

Trade name: Standard sample for LC/MS**Product no.:** 225-06613-13**Current version :** 3.0.2, issued: 15.09.2021**Replaced version:** 3.0.0, issued: 18.07.2018**Region:** GB**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**

Trade name

Standard sample for LC/MS**1.2 Relevant identified uses of the substance or mixture and uses advised against****Relevant identified uses of the substance or mixture**

General chemical processes

Uses advised against

No data available.

1.3 Details of the supplier of the safety data sheet**Address**

Shimadzu Europa GmbH

Albert-Hahn-Str. 6-10

47269 Duisburg

Telephone no. +49 (0)203 - 7687-0

Fax no. +49 (0)203 - 711045

Information provided by / telephone

Tel.: +49 (0)203 - 7687-0

Advice on Safety Data Sheet

sdb_info@umco.de

1.4 Emergency telephone number

For medical advice (in German and English):

+49 (0)551 192 40 (Giftinformationszentrum Nord)

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****Classification in accordance with Regulation (EC) No 1272/2008 (CLP)**

Acute Tox. 4; H302

Acute Tox. 4; H312

Acute Tox. 4; H332

Eye Irrit. 2; H319

Flam. Liq. 2; H225

Classification information

This product is assessed and classified using the methods and criteria below referred to in Article 9 of Regulation (EC) n° 1272/2008:

Physical hazards: determined through assessment data based on the methods or standards referred to in part 2 of Annex I to CLP

Health hazards and environmental hazards: determined through toxicological and ecotoxicological assessment data based on the methods or standards referred to in Part 3, 4 and 5 of Annex I to CLP.

2.2 Label elements**Labelling according to Regulation (EC) No 1272/2008 (CLP Regulation)****Hazard pictograms**

GHS02



GHS07

Signal word

Danger

Hazardous component(s) to be indicated on label:

acetonitrile

Hazard statement(s)

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 statement(s)

P210

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P280

Wear protective gloves/protective clothing.

P305+P351+P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

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No data available.

SECTION 3: Composition/information on ingredients**3.1 Substances**

Not applicable. The product is not a substance.

3.2 Mixtures**Chemical characterization**

Acetonitrile with 1.0 ng/μl acetophenone (CAS-Nr. 98-86-2)

Hazardous ingredients

No	Substance name		Additional information	
	CAS / EC / Index / REACH no	Classification (EC) 1272/2008 (CLP)	Concentration	%
1	acetonitrile			
	75-05-8 200-835-2 608-001-00-3 -	Acute Tox. 4*; H302 Acute Tox. 4*; H312 Acute Tox. 4*; H332 Eye Irrit. 2; H319 Flam. Liq. 2; H225	< 100.00	wt%

Full Text for all H-phrases and EUH-phrases: pls. see section 16

(*, **, ***, ****) Detailed explanation pls. refer to CLP regulation No. 1272/2008, annex VI, 1.2

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

In case of persisting adverse effects, consult a physician. Remove contaminated clothing and shoes immediately, and launder thoroughly before reusing. If the patient is likely to become unconscious, place and transport in stable sideways position.

After inhalation

Remove affected person from the immediate area. Ensure supply of fresh air. Irregular breathing/no breathing: artificial respiration. Call a doctor immediately.

After skin contact

Wash off immediately with soap and water. Don't use solvents.

After eye contact

Separate eyelids, wash the eyes thoroughly with water (15 min.).

After ingestion

Do not induce vomiting. Call a doctor immediately. Never give anything by mouth to an unconscious person.

4.2 Most important symptoms and effects, both acute and delayed

No data available.

4.3 Indication of any immediate medical attention and special treatment needed

No data available.

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

Alcohol-resistant foam; Extinguishing powder; Carbon dioxide; Water spray jet

Unsuitable extinguishing media

High power water jet

5.2 Special hazards arising from the substance or mixtureIn the event of fire, the following can be released: Carbon monoxide (CO); Carbon dioxide (CO₂); Combustion products of this material have to be classed invariably as respiratory poison.**5.3 Advice for firefighters**

Use self-contained breathing apparatus. Cool endangered containers with water spray jet. Suppress gases/vapours/mists with water spray jet. Wear protective clothing.

