



SAFETY DATA SHEET

Caffeine

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

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

1.1. Product identifier

Product name	Caffeine
Chemical name	1,3,7-Trimethylxanthine
Synonyms; trade names	3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione
CAS number	58-08-2
EU index number	613-086-00-5
EC number	200-362-1

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

Identified uses	For research purposes only.
Uses advised against	Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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1.4. Emergency telephone number

+44 (0) 7769276927

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (SI 2019 No. 720)

Physical hazards	Not Classified
Health hazards	Acute Tox. 4 - H302 Acute Tox. 4 - H332
Environmental hazards	Not Classified

2.2. Label elements

EC number	200-362-1
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Hazard pictograms



Signal word	Warning
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Caffeine

Hazard statements	H302+H332 Harmful if swallowed or if inhaled.
Precautionary statements	P261 Avoid breathing dust. P264 Wash contaminated skin thoroughly after handling. P271 Use only outdoors or in a well-ventilated area. P280 Wear protective clothing and gloves. P301+P312 IF SWALLOWED: Call a POISON CENTRE/doctor if you feel unwell. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. P330 Rinse mouth. P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	Caffeine
Chemical name	1,3,7-Trimethylxanthine
EU index number	613-086-00-5
CAS number	58-08-2
EC number	200-362-1
Chemical formula	C ₈ H ₁₀ N ₄ O ₂

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	If in doubt, get medical attention promptly. Show this Safety Data Sheet to the medical personnel.
Inhalation	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Maintain an open airway. Loosen tight clothing such as collar, tie or belt. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention. Place unconscious person on their side in the recovery position and ensure breathing can take place.
Ingestion	Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Never give anything by mouth to an unconscious person. Place unconscious person on their side in the recovery position and ensure breathing can take place. Keep affected person under observation. Get medical attention if symptoms are severe or persist.
Skin contact	Rinse with water.
Eye contact	Remove any contact lenses and open eyelids wide apart. Rinse with water. Get medical attention if any discomfort continues.
Protection of first aiders	First aid personnel should wear appropriate protective equipment during any rescue.

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

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Headache. Exhaustion and weakness.

Caffeine

Ingestion	May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.
Skin contact	Prolonged contact may cause dryness of the skin.
Eye contact	May be slightly irritating to eyes.

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

Notes for the doctor	Treat symptomatically.
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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
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Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.
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5.2. Special hazards arising from the substance or mixture

Specific hazards	This product is toxic.
Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Toxic gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO ₂). Nitrous gases (NO _x).

5.3. Advice for firefighters

Protective actions during firefighting	Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Ventilate closed spaces before entering them. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.
Special protective equipment for firefighters	Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions	Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of dust. Use suitable respiratory protection if ventilation is inadequate.
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6.2. Environmental precautions

Environmental precautions	Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.
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6.3. Methods and material for containment and cleaning up

Methods for cleaning up	Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Provide adequate ventilation. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.
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6.4. Reference to other sections

Reference to other sections	For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.
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Caffeine

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions	Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.
Advice on general occupational hygiene	Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions	Store away from incompatible materials (see Section 10). Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.
Storage class	Chemical storage.

7.3. Specific end use(s)

Specific end use(s)	The identified uses for this product are detailed in Section 1.2.
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SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

8.2. Exposure controls

Protective equipment



Appropriate engineering controls	Provide adequate general and local exhaust ventilation. Ensure the ventilation system is regularly maintained and tested. Good general ventilation should be adequate to control worker exposure to airborne contaminants. Observe any occupational exposure limits for the product or ingredients.
Eye/face protection	Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses.
Hand protection	No specific hand protection recommended.
Other skin and body protection	Wear appropriate clothing to prevent repeated or prolonged skin contact.
Hygiene measures	Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.
Respiratory protection	Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.
Environmental exposure controls	Keep container tightly sealed when not in use. 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.

Caffeine

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Crystalline powder.
Colour	White.
Odour	Odourless.
Odour threshold	No information available.
pH	pH (diluted solution): 5.5 - 6.5 , 20g/l (20°C/68°F)
Melting point	234 - 239°C/453.2 - 462.2°F
Initial boiling point and range	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Upper/lower flammability or explosive limits	No information available.
Vapour pressure	No information available.
Vapour density	No information available.
Relative density	1.23
Solubility(ies)	Slightly soluble in the following materials: Ethanol. Water
Partition coefficient	No information available.
Auto-ignition temperature	540°C/1004°F
Decomposition Temperature	No information available.

