thoroughly after handling.
5.0 mM Purine	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. P241 - Use explosion-proof electrical, ventilating or

Section 2. Hazards identification

			lighting equipment. P242 - Use non-sparking tools. P243 - Take action to prevent static discharges. P233 - Keep container tightly closed. P261 - Avoid breathing vapor. P270 - Do not eat, drink or smoke when using this product. P264 - Wash thoroughly after handling.
		2.5 mM Hexakis	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. P241 - Use explosion-proof electrical, ventilating or lighting equipment. P242 - Use non-sparking tools. P243 - Take action to prevent static discharges. P233 - Keep container tightly closed. P261 - Avoid breathing vapor. P270 - Do not eat, drink or smoke when using this product. P264 - Wash thoroughly after handling.
Response	:	100 mM Ammonium Trifluoroacetate	P304 + P312 - IF INHALED: Call a POISON CENTER or doctor if you feel unwell. P302 + P312 - IF ON SKIN: Call a POISON CENTER or doctor if you feel unwell. P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P337 + P313 - If eye irritation persists: Get medical advice or attention.
		5.0 mM Purine	P304 + P312 - IF INHALED: Call a POISON CENTER or doctor if you feel unwell. P302 + P312 - IF ON SKIN: Call a POISON CENTER or doctor if you feel unwell. P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P337 + P313 - If eye irritation persists: Get medical advice or attention.
		2.5 mM Hexakis	P304 + P312 - IF INHALED: Call a POISON CENTER or doctor if you feel unwell. P302 + P312 - IF ON SKIN: Call a POISON CENTER or doctor if you feel unwell. P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P337 + P313 - If eye irritation persists: Get medical advice or attention.
Storage	:	100 mM Ammonium Trifluoroacetate	P403 + P235 - Store in a well-ventilated place. Keep cool.
		5.0 mM Purine	P403 + P235 - Store in a well-ventilated place. Keep cool.
		2.5 mM Hexakis	P403 + P235 - Store in a well-ventilated place. Keep cool.
Disposal	:		

Section 2. Hazards identification

	100 mM Ammonium Trifluoroacetate	P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
	5.0 mM Purine	P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
	2.5 mM Hexakis	P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
Supplemental label elements :	100 mM Ammonium Trifluoroacetate	None known.
	5.0 mM Purine	None known.
	2.5 mM Hexakis	None known.

2.3 Other hazards

Hazards not otherwise classified :	100 mM Ammonium Trifluoroacetate	None known.
	5.0 mM Purine	None known.
	2.5 mM Hexakis	None known.

Section 3. Composition/information on ingredients

Substance/mixture :	100 mM Ammonium Trifluoroacetate	Mixture
	5.0 mM Purine	Mixture
	2.5 mM Hexakis	Mixture

Ingredient name	%	CAS number
100 mM Ammonium Trifluoroacetate		
Acetonitrile	≥90	75-05-8
5.0 mM Purine		
Acetonitrile	≥90	75-05-8
2.5 mM Hexakis		
Acetonitrile	≥90	75-05-8

Any concentration shown as a range is to protect confidentiality or is due to batch variation.

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified and hence require reporting in this section.

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

Section 4. First aid measures

4.1 Description of necessary first aid measures

Eye contact :	100 mM Ammonium Trifluoroacetate	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.
	5.0 mM Purine	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.

Section 4. First aid measures

		2.5 mM Hexakis	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	:	100 mM Ammonium Trifluoroacetate	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.
		5.0 mM Purine	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.
		2.5 mM Hexakis	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.

Section 4. First aid measures

			The exposed person may need to be kept under medical surveillance for 48 hours.
Skin contact	:	100 mM Ammonium Trifluoroacetate	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.
		5.0 mM Purine	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.
		2.5 mM Hexakis	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	:	100 mM Ammonium Trifluoroacetate	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.
		5.0 mM Purine	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.
		2.5 mM Hexakis	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

Section 4. First aid measures

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.

4.2 Most important symptoms/effects, acute and delayed

Potential acute health effects

Eye contact	:	100 mM Ammonium Trifluoroacetate	Causes serious eye irritation.
		5.0 mM Purine	Causes serious eye irritation.
		2.5 mM Hexakis	Causes serious eye irritation.
Inhalation	:	100 mM Ammonium Trifluoroacetate	Harmful if inhaled.
		5.0 mM Purine	Harmful if inhaled.
		2.5 mM Hexakis	Harmful if inhaled.
Skin contact	:	100 mM Ammonium Trifluoroacetate	Harmful in contact with skin.
		5.0 mM Purine	Harmful in contact with skin.
		2.5 mM Hexakis	Harmful in contact with skin.
Ingestion	:	100 mM Ammonium Trifluoroacetate	Harmful if swallowed.
		5.0 mM Purine	Harmful if swallowed.
		2.5 mM Hexakis	Harmful if swallowed.