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures****For non-emergency personnel**

Refer to protective measures listed in sections 7 and 8. Avoid contact with skin, eyes and clothing. Ensure adequate ventilation. Keep

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away from ignition sources.

For emergency responders

No data available. Personal protective equipment (PPE) - see Section 8.

6.2 Environmental precautions

Do not discharge into the drains/surface waters/groundwater. Do not discharge into the subsoil/soil.

6.3 Methods and material for containment and cleaning up

Pick up with absorbent material (e.g., sand, sawdust, general-purpose binder). Send in suitable containers for recovery or disposal.

6.4 Reference to other sections

No data available.

SECTION 7: Handling and storage**7.1 Precautions for safe handling****Advice on safe handling**

Provide good ventilation at the work area (local exhaust ventilation, if necessary). If workplace exposure limits are exceeded, respiratory protection approved for this particular job must be worn. Risks inherent to handling the product must be minimised by applying the appropriate protective and preventive measures. Working processes should - so far as possible, according to the state of the art - be designed to rule out bodily contact or the release of hazardous substances.

General protective and hygiene measures

Do not eat, drink or smoke during work time. Keep away from foodstuffs and beverages. Avoid contact with eyes and skin. Remove soiled or soaked clothing immediately. Do not inhale vapours. Wash hands before breaks and after work. Provide eye wash fountain in work area. Have emergency shower available.

Advice on protection against fire and explosion

Vapours can form an explosive mixture with air. Take precautionary measures against static charges. Keep away from sources of heat and ignition. Use explosion-proof equipment/fittings and non-sparking tools.

7.2 Conditions for safe storage, including any incompatibilities**Technical measures and storage conditions**

Keep container tightly closed in a cool, well-ventilated place. Protect from heat and direct sunlight.

Requirements for storage rooms and vessels

Containers which are opened must be carefully closed and kept upright to prevent leakage. Always keep in containers of same material as the original.

Incompatible products

Do not store together with:

7.3 Specific end use(s)

No data available.

SECTION 8: Exposure controls/personal protection**8.1 Control parameters****Occupational exposure limit values**

No	Substance name	CAS no.	EC no.
1	acetonitrile	75-05-8	200-835-2
	2006/15/EC		
	Acetonitrile		
	WEL long-term (8-hr TWA reference period)	70	mg/m ³ 40 ppm
	Skin resorption / sensibilisation	Skin	
	List of approved workplace exposure limits (WELs) / EH40		
	Acetonitrile		
	WEL short-term (15 min reference period)	102	mg/m ³ 60 ppm
	WEL long-term (8-hr TWA reference period)	68	mg/m ³ 40 ppm

8.2 Exposure controls**Appropriate engineering controls**

No data available.

Personal protective equipment**Respiratory protection**

If workplace exposure limits are exceeded, a respiration protection approved for this particular job must be worn. In case of aerosol and mist formation, take appropriate measures for breathing protection in the event workplace threshold values are not specified.

Eye / face protection

Safety glasses with side protection shield (EN 166)

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In case of intensive contact, wear protective gloves (EN 374). Sufficient protection is given wearing suitable protective gloves checked according to i.e. EN 374, in the event of risk of skin contact with the product. Before use, the protective gloves should be tested in any case for its specific work-station suitability (i.e. mechanical resistance, product compatibility and antistatic properties). Adhere to the manufacturer's instructions and information relating to the use, storage, care and replacement of protective gloves. Protective gloves shall be replaced immediately when physically damaged or worn. Design operations thus to avoid permanent use of protective gloves.

Appropriate Material

In case of longer-term contact:

Appropriate Material

viton

Appropriate Material

In case of short-term contact / splash protection:

Appropriate Material

nitrile

Other

Normal chemical work clothing.

Environmental exposure controls

No data available.

