



Preparing for the New Era of Laboratories

# SAFETY DATA SHEET (SDS)

According to regulation (EU) no.1907/2006

## **CAFFEINE ANHYDROUS 99% AR**

PRODUCT CODE : O-5295

CAS No : 58-08-2

FORMULA :  $C_8H_{10}N_4O_2$

UN No : not applicable

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SDS Number : 0625

Date : June 3, 2026

Version : 1.0

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

- 1.1 Product Name** : CAFFEINE ANHYDROUS 99% AR
- Synonyms** : 1,3,7-Trimethylxanthine
- CAS No.** : 58-08-2
- HS Code** : 2939.3000
- Chemical Formula** :  $C_8H_{10}N_4O_2$
- Molecular Weight** : 194.19 g/mol
- Product Code** : O-5295
- Brand** : Labotiq
- 1.2 Manufacturer** : Labotiq
- Address** : Jl.Terapi Raya AD2-Bumi Menteng Asri Bogor, Jawa Barat Indonesia – 16111
- Website** : [www.labotiq.net](http://www.labotiq.net)
- Email** : [labotiq.id@gmail.com](mailto:labotiq.id@gmail.com)
- For information** : Phone : (+62-251) 839110, 8311662, Fax : (+62-251) 83135710
- Emergency number** : +6281316894650
- 1.3 Application** : Laboratory chemicals, Manufacture of substances

### SECTION 2: Hazards identification

#### 2.1 Classification of the substance or mixture

**Classification according to Regulation (EC) No 1272/2008**

Acute toxicity, (Category 4) H302: Harmful if swallowed.

For the full text of the H-Statements mentioned in this Section, see Section 16

#### 2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal word

Warning

Hazard statement(s)

H302

Harmful if swallowed

Precautionary statement(s)

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P301 + P312

IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.

P501

Dispose of contents/ container to an approved waste disposal plant.

Supplemental Hazard Statements

none

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Reduced labelling ( $\leq 125$  ml)  
Hazard pictograms



|                                |         |
|--------------------------------|---------|
| Signal Word                    | Warning |
| Hazard Statements              | none    |
| Precautionary Statements       | none    |
| Supplemental Hazard Statements | none    |

### 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                           |
|------------------|---------------------------|
| Synonyms         | : 1,3,7-Trimethylxanthine |
| Formula          | : $C_8H_{10}N_4O_2$       |
| Molecular weight | : 194.19 g/mol            |
| CAS-No.          | : 58-08-2                 |

### 3.2 Mixture

Hazardous ingredients according to Regulation (EC) No 1272/2008

| Component                                                                 | Classification     | Concentration |
|---------------------------------------------------------------------------|--------------------|---------------|
| Caffeine<br>CAS-No. 58-08-2<br>EC-No. 200-362-1<br>Index-No. 613-086-00-5 | Acute Tox. 4; H302 | $\leq 100$ %  |

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### General advice

Show this safety data sheet to the doctor in attendance.

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**If inhaled**

After inhalation: fresh air.

**In case of skin contact**

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

**In case of eye contact**

After eye contact: rinse out with plenty of water. Remove contact lenses.

**If swallowed**

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

**4.2 Most important symptoms and effects, both acute and delayed**

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

**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**Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder**Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

**5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Risk of dust explosion.

Development of hazardous combustion gases or vapours possible in the event of fire.

**5.3 Advice for firefighters**

In the event of fire, wear self-contained breathing apparatus.

**5.4 Further information**

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

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**6.3 Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

**6.4 Reference to other sections**

For disposal see section 13.

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

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

**Hygiene measures**

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance. For precautions see section 2.2.

**7.2 Conditions for safe storage, including any incompatibilities****Storage conditions**

Tightly closed. Dry.

**Storage class**

Storage class (TRGS 510): 11: Combustible Solids

**7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

**SECTION 8: Exposure controls/personal protection****8.1 Control parameters**

Ingredients with workplace control parameters

**8.2 Exposure control****Appropriate engineering controls**

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

**Personal protective equipment****Eye/face protection**

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

**Skin protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

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**Full contact**

Material: Nitrile rubber  
 Minimum layer thickness: 0.11 mm  
 Break through time: 480 min  
 Material tested: Dermatril® (KCL 740, Size M)

**Splash contact**

Material: Nitrile rubber  
 Minimum layer thickness: 0.11 mm  
 Break through time: 480 min  
 Material tested: Dermatril® (KCL 740, Size M)

**Body Protection**

protective clothing

**Respiratory protection**

required when dusts are generated.  
 Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.  
 Recommended Filter type: Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

**Control of environmental exposure**

Do not let product enter drains.

### SECTION 9: Physical and chemical properties

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

|                                              |                                                  |
|----------------------------------------------|--------------------------------------------------|
| Appearance                                   | Form: Crystalline powder                         |
| Odour                                        | Colour: colourless                               |
| Odour Threshold                              | odourless                                        |
| pH                                           | No data available                                |
| Melting point/freezingpoint                  | No data available                                |
| Initial boiling point and boiling range      | Melting point/ range: 234 - 236,5 °C - lit.      |
| Flash point                                  | No data available                                |
| Evaporation rate                             | Not applicable                                   |
| Flammability (solid, gas)                    | No data available                                |
| Upper/lower flammability or explosive limits | May form combustible dust concentrations in air. |
| Vapour pressure                              | No data available                                |
| Vapour density                               | No data available                                |
| Density                                      | No data available                                |
| Relative density                             | 1,23 g/cm <sup>3</sup> at 18 °C                  |
| Water solubility                             | 1,23 at 18 °C                                    |
| Partition coefficient: noctanol/water        | No data available                                |
| Auto-ignition temperature                    | No data available                                |
| Decomposition temperature                    | No data available                                |
| Viscosity                                    | No data available                                |

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Explosive properties  
Oxidizing properties

Not classified as explosive.  
none

**9.2 Other safety information**

No data available

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

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

**10.2 Chemical stability**

The product is chemically stable under standard ambient conditions (room temperature).