Over-exposure signs/symptoms

Eye contact	:	100 mM Ammonium Trifluoroacetate	Adverse symptoms may include the following: pain or irritation watering redness
		5.0 mM Purine	Adverse symptoms may include the following: pain or irritation watering redness
		2.5 mM Hexakis	Adverse symptoms may include the following: pain or irritation watering redness
Inhalation	:	100 mM Ammonium Trifluoroacetate	No specific data.
		5.0 mM Purine	No specific data.
		2.5 mM Hexakis	No specific data.
Skin contact	:	100 mM Ammonium Trifluoroacetate	No specific data.
		5.0 mM Purine	No specific data.
		2.5 mM Hexakis	No specific data.
Ingestion	:	100 mM Ammonium Trifluoroacetate	No specific data.
		5.0 mM Purine	No specific data.
		2.5 mM Hexakis	No specific data.

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Section 4. First aid measures

Notes to physician	:	100 mM Ammonium Trifluoroacetate	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.
		5.0 mM Purine	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.
		2.5 mM Hexakis	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	:	100 mM Ammonium Trifluoroacetate	No specific treatment.
		5.0 mM Purine	No specific treatment.
		2.5 mM Hexakis	No specific treatment.
Protection of first-aiders	:	100 mM Ammonium Trifluoroacetate	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.
		5.0 mM Purine	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.
		2.5 mM Hexakis	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.

See toxicological information (Section 11)

Section 5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media	:	100 mM Ammonium Trifluoroacetate	Use dry chemical, CO_2, water spray (fog) or foam.
		5.0 mM Purine	Use dry chemical, CO_2, water spray (fog) or foam.
		2.5 mM Hexakis	Use dry chemical, CO_2, water spray (fog) or foam.
Unsuitable extinguishing media	:	100 mM Ammonium Trifluoroacetate	Do not use water jet.
		5.0 mM Purine	Do not use water jet.
		2.5 mM Hexakis	Do not use water jet.

5.2 Special hazards arising from the substance or mixture

Section 5. Fire-fighting measures

Specific hazards arising from the chemical	:	100 mM Ammonium Trifluoroacetate	Highly flammable liquid and vapor. 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.
		5.0 mM Purine	Highly flammable liquid and vapor. 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.
		2.5 mM Hexakis	Highly flammable liquid and vapor. 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 thermal decomposition products	:	100 mM Ammonium Trifluoroacetate	Decomposition products may include the following materials: carbon dioxide carbon monoxide nitrogen oxides cyanides
		5.0 mM Purine	Decomposition products may include the following materials: carbon dioxide carbon monoxide nitrogen oxides cyanides
		2.5 mM Hexakis	Decomposition products may include the following materials: carbon dioxide carbon monoxide nitrogen oxides cyanides

5.3 Advice for firefighters

Special protective actions for fire-fighters	:	100 mM Ammonium Trifluoroacetate	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.
		5.0 mM Purine	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.
		2.5 mM Hexakis	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.

Section 5. Fire-fighting measures

Special protective equipment for fire-fighters	:	100 mM Ammonium Trifluoroacetate	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
		5.0 mM Purine	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
		2.5 mM Hexakis	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel	:	100 mM Ammonium Trifluoroacetate	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 spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
		5.0 mM Purine	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 spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
		2.5 mM Hexakis	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 spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
For emergency responders	:	100 mM Ammonium Trifluoroacetate	If specialized 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".
		5.0 mM Purine	If specialized 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".
		2.5 mM Hexakis	If specialized 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".

Section 6. Accidental release measures

6.2 Environmental precautions

100 mM Ammonium Trifluoroacetate	Avoid dispersal of spilled 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).
5.0 mM Purine	Avoid dispersal of spilled 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).
2.5 mM Hexakis	Avoid dispersal of spilled 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 materials for containment and cleaning up

Methods for cleaning up

100 mM Ammonium Trifluoroacetate	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.
5.0 mM Purine	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.
2.5 mM Hexakis	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.

Section 7. Handling and storage

7.1 Precautions for safe handling

Protective measures

100 mM Ammonium Trifluoroacetate	Put on appropriate personal protective equipment (see Section 8). Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor 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. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Empty containers retain product residue and can be hazardous. Do not reuse container.

