

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

1.1. Product identifier

Product form	: Substance
Substance name	: CAFFEINE
Chemical name	: caffeine
EC Index-No.	: 613-086-00-5
EC-No.	: 200-362-1
CAS-No.	: 58-08-2
Product code	: B2030, B2104, B2216
Product group	: End product

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

1.2.1. Relevant identified uses

Main use category	: Professional use
Use of the substance/mixture	: Laboratory chemicals
Function or use category	: Laboratory chemicals

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Elemental Microanalysis Ltd
1 Hameldown Road
Okehampton – Devon EX20 1UB
GB United Kingdom
T +44 1837 54446
enquiries@microanalysis.co.uk - <https://www.elementalmicroanalysis.com/>

1.4. Emergency telephone number

Emergency number : +44 (0) 7990 767375

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

Signal word (CLP) : Warning
Hazard statements (CLP) : H302 - Harmful if swallowed.
Precautionary statements (CLP) : P264 - Wash hands thoroughly after handling.
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER, a doctor.
P321 - Specific treatment (see supplemental first aid instruction on this label).

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2.3. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
CAFFEINE	CAS-No.: 58-08-2 EC-No.: 200-362-1 EC Index-No.: 613-086-00-5	100	Acute Tox. 4 (Oral), H302 (ATE=185 mg/kg bodyweight)

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

3.2. Mixtures

Not applicable

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 skin with plenty of water.
First-aid measures after eye contact	: Rinse eyes with water as a precaution.
First-aid measures after ingestion	: Rinse mouth. Call a poison center or a doctor if you feel unwell.

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

No additional information available

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 : Water spray. Dry powder. Foam.

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 attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Ventilate spillage area.

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6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

6.2. Environmental precautions

Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Mechanically recover the product.
Other information : 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.
Hygiene measures : Do not eat, drink or smoke when using this product. 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 cool.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.1.1 National occupational exposure and biological limit values

No additional information available

8.1.2. Recommended monitoring procedures

No additional information available

8.1.3. Air contaminants formed

No additional information available

8.1.4. DNEL and PNEC

CAFFEINE (58-08-2)	
DNEL/DMEL (Workers)	
Long-term - systemic effects, dermal	25.17 mg/kg bodyweight/day
Long-term - systemic effects, inhalation	44.37 mg/m ³
PNEC (Water)	
PNEC aqua (freshwater)	0.087 mg/l
PNEC aqua (marine water)	0.0087 mg/l
PNEC aqua (intermittent, freshwater)	0.87 mg/l
PNEC (Sediment)	
PNEC sediment (freshwater)	0.4 mg/kg dwt

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CAFFEINE (58-08-2)	
PNEC (Soil)	
PNEC soil	0.0289 mg/kg dwt
PNEC (STP)	
PNEC sewage treatment plant	10 mg/l

8.1.5. Control banding

No additional information available

8.2. Exposure controls

8.2.1. Appropriate engineering controls

Appropriate engineering controls:

Ensure good ventilation of the work station.

8.2.2. Personal protection equipment

Personal protective equipment symbol(s):



8.2.2.1. Eye and face protection

Eye protection:

Safety glasses

8.2.2.2. Skin protection

Skin and body protection:

Wear suitable protective clothing

Hand protection:

Protective gloves

8.2.2.3. Respiratory protection

Respiratory protection:

In case of insufficient ventilation, wear suitable respiratory equipment

8.2.2.4. Thermal hazards

No additional information available

8.2.3. 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	: Not available
Molecular mass	: 194.19 g/mol
Odour	: Not available
Odour threshold	: Not available
Melting point	: 237.7 – 239 °C Sublimation: 'yes'
Freezing point	: Not applicable
Boiling point	: Not available
Flammability	: Non flammable.
Explosive limits	: Not applicable
Lower explosion limit	: Not applicable

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Upper explosion limit	: Not applicable
Flash point	: Not applicable
Auto-ignition temperature	: 925 °C
Decomposition temperature	: Not available
pH	: 6.9
pH solution	: Not available
Viscosity, kinematic	: Not applicable
Solubility	: Water: 2.17 g/100ml
Partition coefficient n-octanol/water (Log Kow)	: Not available
Partition coefficient n-octanol/water (Log Pow)	: -0.07
Vapour pressure	: 0.000000047 hPa Temp.: 25 °C
Vapour pressure at 50°C	: Not available
Density	: Not available
Relative density	: 1.23 Type: 'relative density' Temp.: 18 °C
Relative vapour density at 20°C	: 6.7
Particle size	: Not available

9.2. Other information

9.2.1. Information with regard to physical hazard classes

No additional information available

9.2.2. Other safety characteristics

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.

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

None under recommended storage and handling conditions (see section 7).

10.5. Incompatible materials

No additional information available

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

CAFFEINE (58-08-2)

LD50 oral rat	200 – 400 mg/kg bodyweight Animal: rat, Guideline: OECD Guideline 401 (Acute Oral Toxicity)
LD50 oral	185 mg/kg bodyweight Animal: mouse, Guideline: OECD Guideline 401 (Acute Oral Toxicity), 95% CL: 100 - 240

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CAFFEINE (58-08-2)	
LD50 dermal rat	> 2000 mg/kg bodyweight Animal: rat, Guideline: OECD Guideline 402 (Acute Dermal Toxicity)
LC50 Inhalation - Rat	≈ 4.94 mg/l air Animal: rat, Guideline: OECD Guideline 403 (Acute Inhalation Toxicity)

Skin corrosion/irritation	: Not classified pH: 6.9
Serious eye damage/irritation	: Not classified pH: 6.9
Respiratory or skin sensitisation	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified

CAFFEINE (58-08-2)	
IARC group	3 - Not classifiable
Reproductive toxicity	: Not classified
STOT-single exposure	: Not classified
STOT-repeated exposure	: Not classified

CAFFEINE (58-08-2)	
NOAEL (subchronic, oral, animal/male, 90 days)	≥ 167.4 mg/kg bodyweight Animal: mouse, Animal sex: male, Guideline: other:
NOAEL (subchronic, oral, animal/female, 90 days)	≥ 179.4 mg/kg bodyweight Animal: mouse, Animal sex: female, Guideline: other:
Aspiration hazard	: Not classified

CAFFEINE (58-08-2)	
Viscosity, kinematic	Not applicable

11.2. Information on other hazards

No additional information available

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 (chronic)	: Not classified
Not rapidly degradable	

CAFFEINE (58-08-2)	
LC50 - Fish [1]	≈ 87 mg/l Test organisms (species): Leuciscus idus
EC50 - Crustacea [1]	182 mg/l Test organisms (species): Daphnia magna
EC50 72h - Algae [1]	> 100 mg/l Test organisms (species): Desmodesmus subspicatus (previous name: Scenedesmus subspicatus)

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

CAFFEINE (58-08-2)	
Partition coefficient n-octanol/water (Log Pow)	-0.07

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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 : Dispose of contents/container in accordance with licensed collector's sorting instructions.

SECTION 14: Transport information

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

ADR	IMDG	IATA	ADN	RID
14.1. UN number or ID number				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.2. UN proper shipping name				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.3. Transport hazard class(es)				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.4. Packing group				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.5. Environmental hazards				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
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

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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

15.1.1. 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)

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)

15.1.2. National regulations

No additional information available

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

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Abbreviations and acronyms:

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
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 disrupting properties

Full text of H- and EUH-statements:

Acute Tox. 4 (Oral)	Acute toxicity (oral), Category 4
H302	Harmful if swallowed.

The classification complies with : ATP 12

Safety Data Sheet (SDS)_EMAL, 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.