**10.3 Possibility of hazardous reactions**

Violent reactions possible with: Strong oxidizing agents

**10.4 Conditions to avoid**

No data available

**10.5 Incompatible materials**

No data available

**10.6 Hazardous decomposition products**

in the event of fire: See section 5.

**SECTION 11: Toxicological information****Mixture****Acute toxicity**

LD50 Oral - Rat - male and female - 367,7 mg/kg

(OECD Test Guideline 401)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Acute toxicity estimate Oral - 367,7 mg/kg

(ATE value derived from LD50/LC50 value)

LC50 Inhalation - Rat - male and female - 4 h - 4,94 mg/l - aerosol

(OECD Test Guideline 403)

LD50 Dermal - Rat - male and female - &gt; 2.000 mg/kg

(OECD Test Guideline 402)

**Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

**Respiratory or skin sensitisation**

Local lymph node assay (LLNA) - Mouse

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Result: negative  
(OECD Test Guideline 429)

**Germ cell mutagenicity**

Test Type: In vitro mammalian cell gene mutation test  
Test system: mouse lymphoma cells  
Metabolic activation: without metabolic activation  
Method: OECD Test Guideline 476  
Result: negative  
Test Type: Ames test  
Test system: Escherichia coli/Salmonella typhimurium  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 471  
Result: negative  
Test Type: Chromosome aberration test in vitro  
Test system: Human lymphocytes  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 473  
Result: negative  
Test Type: Chromosome aberration test in vitro  
Test system: Chinese hamster lung cells  
Metabolic activation: without metabolic activation  
Method: OECD Test Guideline 473  
Result: positive  
Test Type: Chromosome aberration test  
Species: Mouse  
Application Route: Intraperitoneal  
Result: negative  
Remarks: (ECHA)  
Test Type: dominant lethal test  
Species: Mouse  
Application Route: Gavage  
Result: negative  
Remarks: (ECHA)  
Test Type: Micronucleus test  
Species: Mouse  
Cell type: Red blood cells (erythrocytes)  
Application Route: Oral  
Method: OECD Test Guideline 474  
Result: Positive results were obtained in some in vivo tests.  
Test Type: Chromosome aberration test  
Species: Rat  
Application Route: Oral  
Result: negative  
Remarks: (ECHA)

**Carcinogenicity**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available



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**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

Endocrine disrupting properties

Product:

Assessment :

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Repeated dose toxicity - Mouse - male and female - Oral - 90 d - No observed adverse effect level - 167,4 - 179,4 mg/kg

Remarks: (ECHA)

RTECS: EV6475000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption of toxic quantities:

Diarrhoea

Vomiting

agitation

Headache

Systemic effects:

drop in blood pressure

tachycardia

collapse

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

**SECTION 12: Ecological information****12.1 Toxicity**

Toxicity to fish

static test LC50 - *Leuciscus idus* (Golden orfe) - ca. 87 mg/l - 96 h  
(DIN 38412 part 15)

static test NOEC - *Leuciscus idus* (Golden orfe) - 46 mg/l - 96 h  
(DIN 38412 part 15)

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - *Daphnia magna* (Water flea) - 182 mg/l - 48 h  
(DIN 38412)

Toxicity to algae static test

ErC50 - *Desmodesmus subspicatus* (green algae) - > 100 mg/l - 72 h  
(OECD Test Guideline 201)

Toxicity to bacteria EC50 - activated sludge - > 1.000 mg/l - 3 h  
(OECD Test Guideline 209)

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**12.2 Persistence and degradability**

Biodegradability aerobic - Exposure time 22 d  
 Result: 90 - 100 % - Readily biodegradable.  
 (OECD Test Guideline 301A)

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**12.6 Other adverse effects**

Discharge into the environment must be avoided.

**Endocrine disrupting properties****Product:**

Assessment :

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission. Delegated regulation (EU) 2017/2100 or Commission. Regulation (EU) 2018/605 at levels of 0.1% or higher.

### SECTION 13: Disposal considerations

**13.1 Waste treatment methods**

No data available

### SECTION 14: Transport information

**14.1 UN number**

ADR/RID: -

IMDG: -

IATA: -

**14.2 UN proper shipping name**

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

**14.3 Transport hazard class(es)**

ADR/RID: -

IMDG: -

IATA: -

**14.4 Packaging group**

ADR/RID: -

IMDG: -

IATA: -

**14.5 Environmental hazards**

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

**14.6 Special precautions for user****Further information**

No data available

### SECTION 15: Regulatory information

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

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

**15.2 Chemical safety assessment**

For this product a chemical safety assessment was not carried out

**SECTION 16: Other information****Full text of H-Statements referred to under sections 2 and 3.**

H302 Harmful if swallowed.

**National Fire Protection Association (U.S.A.):**

Health: 2

Flammability: 0

Reactivity: 0

**Further information**

*The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Labotiq shall not be held liable for any damage resulting from handling or from contact with the above product.*

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