SECTION 9: Physical and chemical properties**9.1 Information on basic physical and chemical properties**

State of aggregation			
liquid			
Form/Colour			
liquid			
colourless			
Odour			
aromatic			
pH value			
No data available			
Boiling point / boiling range			
Value	82	°C	
Melting point/freezing point			
Value	-45	°C	
Decomposition temperature			
No data available			
Flash point			
Value	9.5	°C	
Ignition temperature			
Value	524	°C	
Flammability			
No data available			
Lower explosion limit			
Value	4.4	% vol	
Upper explosion limit			
Value	16	% vol	
Vapour pressure			
Value	9.7	kPa	
Reference temperature	20	°C	
Relative vapour density			
No data available			
Relative density			
No data available			
Density			
Value	0.780	-	0.784 g/cm³
Reference temperature	20	°C	
Solubility in water			
Comments	miscible in all proportions		
Solubility			
No data available			
Partition coefficient n-octanol/water (log value)			

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No	Product Name
1	Standard sample for LC/MS
log Pow	-0.34
Viscosity	
Value	0.39 mPa*s
Reference temperature	20 °C
Type	dynamic
Particle characteristics	
No data available	

9.2 Other information

Other information
The physical data is that of the main component/s.

SECTION 10: Stability and reactivity**10.1 Reactivity**

No data available.

10.2 Chemical stability

Stable if stored and handled properly.

10.3 Possibility of hazardous reactions

No data available.

10.4 Conditions to avoid

Heat, naked flames or other ignition sources, electrostatic charge and discharge, formation of vapours/aerosols. Protect from sun.

10.5 Incompatible materials

Acids; Alkalies; Reactions with alkali metals. Reducing agents

10.6 Hazardous decomposition products

Carbon monoxide and carbon dioxide; Nitrous gases; cyanides

SECTION 11: Toxicological information**11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008**

Acute oral toxicity (result of the ATE calculation for the mixture)			
No	Product Name		
1	Standard sample for LC/MS		
ATE (Mixture)		500.05	
Method		Calculation method according Regulation (EC) No 1272/2008, (CLP), annex I, part 3, section 3.1.3.6.	
Acute oral toxicity			
No	Product Name		
1	Standard sample for LC/MS		
LD50		2460	mg/kg
Species		rat	
Acute dermal toxicity (result of the ATE calculation for the mixture)			
No	Product Name		
1	Standard sample for LC/MS		
ATE (Mixture)		1100.11	
Method		Calculation method according Regulation (EC) No 1272/2008, (CLP), annex I, part 3, section 3.1.3.6.	
Acute dermal toxicity			
No	Product Name		
1	Standard sample for LC/MS		
LD50		390	mg/kg
Species		rabbit	
Acute inhalational toxicity (result of the ATE calculation for the mixture)			
No	Product Name		
1	Standard sample for LC/MS		
ATE (Mixture)		11.0011	
Route of exposure / physical form		Vapour	
Method		Calculation method according Regulation (EC) No 1272/2008, (CLP), annex I, part 3, section 3.1.3.6.	

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Acute inhalation toxicity			
No	Product Name		
1	Standard sample for LC/MS		
LC50		17100	ppm
Duration of exposure		4	h
Species	rat		
Skin corrosion/irritation			
No data available			
Serious eye damage/irritation			
No data available			
Respiratory or skin sensitisation			
No data available			
Germ cell mutagenicity			
No data available			
Reproduction toxicity			
No data available			
Carcinogenicity			
No data available			
STOT - single exposure			
No data available			
STOT - repeated exposure			
No data available			
Aspiration hazard			
No data available			
Delayed and immediate effects as well as chronic effects from short and long-term exposure			
Inhalation of vapours may lead to headache, drowsiness and dizziness. Inhalation of vapours in higher concentration may lead to irritation of eyes, nose and respiratory tract. Repeated and prolonged skin contact may cause removal of natural fat from the skin and irritation of the skin. Eye contact with the product may lead to irritation.			

11.2 Information on other hazards**Endocrine disrupting properties**

No data available.

Other information

The toxicological information is based on the main components.

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish (acute)			
No	Product Name		
1	Standard sample for LC/MS		
LC50	>	100	mg/l
Duration of exposure		96	h
Species	Killifish		
Toxicity to fish (chronic)			
No data available			
Toxicity to Daphnia (acute)			
No	Product Name		
1	Standard sample for LC/MS		
EC50		100	mg/l
Duration of exposure		96	h
Species	Daphnia magna		
Toxicity to Daphnia (chronic)			
No data available			
Toxicity to algae (acute)			
No	Product Name		
1	Standard sample for LC/MS		
EC0		7300	mg/l
Species	Scenedesmus quadricauda		
Toxicity to algae (chronic)			

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No data available			
Bacteria toxicity			
No	Product Name		
1	Standard sample for LC/MS		
EC0		680	mg/l
Species	Pseudomonas putida		

12.2 Persistence and degradability

Biodegradability	
No	Product Name
1	Standard sample for LC/MS
Evaluation	readily degradable

12.3 Bioaccumulative potential

Partition coefficient n-octanol/water (log value)	
No	Product Name
1	Standard sample for LC/MS
log Pow	-0.34

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

No data available.