Section 7. Handling and storage

	5.0 mM Purine	Put on appropriate personal protective equipment (see Section 8). Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor 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. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Empty containers retain product residue and can be hazardous. Do not reuse container.
	2.5 mM Hexakis	Put on appropriate personal protective equipment (see Section 8). Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor 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. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Empty containers retain product residue and can be hazardous. Do not reuse container.
Advice on general occupational hygiene :	100 mM Ammonium Trifluoroacetate	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.
	5.0 mM Purine	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.
	2.5 mM Hexakis	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.

Section 7. Handling and storage

7.2 Conditions for safe storage, including any incompatibilities	: 100 mM Ammonium Trifluoroacetate	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 oxidizing 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 unlabeled containers. Use appropriate containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.
	5.0 mM Purine	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 oxidizing 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 unlabeled containers. Use appropriate containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.
	2.5 mM Hexakis	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 oxidizing 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 unlabeled containers. Use appropriate containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.

7.3 Specific end use(s)

Recommendations	: 100 mM Ammonium Trifluoroacetate	Industrial applications, Professional applications.
	5.0 mM Purine	Industrial applications, Professional applications.
	2.5 mM Hexakis	Industrial applications, Professional applications.
Industrial sector specific solutions	: 100 mM Ammonium Trifluoroacetate	Not available.
	5.0 mM Purine	Not available.
	2.5 mM Hexakis	Not available.

Section 8. Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limits

Ingredient name	Exposure limits
100 mM Ammonium Trifluoroacetate Acetonitrile	**ACGIH TLV (United States, 1/2024).** **Absorbed through skin.** TWA: 20 ppm 8 hours. **OSHA PEL 1989 (United States, 3/1989).** TWA: 40 ppm 8 hours. TWA: 70 mg/m³ 8 hours. STEL: 60 ppm 15 minutes. STEL: 105 mg/m³ 15 minutes. **NIOSH REL (United States, 10/2020).** TWA: 20 ppm 10 hours. TWA: 34 mg/m³ 10 hours. **OSHA PEL (United States, 5/2018).** TWA: 40 ppm 8 hours. TWA: 70 mg/m³ 8 hours. **CAL OSHA PEL (United States, 5/2018).** **Absorbed through skin.** STEL: 105 mg/m³ 15 minutes. STEL: 60 ppm 15 minutes. TWA: 70 mg/m³ 8 hours. TWA: 40 ppm 8 hours.
5.0 mM Purine Acetonitrile	**ACGIH TLV (United States, 1/2024).** **Absorbed through skin.** TWA: 20 ppm 8 hours. **OSHA PEL 1989 (United States, 3/1989).** TWA: 40 ppm 8 hours. TWA: 70 mg/m³ 8 hours. STEL: 60 ppm 15 minutes. STEL: 105 mg/m³ 15 minutes. **NIOSH REL (United States, 10/2020).** TWA: 20 ppm 10 hours. TWA: 34 mg/m³ 10 hours. **OSHA PEL (United States, 5/2018).** TWA: 40 ppm 8 hours. TWA: 70 mg/m³ 8 hours. **CAL OSHA PEL (United States, 5/2018).** **Absorbed through skin.** STEL: 105 mg/m³ 15 minutes. STEL: 60 ppm 15 minutes. TWA: 70 mg/m³ 8 hours. TWA: 40 ppm 8 hours.
2.5 mM Hexakis Acetonitrile	**ACGIH TLV (United States, 1/2024).** **Absorbed through skin.** TWA: 20 ppm 8 hours. **OSHA PEL 1989 (United States, 3/1989).** TWA: 40 ppm 8 hours. TWA: 70 mg/m³ 8 hours. STEL: 60 ppm 15 minutes. STEL: 105 mg/m³ 15 minutes. **NIOSH REL (United States, 10/2020).**

Section 8. Exposure controls/personal protection

	TWA: 20 ppm 10 hours. TWA: 34 mg/m³ 10 hours. **OSHA PEL (United States, 5/2018).** TWA: 40 ppm 8 hours. TWA: 70 mg/m³ 8 hours. **CAL OSHA PEL (United States, 5/2018).** **Absorbed through skin.** STEL: 105 mg/m³ 15 minutes. STEL: 60 ppm 15 minutes. TWA: 70 mg/m³ 8 hours. TWA: 40 ppm 8 hours.

Biological exposure indices

No exposure indices known.

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, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

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.

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.

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.

Section 8. Exposure controls/personal protection

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.

