

Safety Data Sheet

according to HPR, Schedule 1

Printing date 07/04/2024

Version Number 5

Reviewed on 07/04/2024

1 Identification

- **Product identifier**
- **Trade name:** Carbonyl Compounds Standard (1X1 mL)
- **Part number:** ALD-554A-1
- **Application of the substance / the mixture** Reagents and Standards for Analytical Chemical Laboratory Use
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
Agilent Technologies, Inc.
5301 Stevens Creek Blvd.
Santa Clara, CA 95051 USA
- **Information department:**
Telephone: 800-227-9770
e-mail: pdl-msds_author@agilent.com
- **Emergency telephone number:** CHEMTREC®: 1-800-424-9300

2 Hazard identification

- **Classification of the substance or mixture**



GHS02 Flame

Flammable Liquids - Category 2

H225 Highly flammable liquid and vapour.



GHS08 Health hazard

Carcinogenicity - Category 1A

H350 May cause cancer.



GHS07

Acute Toxicity (Oral) - Category 4

H302 Harmful if swallowed.

Acute Toxicity (Dermal) - Category 4

H312 Harmful in contact with skin.

Eye Irritation - Category 2A

H319 Causes serious eye irritation.

Skin Sensitizer - Category 1

H317 May cause an allergic skin reaction.

- **Label elements**

- **GHS label elements** The product is classified and labeled according to the Globally Harmonized System (GHS).

- **Hazard pictograms**



GHS02



GHS07



GHS08

- **Signal word** Danger

- **Hazard-determining components of labeling:**

acetonitrile

formaldehyde

acetaldehyde

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(E)-2-butenal
valeraldehyde

Hazard statements

- H225 Highly flammable liquid and vapour.
- H302+H312 Harmful if swallowed or in contact with skin.
- H319 Causes serious eye irritation.
- H317 May cause an allergic skin reaction.
- H350 May cause cancer.

Precautionary statements

- P101 If medical advice is needed, have product container or label at hand.
- P102 Keep out of reach of children.
- P103 Read label before use.
- P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
- P241 Use explosion-proof [electrical/ventilating/lighting] equipment.
- P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
- P280 Wear protective gloves/protective clothing/eye protection/face protection.
- P240 Ground and bond container and receiving equipment.
- P233 Keep container tightly closed.
- P242 Use non-sparking tools.
- P243 Take actions to prevent static discharges.
- P264 Wash thoroughly after handling.
- P270 Do not eat, drink or smoke when using this product.
- P272 Contaminated work clothing should not be allowed out of the workplace.
- P201 Obtain special instructions before use.
- P202 Do not handle until all safety precautions have been read and understood.
- P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].
- P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P322 Specific measures (see on this label).
- P301+P312 If swallowed: Call a poison center/doctor if you feel unwell.
- P363 Wash contaminated clothing before reuse.
- P308+P313 IF exposed or concerned: Get medical advice/attention.
- P333+P313 If skin irritation or rash occurs: Get medical advice/attention.
- P337+P313 If eye irritation persists: Get medical advice/attention.
- P330 Rinse mouth.
- P370+P378 In case of fire: Use CO₂, powder or water spray to extinguish.
- P362+P364 Take off contaminated clothing and wash it before reuse.
- P405 Store locked up.
- P403+P235 Store in a well-ventilated place. Keep cool.
- P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

Classification system:
NFPA ratings (scale 0 - 4)


Health = 2
Fire = 3
Reactivity = 0

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· HMIS-ratings (scale 0 - 4)

HEALTH	2	Health = *2
FIRE	3	Fire = 3
REACTIVITY	0	Reactivity = 0

3 Composition/Information on ingredients

- **Chemical characterization: Mixtures**
- **Description:** Mixture of the substances listed below with nonhazardous additions.

