

SAFETY DATA SHEET

according to 1907/2006/EC, Article 3

Version no. : 2.0
Prepared on : 04.03.2026
Revised on : -

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

1.1 Product identifiers

Product name	Caffeine
Product Number	PSR50284
Brand	PureSynth research chemicals
CAS No.	58-08-2

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company	PureSynth Research Chemicals GmbH
	64683 Einhausen Marie-Curie-StraBe. 3, Germany

1.4 Emergency telephone number

Worldwide Helpline No.: 1800-8908-260

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.

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

2.3 Other hazards:

This substance/mixture contains no components considered to be either persistent, bio accumulative and toxic (PBT), or very persistent and very bio accumulative (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. May form explosible dust-air mixture if dispersed.

SECTION 3: Composition / information on ingredients

3.1 Substances

Common names & Synonyms	Mol. formula	CAS number
Caffeine free base	C ₈ H ₁₀ N ₄ O ₂	58-08-2
Component	Classification	Concentration
Caffeine	Acute Tox. 4; H302	<= 100 %

SECTION 4: First aid measures

Description of first aid measures

General advice	Show this safety data sheet to the doctor in attendance.
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.
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
Indication of any immediate medical attention and special treatment needed	No data available

SECTION 5: Firefighting measures

Extinguishing media	
Suitable extinguishing media	
Unsuitable extinguishing media	Water Foam Carbon dioxide (CO ₂) Dry powder For this substance/mixture no limitations of extinguishing agents are given.
Special hazards arising from the substance or mixture	Carbon oxides Nitrogen oxides (NO _x) Combustible. Risk of dust explosion. Development of hazardous combustion gases or vapours possible in the event of fire.
Advice for fire-fighters	In the event of fire, wear self-contained breathing apparatus.
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

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.
Environmental precautions	Do not let product enter drains.
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.
Reference to other sections	For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling	<p>Advice on protection against fire and explosion Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.</p> <p>Hygiene measures Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance. For precautions see section 2.2.</p>
Conditions for safe storage, including any incompatibilities	Tightly closed. Dry.
Specific end use(s)	Storage class (TRGS 510): 11: Combustible Solids Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls / Personal protection

Control parameters	Components with workplace control parameters
Exposure controls	
Appropriate engineering controls	No data available
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	<p>This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves</p> <p>Full contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min</p> <p>This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves</p> <p>Splash contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min</p>
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

Appearance	Form: Crystalline powder
	Colour:
Odour	Odourless
pH - Value	No data available
Density	1.23 g/cm ³ at 18 °C
Boiling Point	No data available
Melting Point	No data available
Solubility in water	No data available
Flash point	No data available
Vapour pressure	No data available
Auto -ignition temperature	No data available
Vapour density	No data available
Flammability (solid, gas)	May form combustible dust concentrations in air.
Evaporation rate	No data available
Partition coefficient: n- octanol / water	No data available
Viscosity	No data available
Explosive properties	No data available
Upper / lower flammability or explosive limits	No data available
Oxidizing properties	No data available
Other safety information: No data available	

SECTION 10: Stability and reactivity

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.
Chemical stability	The product is chemically stable under standard ambient conditions (room temperature).
Possibility of hazardous reactions	Violent reactions possible with: Strong oxidizing agents
Condition to avoid	no information available
Incompatible materials	No data available
Hazardous decomposition products	In the event of fire: see section 5

SECTION 11: Toxicological information

Acute toxicity	LD50 Oral - Rat - male and female – 367.7 mg/kg (OECD Test Guideline 401)
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	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 - > 2000 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 sensitization	Local lymph node assay (LLNA) - Mouse 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

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional 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.

Repeated dose toxicity - Mouse - male and female - Oral - 90 d - No observed adverse effect level – 167.4 – 179.4 mg/kg

Remarks: (ECHA)

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

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 - > 1000 mg/l - 3 h (OECD Test Guideline 209)

Persistence and degradability

Biodegradability aerobic - Exposure time 22 d

Result: 90 - 100 % - Readily biodegradable.

(OECD Test Guideline 301A)

Biodegradability

No data available

Bioaccumulation

No data available

Mobility in soil

No data available

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.

Endocrine disrupting properties

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.

Other adverse effects

Discharge into the environment must be avoided

SECTION 13: Disposal considerations

Waste treatment methods No data available

SECTION 14: Transport information

	UN no.	UN proper shipping name	Hazard Class(es)	Packaging group	Marine Pollutant
ADR / RID	-	Not dangerous goods	-	-	no
IMDG	-	Not dangerous goods	-	-	no
IATA	-	Not dangerous goods	-	-	no

SECTION 15: Regulatory information

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

This material safety data sheet 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

The information in this SDS 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. The user must be determined suitability of this information for his application.