Section 9. Physical and chemical properties and safety characteristics

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

Appearance

Physical state	:	100 mM Ammonium Trifluoroacetate	Liquid.
		5.0 mM Purine	Liquid.
		2.5 mM Hexakis	Liquid.
Color	:	100 mM Ammonium Trifluoroacetate	Not available.
		5.0 mM Purine	Not available.
		2.5 mM Hexakis	Not available.
Odor	:	100 mM Ammonium Trifluoroacetate	Not available.
		5.0 mM Purine	Not available.
		2.5 mM Hexakis	Not available.
Odor threshold	:	100 mM Ammonium Trifluoroacetate	Not available.
		5.0 mM Purine	Not available.
		2.5 mM Hexakis	Not available.
pH	:	100 mM Ammonium Trifluoroacetate	Not available.
		5.0 mM Purine	Not available.
		2.5 mM Hexakis	Not available.
Melting point/freezing point	:	100 mM Ammonium Trifluoroacetate	-41.9°C (-43.4°F)
		5.0 mM Purine	-41.9°C (-43.4°F)
		2.5 mM Hexakis	-41.9°C (-43.4°F)
Boiling point, initial boiling point, and boiling range	:	100 mM Ammonium Trifluoroacetate	81.7°C (179.1°F)
		5.0 mM Purine	81.7°C (179.1°F)
		2.5 mM Hexakis	81.7°C (179.1°F)
Flash point	:	100 mM Ammonium Trifluoroacetate	Closed cup: 5.85°C (42.5°F)
		5.0 mM Purine	Closed cup: 5.85°C (42.5°F)
		2.5 mM Hexakis	Closed cup: 5.85°C (42.5°F)
Evaporation rate	:	100 mM Ammonium Trifluoroacetate	Not available.
		5.0 mM Purine	Not available.
		2.5 mM Hexakis	Not available.
Flammability	:	100 mM Ammonium Trifluoroacetate	Not applicable.
		5.0 mM Purine	Not applicable.
		2.5 mM Hexakis	Not applicable.
Lower and upper explosion limit/flammability limit	:	100 mM Ammonium Trifluoroacetate	Not available.
		5.0 mM Purine	Not available.
		2.5 mM Hexakis	Not available.
Vapor pressure	:		

Section 9. Physical and chemical properties and safety characteristics

Ingredient name	Vapor Pressure at 20˚C			Vapor pressure at 50˚C		
	mm Hg	kPa	Method	mm Hg	kPa	Method
100 mM Ammonium Trifluoroacetate						
Acetonitrile	70.88853	9.5	-	-	-	-
water	17.5	2.3	-	92.258	12.3	-
5.0 mM Purine						
Acetonitrile	70.88853	9.5	-	-	-	-
water	17.5	2.3	-	92.258	12.3	-
2.5 mM Hexakis						
Acetonitrile	70.88853	9.5	-	-	-	-

Relative vapor density :

100 mM Ammonium Trifluoroacetate	Not available.
5.0 mM Purine	Not available.
2.5 mM Hexakis	Not available.

Relative density :

100 mM Ammonium Trifluoroacetate	Not available.
5.0 mM Purine	Not available.
2.5 mM Hexakis	Not available.

Solubility(ies) :

Media	Result
100 mM Ammonium Trifluoroacetate	
methanol	Soluble
acetone	Soluble
water	Soluble
5.0 mM Purine	
water	Soluble
methanol	Soluble
acetone	Soluble
2.5 mM Hexakis	
methanol	Soluble
acetone	Soluble
water	Soluble

Partition coefficient: n-octanol/water :

100 mM Ammonium Trifluoroacetate	Not applicable.
5.0 mM Purine	Not applicable.
2.5 mM Hexakis	Not applicable.

Auto-ignition temperature :

2.5 mM Hexakis	524°C (975.2°F)

Section 9. Physical and chemical properties and safety characteristics

Ingredient name	°C	°F	Method
100 mM Ammonium Trifluoroacetate			
Acetonitrile	524	975.2	-
5.0 mM Purine			
Acetonitrile	524	975.2	-

Decomposition temperature :
- 100 mM Ammonium Trifluoroacetate: Not available.
- 5.0 mM Purine: Not available.
- 2.5 mM Hexakis: Not available.

Viscosity :
- 100 mM Ammonium Trifluoroacetate: Not available.
- 5.0 mM Purine: Not available.
- 2.5 mM Hexakis: Not available.

Particle characteristics

Median particle size :
- 100 mM Ammonium Trifluoroacetate: Not applicable.
- 5.0 mM Purine: Not applicable.
- 2.5 mM Hexakis: Not applicable.

Section 10. Stability and reactivity

10.1 Reactivity :
- 100 mM Ammonium Trifluoroacetate: No specific test data related to reactivity available for this product or its ingredients.
- 5.0 mM Purine: No specific test data related to reactivity available for this product or its ingredients.
- 2.5 mM Hexakis: No specific test data related to reactivity available for this product or its ingredients.

