SAFETY DATA SHEET (SDS)

in accordance with Regulation (EC) No 1907/2006 (REACH), Annex II — Regulation (EU) 2020/878

Date: 26.10.2026 | Version: 13 | EN

caffeine

1,3,7-trimethylpurine-2,6-dione

CAS 58-08-2

$C_8H_{10}N_4O_2$ | EC 200-362-1

MOLAR MASS	LOGP
194.19	-0.07 (pomiar: Merck Index 15th ed. (2013))

HAZARD CLASSIFICATION (GHS / CLP)



Warning

H302

Hazard class scope limited to the harmonised classification (CLP Annex VI); classes outside the harmonised entry may require supplier self-classification (CLP Art. 4(3)) — verify with the supplier safety data sheet.

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

1.1 Substance name	caffeine
1.1 IUPAC name	1,3,7-trimethylpurine-2,6-dione
1.1 CAS number	58-08-2
1.1 EC number	200-362-1
1.1 PubChem CID	2519
1.1 InChIKey	RYYVLZVUVIJVGH-UHFFFAOYSA-N
1.1 SMILES	CN1C=NC2=C1C(=O)N(C(=O)N2C)C
1.1 Molecular formula	$C_8H_{10}N_4O_2$ [7]
1.1 Molar mass	194.19 g/mol [7]
1.1 Exact mass	194.0804 Da [7]

1.2 Uses

For laboratory and research purposes. Not for use in the production of food, medicines or cosmetics without appropriate authorisation.

1.3 Details of the supplier

REFERENCE COPY — NO SUPPLIER DETAILS — NOT FOR DISTRIBUTION	Supplier details are not included in this reference copy. The supplier placing the substance on the market must complete this section and remains responsible for the sheet under REACH. MolGod.org prepares documentation and is not the supplier of this substance.

1.4 Emergency telephone number

Emergency telephone	112 (EU-wide emergency number)

Contact the poison centre designated in the country of placing on the market (CLP Art. 45).

2. Hazards identification

GHS:



PPE:



Prohibitions:



Warning

Hazard statements (H) [3][4][10]

H302	Harmful if swallowed

Precautionary statements (P) [3][4][10]

P264	Wash thoroughly after handling
P270	Do not eat, drink or smoke when using this product
P301+P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P330	Rinse mouth
P501	Dispose of contents/container to an approved waste collection point

Hazard class scope limited to the harmonised classification (CLP Annex VI); classes outside the harmonised entry may require supplier self-classification (CLP Art. 4(3)) — verify with the supplier safety data sheet.

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3. Composition/information on ingredients

Substance type	pure substance
CAS Number	58-08-2
EC number	200-362-1
Molecular formula	$C_8H_{10}N_4O_2$
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	613-086-00-5

4. First aid measures



Inhalation

Move the affected person to fresh air. Keep at rest. If not breathing: artificial respiration (qualified personnel only). [1][2][14]

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). [1][2][14]

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [1][2][14]

Ingestion

Do NOT induce vomiting (unless directed by a physician). Rinse mouth with water. Never give anything by mouth to an unconscious person. Emergency number: 112 (EU-wide). Contact the poison centre designated in your country (CLP Art. 45). [1][2][14]

Symptoms and effects

nausea, vomiting, diarrhoea. [3][10]

Notes for physician

Requires verification

Emergency numbers: Emergency: 112 (EU-wide). Poison centre: as designated in the country of placing on the market (CLP Art. 45).

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5. Firefighting measures

Suitable extinguishing media	Adapt extinguishing media to surroundings. CO2, dry powder, foam.
Unsuitable extinguishing media	No specific restrictions.
Specific hazards	Thermal decomposition products: CO, CO2, NOx. [15]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing dust. [1][2][14]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][14]
Methods for containment and cleaning up	1. Ensure ventilation 2. Protective equipment: nitrile gloves, P2 half mask 3. Collect mechanically into closable bags, avoiding dust formation 4. Rinse residues with water 5. NOTE: the lethal dose in humans is estimated at 150–200 mg/kg bw, usually ≥5 g (Willson 2018, doi:10.1016/j.toxrep.2018.11.002)
Related sections	8; 13
Large spill	1. Remove uninvolved persons from the area 2. Protective equipment: nitrile gloves, goggles, P2 half mask, protective clothing 3. Collect mechanically into labelled, closable containers, avoiding dust formation 4. Prevent entry into drains; notify the competent authority if released into the environment
Absorbent	dry vacuum with HEPA filter
HAZMAT response required	No
Required PPE	Gloves: nitrile powder free; Safety goggles: Yes; Respiratory protection: dust mask P2; Protective clothing: lab coat

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7. Handling and storage

Precautions	Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2][14]
Storage temperature	Store at temperature below 25°C. [1][2][14]
Humidity	Store in a dry place (<60% RH). [1][2][14]
Light	Protect from direct sunlight. [1][2][14]

Store in a dry, cool place, away from food and drink. Protect from light.

Incompatible materials	Strong oxidizers. [15]

8. Exposure controls/personal protection

8.1 Control parameters

OEL — NDS (Poland)	No NDS (OEL) value in the available working list — verify in the current MRPiPS regulation before use; do not assume the absence of a limit value.
OEL (EU)	The EU OEL value has not been verified against the available dataset — check the IOELV/BOELV directives; do not assume the absence of a value.
DNEL	No data available.
PNEC	No data available.

