

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878 SDS Reference Number: 02429 Issue date: 5/16/2016 Revision date: 8/8/2024 Supersedes version of: 9/25/2023 Version: 2.0

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

1.1. Product identifier

Product form : Substance

Trade name : CAFFEINE ANHYDROUS EXTRA PURE

 EC Index-No.
 : 613-086-00-5

 EC-No.
 : 200-362-1

 CAS-No.
 : 58-08-2

 Product code
 : 02429

 Formula
 : C8H10N4O2

Chemical structure

H₃C N CH₃

Synonyms : 3,7-Dihydro-1,3,7-Trimethyl-1H-Purine-2,6-Dione; 1,3,7-Trimethyl xanthine; Methyl

theobromide

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

Relevant identified uses

Use of the substance/mixture : Laboratory chemicals, Manufacture of substances

1.3. Details of the supplier of the safety data sheet

LOBA CHEMIE PVT.LTD.

107 Wode House Road, Jehangir Villa, Colaba

400005 Mumbai

INDIA

T +91 22 6663 6663, F +91 22 6663 6699

info@lobachemie.com, www.lobachemie.com

1.4. Emergency telephone number

Emergency number : + 91 22 6663 6663 (9:00am - 6:00 pm)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute toxicity (oral), Category 4 H302

Full text of H- and EUH-statements: see section 16

Adverse physicochemical, human health and environmental effects

Harmful if swallowed.

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :

GHS07

Warning

Signal word (CLP)

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Hazard statements (CLP) : H302 - Harmful if swallowed

Precautionary statements (CLP) : P264 - Wash hands thoroughly after handling.

P270 - Do not eat, drink or smoke when using this product.

P301+P312 - IF SWALLOWED: Call a POISON CENTRE or doctor if you feel unwell. P501 - Dispose of contents/container to hazardous or special waste collection point, in

accordance with local, regional, national and/or international regulation.

2.3. Other hazards

Contains no PBT and/or vPvB substances ≥ 0.1% assessed in accordance with REACH Annex XIII

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name : CAFFEINE ANHYDROUS

CAS-No. : 58-08-2 EC-No. : 200-362-1 EC Index-No. : 613-086-00-5

Name	Product identifier	%
CAFFEINE ANHYDROUS	CAS-No.: 58-08-2 EC-No.: 200-362-1 EC Index-No.: 613-086-00-5	100

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : Call a poison center or a doctor if you feel unwell.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing.

First-aid measures after skin contact : Wash with plenty of water/.... Get medical advice/attention. Wash skin with plenty of water. First-aid measures after eye contact : Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy

to do. Continue rinsing. Get medical advice/attention.

First-aid measures after ingestion : Rinse mouth. Call a POISON CENTER/doctor if you feel unwell. Call a poison center or a

doctor if you feel unwell.

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

Symptoms/effects after ingestion : Harmful if swallowed.

4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide. Dry powder. Foam. Water spray.

Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Hazardous decomposition products in case of fire : Toxic fumes may be released.

5.3. Advice for firefighters

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

Do not attempt to take action without suitable protective equipment. Self-contained

breathing apparatus. Complete protective clothing.

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SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Emergency procedures : Ventilate spillage area. Evacuate unnecessary personnel.

For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Use personal protective

equipment as required. For further information refer to section 8: "Exposure

controls/personal protection".

6.2. Environmental precautions

Avoid release to the environment.

Other information

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Mechanically recover the product. On land, sweep or shovel into suitable containers. Soak

up spills with inert solids, such as clay or diatomaceous earth as soon as possible.

: Dispose of materials or solid residues at an authorized site.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Ensure good ventilation of the work station. Wear personal protective equipment. Avoid

contact with skin and eyes. Do not breathe vapours. Provide good ventilation in process

area to prevent formation of vapour.

Hygiene measures : Do not eat, drink or smoke when using this product. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Always

wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store in a well-ventilated place. Keep container tightly closed. Store in a well-ventilated

place. Keep cool.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls

Appropriate engineering controls:

Ensure good ventilation of the work station.