10.2 Chemical stability :
- 100 mM Ammonium Trifluoroacetate: The product is stable.
- 5.0 mM Purine: The product is stable.
- 2.5 mM Hexakis: The product is stable.

10.3 Possibility of hazardous reactions :
- 100 mM Ammonium Trifluoroacetate: Under normal conditions of storage and use, hazardous reactions will not occur.
- 5.0 mM Purine: Under normal conditions of storage and use, hazardous reactions will not occur.
- 2.5 mM Hexakis: Under normal conditions of storage and use, hazardous reactions will not occur.

10.4 Conditions to avoid :
- 100 mM Ammonium Trifluoroacetate: Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.
- 5.0 mM Purine: Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.
- 2.5 mM Hexakis: Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.

Section 10. Stability and reactivity

10.5 Incompatible materials	:	100 mM Ammonium Trifluoroacetate	Reactive or incompatible with the following materials: oxidizing materials
		5.0 mM Purine	Reactive or incompatible with the following materials: oxidizing materials
		2.5 mM Hexakis	Reactive or incompatible with the following materials: oxidizing materials
10.6 Hazardous decomposition products	:	100 mM Ammonium Trifluoroacetate	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
		5.0 mM Purine	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
		2.5 mM Hexakis	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	Species	Dose	Exposure
100 mM Ammonium Trifluoroacetate				
Acetonitrile	LC50 Inhalation Vapor LD50 Oral	Rat Rat	17100 ppm 2460 mg/kg	4 hours -
5.0 mM Purine				
Acetonitrile	LC50 Inhalation Vapor LD50 Oral	Rat Rat	17100 ppm 2460 mg/kg	4 hours -
2.5 mM Hexakis				
Acetonitrile	LC50 Inhalation Vapor LD50 Oral	Rat Rat	17100 ppm 2460 mg/kg	4 hours -

Irritation/Corrosion

Product/ingredient name	Result	Species	Score	Exposure	Observation
100 mM Ammonium Trifluoroacetate					
Acetonitrile	Eyes - Moderate irritant	Rabbit	-	24 hours 100 uL	-
5.0 mM Purine					
Acetonitrile	Eyes - Moderate irritant	Rabbit	-	24 hours 100 uL	-
2.5 mM Hexakis					
Acetonitrile	Eyes - Moderate irritant	Rabbit	-	24 hours 100 uL	-

Sensitization

Not available.

Mutagenicity

Section 11. Toxicological information

Conclusion/Summary : Not available.

Carcinogenicity

Conclusion/Summary : Not available.

Reproductive toxicity

Conclusion/Summary : Not available.

Teratogenicity

Conclusion/Summary : Not available.

Specific target organ toxicity (single exposure)

Not available.

Specific target organ toxicity (repeated exposure)

Not available.

Aspiration hazard

Not available.

Information on the likely routes of exposure	:	100 mM Ammonium Trifluoroacetate	Routes of entry anticipated: Oral, Dermal, Inhalation, Eyes.
		5.0 mM Purine	Routes of entry anticipated: Oral, Dermal, Inhalation, Eyes.
		2.5 mM Hexakis	Routes of entry anticipated: Oral, Dermal, Inhalation, Eyes.

Potential acute health effects

Eye contact	:	100 mM Ammonium Trifluoroacetate	Causes serious eye irritation.
		5.0 mM Purine	Causes serious eye irritation.
		2.5 mM Hexakis	Causes serious eye irritation.
Inhalation	:	100 mM Ammonium Trifluoroacetate	Harmful if inhaled.
		5.0 mM Purine	Harmful if inhaled.
		2.5 mM Hexakis	Harmful if inhaled.
Skin contact	:	100 mM Ammonium Trifluoroacetate	Harmful in contact with skin.
		5.0 mM Purine	Harmful in contact with skin.
		2.5 mM Hexakis	Harmful in contact with skin.
Ingestion	:	100 mM Ammonium Trifluoroacetate	Harmful if swallowed.
		5.0 mM Purine	Harmful if swallowed.
		2.5 mM Hexakis	Harmful if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact	:	100 mM Ammonium Trifluoroacetate	Adverse symptoms may include the following: pain or irritation watering redness
		5.0 mM Purine	Adverse symptoms may include the following: pain or irritation watering redness
		2.5 mM Hexakis	Adverse symptoms may include the following: pain or irritation watering redness

Section 11. Toxicological information

Inhalation	:	100 mM Ammonium Trifluoroacetate	No specific data.
		5.0 mM Purine	No specific data.
		2.5 mM Hexakis	No specific data.
Skin contact	:	100 mM Ammonium Trifluoroacetate	No specific data.
		5.0 mM Purine	No specific data.
		2.5 mM Hexakis	No specific data.
Ingestion	:	100 mM Ammonium Trifluoroacetate	No specific data.
		5.0 mM Purine	No specific data.
		2.5 mM Hexakis	No specific data.