12.6 Endocrine disrupting properties

No data available.

12.7 Other adverse effects

No data available.

12.8 Other information

Other information	
Do not discharge product unmonitored into the environment.	
Ecological data refers to the main components.	

SECTION 13: Disposal considerations**13.1 Waste treatment methods****Product**

Allocation of a waste code number, according to the European Waste Catalogue, should be carried out in agreement with the regional waste disposal company.

Packaging

Residues must be removed from packaging and when emptied completely disposed of in accordance with the regulations for waste removal. Incompletely emptied packaging must be disposed of in the form of disposal specified by the regional disposer.

SECTION 14: Transport information**14.1 Transport ADR/RID/ADN**

Class	3
Classification code	F1
Packing group	II
Hazard identification no.	33
UN number	UN1648
Proper shipping name	ACETONITRILE
Tunnel restriction code	D/E
Label	3

14.2 Transport IMDG

Class	3
Packing group	II
UN number	UN1648
Proper shipping name	ACETONITRILE
EmS	F-E, S-D
Label	3

14.3 Transport ICAO-TI / IATA

Class	3
Packing group	II
UN number	UN1648

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Proper shipping name
Label

Acetonitrile
3

14.4 Other information

No data available.

14.5 Environmental hazards

Information on environmental hazards, if relevant, please see 14.1 - 14.3.

14.6 Special precautions for user

No data available.

14.7 Maritime transport in bulk according to IMO instruments

Not relevant

SECTION 15: Regulatory information**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulations****Regulation (EC) No 1907/2006 (REACH) Annex XIV (List of substances subject to authorisation)**

According to the data available and/or specifications supplied by upstream suppliers, this product does not contain any substances considered as substances requiring authorisation as listed on Annex XIV of the REACH regulation (EC) 1907/2006.

REACH candidate list of substances of very high concern (SVHC) for authorisation

According to available data and the information provided by preliminary suppliers, the product does not contain substances that are considered substances meeting the criteria for inclusion in annex XIV (List of Substances Subject to Authorisation) as laid down in Article 57 and article 59 of REACH (EC) 1907/2006.

Regulation (EC) No 1907/2006 (REACH) Annex XVII: RESTRICTIONS ON THE MANUFACTURE, PLACING ON THE MARKET AND USE OF CERTAIN DANGEROUS SUBSTANCES, MIXTURES AND ARTICLES

The product is considered being subject to REACH regulation (EC) 1907/2006 annex XVII.	No 3, 40
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Directive 2012/18/EU on the control of major-accident hazards involving dangerous substances

This product is subject to Part I of Annex I, risk category:	P5b
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15.2 Chemical safety assessment

No data available.

SECTION 16: Other information**Sources of key data used to compile the data sheet:**

Regulation (EC) No 1907/2006 (REACH), 1272/2008 (CLP) as amended in each case.

Directives 2000/39/EC, 2006/15/EC, 2009/161/EU, (EU) 2017/164.

National Threshold Limit Values of the corresponding countries as amended in each case.

Transport regulations according to ADR, RID, IMDG, IATA as amended in each case.

The data sources used to determine physical, toxic and ecotoxic data, are indicated directly in the corresponding section.

Full text of the H- and EUH- phrases drawn up in sections 2 and 3 (provided not already drawn up in these sections)

H302	Harmful if swallowed.
H312	Harmful in contact with skin.
H332	Harmful if inhaled.

Creation of the safety data sheet

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This information is based on our present knowledge and experience.

The safety data sheet describes products with a view to safety requirements.

It does not however, constitute a guarantee for any specific product properties and shall not establish a legally valid contractual relationship.

Alterations/supplements:

Alterations to the previous edition are marked in the left-hand margin.

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