9.2. Other information

Molecular weight	194.19
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SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity	See the other subsections of this section for further details.
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10.2. Chemical stability

Stability	Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.
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10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	Violent reactions possible with: Strong oxidising agents.
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10.4. Conditions to avoid

Conditions to avoid	Avoid the accumulation of dust. Avoid dust close to ignition sources. Avoid excessive heat for prolonged periods of time.
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10.5. Incompatible materials

Materials to avoid	Avoid contact with strong oxidising agents.
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Caffeine

10.6. Hazardous decomposition products

Hazardous decomposition products	Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Toxic gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO ₂). Nitrous gases (NO _x).
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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Summary Harmful if swallowed.

Acute toxicity oral (LD₅₀ mg/kg) 367.7

Species Rat

ATE oral (mg/kg) 500.0

Acute toxicity - dermal

Summary Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Summary Harmful if inhaled.

Acute toxicity inhalation (LC₅₀ dust/mist mg/l) 4.94

Species Rat

ATE inhalation (dusts/mists mg/l) 4.94

Skin corrosion/irritation

Summary Based on available data the classification criteria are not met.

Serious eye damage/irritation

Summary Based on available data the classification criteria are not met.

Respiratory sensitisation

Summary Based on available data the classification criteria are not met.

Skin sensitisation

Summary Based on available data the classification criteria are not met.

Germ cell mutagenicity

Summary Based on available data the classification criteria are not met.

Carcinogenicity

Summary Based on available data the classification criteria are not met.

IARC carcinogenicity None of the ingredients are listed or exempt.

Reproductive toxicity

Summary Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

Summary Based on available data the classification criteria are not met.

Specific target organ toxicity - repeated exposure

Summary Based on available data the classification criteria are not met.

Caffeine

Aspiration hazard

Summary Not relevant. Solid.

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Headache. Exhaustion and weakness.
Ingestion	May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.
Skin contact	Prolonged contact may cause dryness of the skin.
Eye contact	May be slightly irritating to eyes.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.

SECTION 12: Ecological information

Ecotoxicity Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

12.1. Toxicity

Acute aquatic toxicity

Summary Based on available data the classification criteria are not met.

Acute toxicity - fish LC₅₀, 96 hours: 87 mg/l, Leuciscus idus (Golden orfe)
NOEC, 96 hours: 46 mg/l, Leuciscus idus (Golden orfe)

Acute toxicity - aquatic invertebrates EC₅₀, 48 hours: 182 mg/l, Daphnia magna

Acute toxicity - aquatic plants NOEC, 72 hours: 6.25 mg/l, Desmodesmus subspicatus

Chronic aquatic toxicity

Summary Based on available data the classification criteria are not met.

12.2. Persistence and degradability

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient No information available.

12.4. Mobility in soil

Mobility No data available.

12.5. Results of PBT and vPvB assessment

12.6. Other adverse effects

Other adverse effects Avoid discharge into drains and the aquatic environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Caffeine

General information	The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.
Disposal methods	Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

SECTION 14: Transport information

General	The product is not covered by international regulations on the transport of dangerous goods (IMDG, IATA, ADR/RID).
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14.1. UN number

Not applicable.

14.2. UN proper shipping name

Not applicable.

14.3. Transport hazard class(es)

No transport warning sign required.

14.4. Packing group

Not applicable.

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

14.6. Special precautions for user

Not applicable.

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Not applicable.

Annex II of MARPOL 73/78
and the IBC Code

SECTION 15: Regulatory information

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

National regulations	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits.
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15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

Caffeine

EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road. ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways. RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail. IATA: International Air Transport Association. ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air. IMDG: International Maritime Dangerous Goods. CAS: Chemical Abstracts Service. ATE: Acute Toxicity Estimate. LC50: Lethal Concentration to 50 % of a test population. LD50: Lethal Dose to 50% of a test population (Median Lethal Dose). EC ₅₀ : 50% of maximal Effective Concentration. PBT: Persistent, Bioaccumulative and Toxic substance. vPvB: Very Persistent and Very Bioaccumulative.
Classification abbreviations and acronyms	Acute Tox. = Acute toxicity
Classification procedures according to SI 2019 No. 720	Acute Tox. 4 - H332: Acute Tox. 4 - H302: : Expert judgement.
Training advice	Only trained personnel should use this material.
Revision date	08/07/2022
Revision	1
SDS number	1117
Hazard statements in full	H302 Harmful if swallowed. H332 Harmful if inhaled.

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.