· Dangerous components:

75-05-8	acetonitrile	80-100% w/w *
50-00-0	formaldehyde	0.1-1% w/w *
75-07-0	acetaldehyde	0.1-1% w/w *
108-94-1	cyclohexanone	0.1-1% w/w *
110-62-3	valeraldehyde	0.1-1% w/w *
123-38-6	propanal	0.1-1% w/w *
123-72-8	butyraldehyde	0.1-1% w/w *
123-73-9	(E)-2-butenal	0.1-1% w/w *

* Actual concentration ranges are withheld as a trade secret.

4 First-aid measures

- **Description of first aid measures**
- **General information:**
Immediately remove any clothing soiled by the product.
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.
- **After inhalation:**
Supply fresh air and to be sure call for a doctor.
In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:**
Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.
- **After swallowing:** Immediately call a doctor.
- **Information for doctor:**
- **Most important symptoms and effects, both acute and delayed** No further relevant information available.
- **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**
CO₂, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **For safety reasons unsuitable extinguishing agents:** Water with full jet

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- **Special hazards arising from the substance or mixture** No further relevant information available.
- **Advice for firefighters**
- **Protective equipment:** No special measures required.

6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**
Wear protective equipment. Keep unprotected persons away.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose contaminated material as waste according to section 13.
Ensure adequate ventilation.
- **Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

7 Handling and storage

- **Handling:**
- **Precautions for safe handling**
Ensure good ventilation/exhaustion at the workplace.
Open and handle receptacle with care.
Prevent formation of aerosols.
- **Information about protection against explosions and fires:**
Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
Keep respiratory protective device available.
- **Conditions for safe storage, including any incompatibilities**
- **Storage:**
- **Requirements to be met by storerooms and receptacles:** Store in a cool location.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:**
Keep receptacle tightly sealed.
Store in cool, dry conditions in well sealed receptacles.
- **Specific end use(s)** No further relevant information available.

8 Exposure controls/ Personal protection

- **Additional information about design of technical systems:** No further data; see section 7.
- **Control parameters**

Components with limit values that require monitoring at the workplace:
75-05-8 acetonitrile

EL	TWA: 20 ppm
	Skin

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EV	TWA: 20 ppm Skin
50-00-0 formaldehyde	
EL	STEL: 0.3 ppm TWA: 0.1 ppm ACGIH A1; IARC 1; S(D), S(R)
EV	STEL: 1.0 ppm
Ceiling	1.5 ppm
75-07-0 acetaldehyde	
EL	Ceiling: 25 ppm IARC 2B, ACGIH A2
EV	Ceiling: 25 ppm
108-94-1 cyclohexanone	
EL	STEL: 50 ppm TWA: 20 ppm Skin
EV	STEL: 50 ppm TWA: 20 ppm Skin
110-62-3 valeraldehyde	
EL	TWA: 50 ppm
EV	TWA: 175 mg/m ³ , 50 ppm
123-38-6 propanal	
EL	TWA: 20 ppm
EV	TWA: 20 ppm

· **Additional information:** The lists that were valid during the creation were used as basis.

· **Exposure controls**

· **Personal protective equipment:**

· **General protective and hygienic measures:**

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Store protective clothing separately.

Avoid contact with the eyes.

Avoid contact with the eyes and skin.

· **Breathing equipment:**

When used as intended with Agilent instruments, the use of the product under normal laboratory conditions and with standard practices does not result in significant airborne exposures and therefore respiratory protection is not needed.

Under an emergency condition where a respirator is deemed necessary, use a NIOSH or equivalent approved device/equipment with appropriate organic or acid gas cartridge.

· **Protection of hands:**

Although not recommended for constant contact with the chemicals or for clean-up, nitrile gloves 11-13 mil thickness are recommended for normal use. The breakthrough time is 1 hr. For cleaning a spill where there is direct contact of the chemical, butyl rubber gloves are recommended 12-15 mil thickness with breakthrough times exceeding 4 hrs. Supplier recommendations should be followed.