Delayed and immediate effects and also 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.

Potential delayed effects : Not available.

Potential chronic health effects

General	:	100 mM Ammonium Trifluoroacetate	No known significant effects or critical hazards.
		5.0 mM Purine	No known significant effects or critical hazards.
		2.5 mM Hexakis	No known significant effects or critical hazards.
Carcinogenicity	:	100 mM Ammonium Trifluoroacetate	No known significant effects or critical hazards.
		5.0 mM Purine	No known significant effects or critical hazards.
		2.5 mM Hexakis	No known significant effects or critical hazards.
Mutagenicity	:	100 mM Ammonium Trifluoroacetate	No known significant effects or critical hazards.
		5.0 mM Purine	No known significant effects or critical hazards.
		2.5 mM Hexakis	No known significant effects or critical hazards.
Reproductive toxicity	:	100 mM Ammonium Trifluoroacetate	No known significant effects or critical hazards.
		5.0 mM Purine	No known significant effects or critical hazards.
		2.5 mM Hexakis	No known significant effects or critical hazards.

Numerical measures of toxicity

Acute toxicity estimates

Product/ingredient name	Oral (mg/kg)	Dermal (mg/kg)	Inhalation (gases) (ppm)	Inhalation (vapors) (mg/l)	Inhalation (dusts and mists) (mg/l)
100 mM Ammonium Trifluoroacetate					
100 mM Ammonium Trifluoroacetate	555.6	1222.2	N/A	12.2	N/A
Acetonitrile	500	1100	N/A	11	N/A
5.0 mM Purine					
5.0 mM Purine	555.6	1222.3	N/A	12.2	N/A
Acetonitrile	500	1100	N/A	11	N/A

Section 11. Toxicological information

2.5 mM Hexakis					
2.5 mM Hexakis	500.0	1100.0	N/A	11.0	N/A
Acetonitrile	500	1100	N/A	11	N/A

Other information : 100 mM Ammonium Trifluoroacetate — Adverse symptoms may include the following: May cause headache, weakness, dizziness, shortness of breath, cyanosis, rapid heart beat, unconsciousness and possible death.

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

2.5 mM Hexakis — 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	Species	Exposure
100 mM Ammonium Trifluoroacetate			
Acetonitrile	Acute IC50 3685000 µg/l Fresh water	Aquatic plants - *Lemna minor*	96 hours
	Acute LC50 3600000 µg/l Fresh water	Daphnia - *Daphnia magna*	48 hours
	Acute LC50 1000 mg/l Fresh water	Fish - *Pimephales promelas*	96 hours
	Chronic NOEC 1000000 µg/l Fresh water	Aquatic plants - *Lemna minor*	96 hours
	Chronic NOEC 160000 µg/l Fresh water	Daphnia - *Daphnia magna*	21 days
5.0 mM Purine			
Acetonitrile	Acute IC50 3685000 µg/l Fresh water	Aquatic plants - *Lemna minor*	96 hours
	Acute LC50 3600000 µg/l Fresh water	Daphnia - *Daphnia magna*	48 hours
	Acute LC50 1000 mg/l Fresh water	Fish - *Pimephales promelas*	96 hours
	Chronic NOEC 1000000 µg/l Fresh water	Aquatic plants - *Lemna minor*	96 hours
	Chronic NOEC 160000 µg/l Fresh water	Daphnia - *Daphnia magna*	21 days
2.5 mM Hexakis			
Acetonitrile	Acute IC50 3685000 µg/l Fresh water	Aquatic plants - *Lemna minor*	96 hours
	Acute LC50 3600000 µg/l Fresh water	Daphnia - *Daphnia magna*	48 hours
	Acute LC50 1000 mg/l Fresh water	Fish - *Pimephales promelas*	96 hours
	Chronic NOEC 1000000 µg/l Fresh water	Aquatic plants - *Lemna minor*	96 hours
	Chronic NOEC 160000 µg/l Fresh water	Daphnia - *Daphnia magna*	21 days

12.2 Persistence and degradability

Product/ingredient name	Test	Result	Dose	Inoculum
100 mM Ammonium Trifluoroacetate				
Acetonitrile	OECD 310 Ready Biodegradability - CO_2 in Sealed Vessels (Headspace Test)	70 % - Readily - 21 days	-	Activated sludge
5.0 mM Purine				