Personal protection equipment

Personal protective equipment symbol(s):







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Eye and face protection

Eye protection:

Chemical goggles or safety glasses

Skin protection

Skin and body protection:

Wear suitable protective clothing

Hand protection:

Protective gloves

Respiratory protection

Respiratory protection:

[In case of inadequate ventilation] wear respiratory protection.

Environmental exposure controls

Environmental exposure controls:

Avoid release to the environment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Solid
Colour : White.

Appearance : Crystalline powder or crystals.

Molecular mass : 194.19 g/mol Odour : Odourless. Odour threshold 29 - 300 ppm Melting point 235 - 237 °C Freezing point Not applicable Boiling point Not available Flammability Non flammable. Lower explosion limit : Not applicable : Not applicable Upper explosion limit : Not applicable Flash point Auto-ignition temperature : Not applicable

pH : 5.5-6.5 pH solution concentration : 1%

Viscosity, kinematic : Not applicable

Solubility : Water: 20 g/l at 20°C - Slightly soluble in water.

: Not available

Partition coefficient n-octanol/water (Log Kow) : Not available

Partition coefficient n-octanol/water (Log Pow) : 0.07

Vapour pressure : 15 mm Hg (89°C)
Vapour pressure at 50°C : Not available
Density : 1.23 g/cm³ at 18°C
Relative density : Not available
Relative vapour density at 20°C : Not applicable
Particle size : Not available

9.2. Other information

Decomposition temperature

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

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10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Air contact. Direct sunlight. Moisture.

10.5. Incompatible materials

Oxidizing agent.

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity (oral) : Harmful if swallowed.

Acute toxicity (dermal) : Not classified

Acute toxicity (inhalation) : Not classified

Skin corrosion/irritation : Not classified

pH: 5.5 – 6.5

Serious eye damage/irritation : Not classified

pH: 5.5 – 6.5

Respiratory or skin sensitisation : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
STOT-single exposure : Not classified
STOT-repeated exposure : Not classified
Aspiration hazard : Not classified

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Viscosity, kinematic Not applicable

11.2. Information on other hazards

Other information

Potential adverse human health effects and

: Harmful if swallowed.

symptoms

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms nor to cause long-term adverse

effects in the environment.

Hazardous to the aquatic environment, short-term

(acute)

: Not classified

Hazardous to the aquatic environment, long-term

: Not classified

(chronic)

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12.2. Persistence and degradability

CAFFEINE ANHYDROUS EXTRA PURE (58-08-2)

Persistence and degradability Rapidly degradable

12.3. Bioaccumulative potential

CAFFEINE ANHYDROUS EXTRA PURE (58-08-2)

Partition coefficient n-octanol/water (Log Pow) 0.07

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Endocrine disrupting properties

No additional information available

12.7. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste treatment methods

Product/Packaging disposal recommendations

- : Dispose of contents/container in accordance with licensed collector's sorting instructions.
- Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation.

SECTION 14: Transport information

In accordance with ADR / IMDG / IATA / ADN / RID

14.1. UN number or ID number

Not regulated for transport

14.2. UN proper shipping name

Proper Shipping Name (ADR) : Not regulated Proper Shipping Name (IMDG) : Not regulated Proper Shipping Name (IATA) : Not regulated Proper Shipping Name (ADN) : Not regulated Proper Shipping Name (RID) : Not regulated

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR) : Not regulated

IMDG

Transport hazard class(es) (IMDG) : Not regulated

IATA

Transport hazard class(es) (IATA) : Not regulated

ADN

Transport hazard class(es) (ADN) : Not regulated

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RID

Transport hazard class(es) (RID) : Not regulated

14.4. Packing group

Packing group (ADR) : Not regulated Packing group (IMDG) : Not regulated Packing group (IATA) : Not regulated Packing group (ADN) : Not regulated Packing group (RID) : Not regulated Packing group (RID) : Not regulated