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- **Material of gloves**
For normal use: nitrile rubber, 11-13 mil thickness
For direct contact with the chemical: butyl rubber, 12-15 mil thickness
- **Penetration time of glove material**
For normal use: nitrile rubber: 1 hour
For direct contact with the chemical: butyl rubber: >4 hours
- **Eye protection:**



Tightly sealed goggles

9 Physical and chemical properties

- **Information on basic physical and chemical properties**
- **General Information**
- **Appearance:**

Form:	Fluid
Color:	Colorless
- **Odor:** Aromatic
- **Odor threshold:** Not determined.
- **pH-value:** Not determined.
- **Change in condition**

Melting point/Melting range:	-46 °C
Boiling point/Boiling range:	81 °C
- **Flash point:** 2 °C
- **Flammability (solid, gaseous):** Highly flammable.
- **Auto igniting:** 525 °C
- **Decomposition temperature:** Not determined.
- **Ignition temperature:** Product is not selfigniting.
- **Danger of explosion:** Product is not explosive. However, formation of explosive air/vapor mixtures are possible.
- **Explosion limits:**

Lower:	4.4 Vol %
Upper:	16 Vol %
- **Vapor pressure at 20 °C:** 0 hPa
- **Vapor pressure at 50 °C:** 330 hPa
- **Density at 20 °C:** 0.78702 g/cm³
- **Relative density** Not determined.
- **Vapor density** Not determined.
- **Evaporation rate** Not determined.
- **Solubility in / Miscibility with Water:** Not miscible or difficult to mix.

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- **Partition coefficient (n-octanol/water):** Not determined.
- **Viscosity:**
 - Dynamic:** Not determined.
 - Kinematic:** Not determined.
- **Solvent content:**
 - Organic solvents:** 0.3 %
- **Other information** No further relevant information available.

10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** No further relevant information available.
- **Hazardous decomposition products:** No dangerous decomposition products known.

11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**

· **LD/LC50 values that are relevant for classification:**

ATE (Acute Toxicity Estimate)

Oral	LD50	1,309 mg/kg
Dermal	LD50	>1,992 mg/kg (rabbit)
Inhalative	LC50/4 h	>139 mg/L

75-05-8 acetonitrile

Oral	LD50	1,320 mg/kg (rat)
Dermal	LD50	>2,000 mg/kg (rabbit)
Inhalative	LC50/4 h	3,587 mg/L (mouse)

50-00-0 formaldehyde

Oral	LD50	100 mg/kg (rat)
Dermal	LD50	270 mg/kg (rabbit)
Inhalative	LC50/4 h	0.588 mg/L (rat)

75-07-0 acetaldehyde

Oral	LD50	1,930 mg/kg (rat)
Dermal	LD50	3,540 mg/kg (rabbit)
Inhalative	LC50/4 h	13,300 mg/L (rat)

108-94-1 cyclohexanone

Oral	LD50	1,534 mg/kg (rat)
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Dermal	LD50	794 mg/kg (rabbit)
Inhalative	LC50/4 h	>6.2 mg/L (rat)
110-62-3 valeraldehyde		
Oral	LD50	6,400 mg/kg (mouse)
		4,581 mg/kg (rat)
Dermal	LD50	4,050 mg/kg (rabbit)
123-38-6 propanal		
Oral	LD50	1,690 mg/kg (rat)
Dermal	LD50	2,460 mg/kg (rabbit)
Inhalative	LC50/4 h	>4.6 mg/L (rat)
123-72-8 butyraldehyde		
Oral	LD50	5,890 mg/kg (rat)
Dermal	LD50	3,560 mg/kg (rabbit)
Inhalative	LC50/4 h	>5.46 mg/L (rat)
123-73-9 (E)-2-butenal		
Oral	LD50	240 mg/kg (mouse)
Dermal	LD50	380 mg/kg (rabbit)
Inhalative	LC50/4 h	0.3 mg/L (rat)

· **Primary irritant effect:**

· **on the skin:** No irritant effect.

· **on the eye:** Irritating effect.

· **Sensitization:** Sensitization possible through skin contact.