Section 12. Ecological information

Acetonitrile	OECD 310 Ready Biodegradability - CO_2 in Sealed Vessels (Headspace Test)	70 % - Readily - 21 days	-	Activated sludge
2.5 mM Hexakis				
Acetonitrile	OECD 310 Ready Biodegradability - CO_2 in Sealed Vessels (Headspace Test)	70 % - Readily - 21 days	-	Activated sludge

Product/ingredient name	Aquatic half-life	Photolysis	Biodegradability
100 mM Ammonium Trifluoroacetate			
Acetonitrile	-	-	Readily
5.0 mM Purine			
Acetonitrile	-	-	Readily
2.5 mM Hexakis			
Acetonitrile	-	-	Readily

12.3 Bioaccumulative potential

Product/ingredient name	$LogP_{ow}$	BCF	Potential
100 mM Ammonium Trifluoroacetate			
Acetonitrile	-0.34	3	Low
5.0 mM Purine			
Acetonitrile	-0.34	3	Low
2.5 mM Hexakis			
Acetonitrile	-0.34	3	Low

12.4 Mobility in soil

Soil/water partition coefficient (K_{OC}) : Not available.

12.5 Other adverse effects : No known significant effects or critical hazards.

Section 13. Disposal considerations

13.1 Waste treatment methods

Disposal methods : The generation of waste should be avoided or minimized wherever possible. 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. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. 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

Section 13. Disposal considerations

cleaned or rinsed out. Empty containers or liners may retain some product residues. Vapor 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 spilled material and runoff and contact with soil, waterways, drains and sewers.

United States - RCRA Toxic hazardous waste "U" List

Ingredient	CAS #	Status	Reference number
100 mM Ammonium Trifluoroacetate Acetonitrile (I,T)	75-05-8	Listed	U003
5.0 mM Purine Acetonitrile (I,T)	75-05-8	Listed	U003
2.5 mM Hexakis Acetonitrile (I,T)	75-05-8	Listed	U003

Disposal should be in accordance with applicable regional, national and local laws and regulations. Local regulations may be more stringent than regional or national requirements.

The information presented below only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations.

Refer to Section 7: HANDLING AND STORAGE and Section 8: EXPOSURE CONTROLS/PERSONAL PROTECTION for additional handling information and protection of employees.

Section 14. Transport information

	DOT Classification	TDG Classification	Mexico Classification	IMDG	IATA
UN number	UN1648	UN1648	UN1648	UN1648	UN1648
UN proper shipping name	Acetonitrile solution	ACETONITRILE solution	ACETONITRILO solution	ACETONITRILE solution	Acetonitrile solution
Transport hazard class(es)	3 	3 	3 	3 	3 
Packing group	II	II	II	II	II
Environmental hazards	No.	No.	No.	No.	No.

Additional information

Remarks: Excepted Quantity

DOT Classification : **Reportable quantity** 5357.2 lbs / 2432.2 kg. Package sizes shipped in quantities less than the product reportable quantity are not subject to the RQ (reportable quantity) transportation requirements.
Limited quantity Yes.
Packaging instruction Exceptions: 150. Non-bulk: 202. Bulk: 242.
Quantity limitation Passenger aircraft/rail: 5 L. Cargo aircraft: 60 L.
Special provisions IB2, T7, TP2

Section 14. Transport information

TDG Classification : Product classified as per the following sections of the Transportation of Dangerous Goods Regulations: 2.18-2.19 (Class 3).
Explosive Limit and Limited Quantity Index 1
Passenger Carrying Road or Rail Index 5

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.

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.

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

U.S. Federal regulations : **TSCA 8(a) PAIR**: Acetonitrile
TSCA 8(a) CDR Exempt/Partial exemption: Not determined
Clean Water Act (CWA) 307: Acetonitrile

Clean Air Act Section 112 (b) Hazardous Air Pollutants (HAPs) : Listed

Clean Air Act Section 602 Class I Substances : Not listed

Clean Air Act Section 602 Class II Substances : Not listed

DEA List I Chemicals (Precursor Chemicals) : Not listed

DEA List II Chemicals (Essential Chemicals) : Not listed

SARA 302/304

Composition/information on ingredients

No products were found.

SARA 304 RQ : Not applicable.