14.5. Environmental hazards

Other information : No supplementary information available

14.6. Special precautions for user

Overland transport

Not regulated

Transport by sea

Not regulated

Air transport

Not regulated

Inland waterway transport

Not regulated

Rail transport

Not regulated

14.7. Maritime transport in bulk according to IMO instruments

Not applicable

SECTION 15: Regulatory information

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

EU-Regulations

REACH Annex XVII (Restriction List)

Not listed on REACH Annex XVII

REACH Annex XIV (Authorisation List)

Not listed on REACH Annex XIV (Authorisation List)

REACH Candidate List (SVHC)

Not listed on the REACH Candidate List

PIC Regulation (Prior Informed Consent)

Not listed on the PIC list (Regulation EU 649/2012)

POP Regulation (Persistent Organic Pollutants)

Not listed on the POP list (Regulation EU 2019/1021)

Ozone Regulation (1005/2009)

Not listed on the Ozone Depletion list (Regulation EU 1005/2009)

Dual-Use Regulation (428/2009)

Contains no substance subject to the COUNCIL REGULATION (EC) No 428/2009 of 5 May 2009 setting up a Community regime for the control of exports, transfer, brokering and transit of dual-use items.

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Explosives Precursors Regulation (2019/1148)

Contains no substance(s) listed on the Explosives Precursors list (Regulation EU 2019/1148 on the marketing and use of explosives precursors)

Drug Precursors Regulation (273/2004)

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances)

National regulations

Germany

Water hazard class (WGK) : WGK 3, Highly hazardous to water (Classification according to AwSV). Hazardous Incident Ordinance (12. BImSchV) : Is not subject to the Hazardous Incident Ordinance (12. BImSchV)

Netherlands

SZW-lijst van kankerverwekkende stoffen : The substance is not listed SZW-lijst van mutagene stoffen : The substance is not listed SZW-lijst van reprotoxische stoffen – Borstvoeding : The substance is not listed SZW-lijst van reprotoxische stoffen – : The substance is not listed

Vruchtbaarheid

SZW-lijst van reprotoxische stoffen – Ontwikkeling : The substance is not listed

Denmark

Danish National Regulations : Young people below the age of 18 years are not allowed to use the product

15.2. Chemical safety assessment

No chemical safety assessment has been carried out

SECTION 16: Other information

Abbreviations and acronyms:		
ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways	
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road	
ATE	Acute Toxicity Estimate	
BCF	Bioconcentration factor	
BLV	Biological limit value	
BOD	Biochemical oxygen demand (BOD)	
COD	Chemical oxygen demand (COD)	
DMEL	Derived Minimal Effect level	
DNEL	Derived-No Effect Level	
EC-No.	European Community number	
EC50	Median effective concentration	
EN	European Standard	
IARC	International Agency for Research on Cancer	
IATA	International Air Transport Association	
IMDG	International Maritime Dangerous Goods	
LC50	Median lethal concentration	
LD50	Median lethal dose	
LOAEL	Lowest Observed Adverse Effect Level	
NOAEC	No-Observed Adverse Effect Concentration	
NOAEL	No-Observed Adverse Effect Level	

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Abbreviations and acronyms:	
NOEC	No-Observed Effect Concentration
OECD	Organisation for Economic Co-operation and Development
OEL	Occupational Exposure Limit
PBT	Persistent Bioaccumulative Toxic
PNEC	Predicted No-Effect Concentration
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail
SDS	Safety Data Sheet
STP	Sewage treatment plant
ThOD	Theoretical oxygen demand (ThOD)
TLM	Median Tolerance Limit
VOC	Volatile Organic Compounds
CAS-No.	Chemical Abstract Service number
N.O.S.	Not Otherwise Specified
vPvB	Very Persistent and Very Bioaccumulative
ED	Endocrine disruptor

Full text of H- and EUH-statements:	
Acute Tox. 4 (Oral)	Acute toxicity (oral), Category 4
H302	Harmful if swallowed.

Safety Data Sheet (SDS), EU

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.