· **Additional toxicological information:**

The product shows the following dangers according to internally approved calculation methods for preparations:

Harmful

Irritant

· **Carcinogenic categories**

· **IARC (International Agency for Research on Cancer)**

50-00-0	formaldehyde	1
75-07-0	acetaldehyde	2B
108-94-1	cyclohexanone	3
123-72-8	butyraldehyde	3

· **NTP (National Toxicology Program)**

50-00-0	formaldehyde	K
75-07-0	acetaldehyde	R

12 Ecological information

· **Toxicity**

· **Aquatic toxicity:** No further relevant information available.

· **Persistence and degradability** No further relevant information available.

· **Behavior in environmental systems:**

· **Bioaccumulative potential** No further relevant information available.

· **Mobility in soil** No further relevant information available.

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- **Additional ecological information:**
- **General notes:**
 Water hazard class 2 (Self-assessment): hazardous for water
 Do not allow product to reach ground water, water course or sewage system.
 Danger to drinking water if even small quantities leak into the ground.
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **Other adverse effects** No further relevant information available.

13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**
 Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

14 Transport information

- | | |
|---|---------------------|
| · Not Regulated, De minimis Quantities | - |
| · UN-Number | |
| · DOT/TDG, ADR, IMDG, IATA | UN1648 |
| · UN proper shipping name | |
| · DOT/TDG | Acetonitrile |
| · ADR | 1648 Acetonitrile |
| · IMDG, IATA | ACETONITRILE |
| · Transport hazard class(es) | |
| · DOT/TDG (Transport dangerous goods): | |
|  | |
| · Class | 3 Flammable liquids |
| · Label | 3 |
| · ADR, IMDG, IATA | |
|  | |
| · Class | 3 Flammable liquids |
| · Label | 3 |
| · Packing group | |
| · DOT/TDG, ADR, IMDG, IATA | II |

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· Environmental hazards:	Not applicable.
· Special precautions for user	Warning: Flammable liquids
· Hazard identification number (Kemler code):	33
· EMS Number:	F-E,S-D
· Stowage Category	B
· Stowage Code	SW2 Clear of living quarters.
· Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
· Transport/Additional information:	
· DOT/TDG	
· Quantity limitations	On passenger aircraft/rail: 5 L On cargo aircraft only: 60 L
· ADR	
· Excepted quantities (EQ)	Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· IMDG	
· Limited quantities (LQ)	1L
· Excepted quantities (EQ)	Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· UN "Model Regulation":	UN 1648 ACETONITRILE, 3, II

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15 Regulatory information

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

· Section 355 (extremely hazardous substances):

50-00-0	formaldehyde
123-73-9	(E)-2-butenal

· Section 313 (Specific toxic chemical listings):

75-05-8	acetonitrile
50-00-0	formaldehyde
75-07-0	acetaldehyde
123-38-6	propanal
123-72-8	butyraldehyde

· TSCA (Toxic Substances Control Act):

All components have the value ACTIVE.

· Canadian substance listings:

· Canadian Domestic Substances List (DSL)

75-05-8	acetonitrile
50-00-0	formaldehyde

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66-25-1	hexanal
75-07-0	acetaldehyde
108-94-1	cyclohexanone
110-62-3	valeraldehyde
111-71-7	heptanal
112-31-2	decanal
123-38-6	propanal
123-72-8	butyraldehyde
124-13-0	octanal
124-19-6	nonanal

· Canadian Non-Domestic Substances List (NDSL)

None of the ingredients is listed.

· Canadian Ingredient Disclosure list (limit 0.1%)

75-05-8	acetonitrile
50-00-0	formaldehyde
108-94-1	cyclohexanone

· Canadian Ingredient Disclosure list (limit 1%)

None of the ingredients is listed.

· National regulations:
· Additional classification according to Decree on Hazardous Materials:

Carcinogenic hazardous material group III (dangerous).

· Information about limitation of use:

Workers are not allowed to be exposed to the hazardous carcinogenic materials contained in this preparation.

Exceptions can be made by the authorities in certain cases.

· Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

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.

· Department issuing SDS: Document Control / Regulatory

· Contact: pdl-acg-regulatory-cq@agilent.com

· Date of the latest revision of the safety data sheet 07/04/2024 / 4

· Abbreviations and acronyms:

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

· * Data compared to the previous version altered.