SARA 311/312

Classification :

100 mM Ammonium Trifluoroacetate	FLAMMABLE LIQUIDS - Category 2 ACUTE TOXICITY (oral) - Category 4 ACUTE TOXICITY (dermal) - Category 4 ACUTE TOXICITY (inhalation) - Category 4 EYE IRRITATION - Category 2A SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2
5.0 mM Purine	FLAMMABLE LIQUIDS - Category 2 ACUTE TOXICITY (oral) - Category 4 ACUTE TOXICITY (dermal) - Category 4 ACUTE TOXICITY (inhalation) - Category 4 EYE IRRITATION - Category 2A SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2
2.5 mM Hexakis	FLAMMABLE LIQUIDS - Category 2 ACUTE TOXICITY (oral) - Category 4 ACUTE TOXICITY (dermal) - Category 4

Section 15. Regulatory information

ACUTE TOXICITY (inhalation) - Category 4
EYE IRRITATION - Category 2A
SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2

Composition/information on ingredients

Name	%	Classification
100 mM Ammonium Trifluoroacetate		
Acetonitrile	≥90	FLAMMABLE LIQUIDS - Category 2 ACUTE TOXICITY (oral) - Category 4 ACUTE TOXICITY (dermal) - Category 4 ACUTE TOXICITY (inhalation) - Category 4 EYE IRRITATION - Category 2A
5.0 mM Purine		
Acetonitrile	≥90	FLAMMABLE LIQUIDS - Category 2 ACUTE TOXICITY (oral) - Category 4 ACUTE TOXICITY (dermal) - Category 4 ACUTE TOXICITY (inhalation) - Category 4 EYE IRRITATION - Category 2A
2.5 mM Hexakis		
Acetonitrile	≥90	FLAMMABLE LIQUIDS - Category 2 ACUTE TOXICITY (oral) - Category 4 ACUTE TOXICITY (dermal) - Category 4 ACUTE TOXICITY (inhalation) - Category 4 EYE IRRITATION - Category 2A

SARA 313

	Product name	CAS number	%
Form R - Reporting requirements	**100 mM Ammonium Trifluoroacetate** Acetonitrile	75-05-8	≥90
	5.0 mM Purine Acetonitrile	75-05-8	≥90
	2.5 mM Hexakis Acetonitrile	75-05-8	≥90
Supplier notification	**100 mM Ammonium Trifluoroacetate** Acetonitrile	75-05-8	≥90
	5.0 mM Purine Acetonitrile	75-05-8	≥90
	2.5 mM Hexakis Acetonitrile	75-05-8	≥90

SARA 313 notifications must not be detached from the SDS and any copying and redistribution of the SDS shall include copying and redistribution of the notice attached to copies of the SDS subsequently redistributed.

State regulations

Massachusetts : The following components are listed: ACETONITRILE

New York : The following components are listed: Acetonitrile

New Jersey : The following components are listed: ACETONITRILE

Pennsylvania : The following components are listed: ACETONITRILE

California Prop. 65

This product does not require a Safe Harbor warning under California Prop. 65.

International regulations

Chemical Weapon Convention List Schedules I, II & III Chemicals

Section 15. Regulatory information

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.

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.

Section 16. Other information

Procedure used to derive the classification

Classification	Justification
100 mM Ammonium Trifluoroacetate	
FLAMMABLE LIQUIDS - Category 2	On basis of test data
ACUTE TOXICITY (oral) - Category 4	Calculation method
ACUTE TOXICITY (dermal) - Category 4	Calculation method
ACUTE TOXICITY (inhalation) - Category 4	Calculation method
EYE IRRITATION - Category 2A	Calculation method
5.0 mM Purine	
FLAMMABLE LIQUIDS - Category 2	On basis of test data
ACUTE TOXICITY (oral) - Category 4	Calculation method
ACUTE TOXICITY (dermal) - Category 4	Calculation method
ACUTE TOXICITY (inhalation) - Category 4	Calculation method
EYE IRRITATION - Category 2A	Calculation method
2.5 mM Hexakis	
FLAMMABLE LIQUIDS - Category 2	On basis of test data
ACUTE TOXICITY (oral) - Category 4	Calculation method
ACUTE TOXICITY (dermal) - Category 4	Calculation method
ACUTE TOXICITY (inhalation) - Category 4	Calculation method
EYE IRRITATION - Category 2A	Calculation method

History

: 05/31/2024

Section 16. Other information

Date of issue/Date of revision

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Version : 11

Key to abbreviations : ATE = Acute Toxicity Estimate
BCF = Bioconcentration Factor
GHS = Globally Harmonized System of Classification and Labelling of Chemicals
IATA = International Air Transport Association
IBC = Intermediate Bulk Container
IMDG = International Maritime Dangerous Goods
LogPow = logarithm of the octanol/water partition coefficient
MARPOL = International Convention for the Prevention of Pollution From Ships, 1973 as modified by the Protocol of 1978. ("Marpol" = marine pollution)
N/A = Not available
UN = United Nations

Indicates information that has changed from previously issued version.

Notice to reader

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