8.2 Personal protective equipment (PPE) [5][6][16]



Chemical-resistant protective gloves
EN ISO 374-1:2016+A1:2018
nitrile powder free

Closed safety spectacles or goggles
EN ISO 16321-1:2022 / EN 166:2001

Closed safety footwear with toe protection
EN ISO 20345:2022 (S2/S3)

9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	solid (white needle-shaped crystals)	
Colour	white	
Odour	bezwonny, gorzki smak	
pH (1% aqueous solution)	6.9	
Melting point	236°C (CRC Handbook of Chemistry and Physics, 94th ed. (2013), p. 3-90) [8] [7]	
Boiling point	178°C (Sublimuje w 178 °C (nie wrze) — The Merck Index, 15th ed. (2013), p. 289) (experimental data) [7]	
Flash point	Not applicable (REACH 9.1(h))	
Flammability	No data available.	
Lower and upper explosion limit	Not applicable (REACH 9.1(g))	
Density (20°C)	1.23 g/cm³ (18 °C; The Merck Index, 15th ed. (2013), p. 289) [7]	
Vapour pressure	≈1.2×10⁻⁷ kPa (9.0×10⁻⁷ mmHg, 25 °C) — Emel'yanenko & Verevkin, J. Chem. Thermodyn. 40 (2008) 1661, doi:10.1016/j.jct.2008.07.002 [7]	
Relative vapour density	Not applicable (REACH 9.1(q))	
Kinematic viscosity	Not applicable (REACH 9.1(l))	
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	
Dissociation constant (pKa)	pKa_1 = 14 / pKa_2 = -0.12 [9]	
Water solubility	21.6 g/L (25 °C) — Yalkowsky, He, Jain, Handbook of Aqueous Solubility Data, 2nd ed. (2010), p. 506 [9][10]	
Particle characteristics	The particle size distribution has not been determined for this commercial form — required under Annex II 9.1(r); to be completed from the supplier's specification.	
log Kow (XLogP3)	-0.07 [7] (Hansch, Leo, Hoekman, Exploring QSAR (1995), p. 44; Sangster: −0.42)	

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Property (item 9.1)	Value	Source
Molar mass	194.19 g/mol [7]	
Molecular formula	$C_8H_{10}N_4O_2$ [7]	
Lipinski rule (RO5)	PASS	

Where a property above reads "No data available", no measured value was found in the public sources consulted for this substance. The property has not been determined by MolGod.org and no value is inferred. "Not applicable" means the property has no meaning for this substance in the form supplied.

10. Stability and reactivity

Reactivity	Stable under normal storage and handling conditions.
Chemical stability	Thermally stable under recommended conditions.
Hazardous reactions	No hazardous reactions known under normal conditions.
Conditions to avoid	High temperatures, direct sunlight, moisture.
Incompatible materials	Strong oxidizers.
Decomposition products	Thermal decomposition products: CO, CO2, NOx.

11. Toxicological information

LD50 (oral)	367 mg/kg (rat) [11]
LD50 (dermal)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Eye irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Sensitisation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Mutagenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Carcinogenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
IARC classification (carcinogenicity)	No individual IARC monograph for this CAS — this is not confirmation of the absence of carcinogenicity (cf. CLP/GHS classification in section 2).
Reproductive toxicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Other information	The lethal dose in humans is estimated at 150–200 mg/kg bw (usually ≥5 g); the minimum lethal blood concentration is about 80 mg/L (Willson 2018, doi: 10.1016/j.toxrep.2018.11.002). Single doses up to 200 mg (about 3 mg/kg bw) and habitual intake up to 400 mg/day in adults (pregnant women: up to 200 mg/day) do not give rise to safety concerns (EFSA 2015, doi:10.2903/j.efsa.2015.4102). Mechanism: non-selective antagonist of adenosine A1 and A2A receptors (Fredholm et al. 1999, PMID 10049999).
STOT — single exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
STOT — repeated exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Aspiration hazard	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]

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12. Ecological information

Aquatic toxicity	LC50 (96 h, Pimephales promelas) 151 mg/L; EC50 (24 h, Daphnia magna) 160 mg/L — Ministry of the Environment, Japan, initial environmental risk assessment, CAS 58-08-2 (env.go.jp/content/000316699.pdf)
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = -0.07 [7]. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [17][18]
Mobility in soil	No data available.
PBT/vPvB assessment	Insufficient data to assess PBT/vPvB.
Endocrine disrupting properties	Reported endocrine effects in aquatic organisms (ecotoxicological data, US EPA ECOTOX; not a regulatory ED classification under 2018/605). [19]

13. Disposal considerations

Disposal method	Hand over for disposal to licensed contractors in accordance with national and local regulations. Do not discharge into sewers.
Waste code (EWC)	16 05 06* — Laboratory and analytical chemicals (e.g. chemical reagents) containing hazardous substances. Verification of the EWC code required. [13]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information

UN number	UN 1544 [7]
Environmental hazard	Not classified as environmentally hazardous for transport (no H400/H410/H411 in CLP Annex VI; no marine pollutant mark required) [3]
Special precautions	Handle as dangerous goods according to the assigned class (ADR/IMDG/IATA); apply the precautions appropriate to that class.
CN/HS code	CN/HS code: verification required in the Eurostat Combined Nomenclature.
Notes	UN number per the indicated source. Verify the transport class and packing group in ADR Table A / UN Model Regulations before shipment. [7]

15. Regulatory information

SVHC status	SVHC status not verified against the available dataset — check the current ECHA Candidate List; do not assume absence. [1]
REACH Annex XIV	Not verified against the ECHA Authorisation List — check REACH Annex XIV. [1]
REACH Annex XVII	Not confirmed in the available Annex XVII dataset — verify against the current ECHA list before placing on the market; do not assume absence of restriction. [1]
EC number type	EINECS

16. Other information

Legal status of classification: harmonised under CLP Annex VI — Reg. (EC) No 1272/2008 (as at the date of issue).Entries with an entry-into-force date after 26.10.2026 were omitted as future (not yet applicable).

Data aggregated automatically from public reference databases (PubChem, ECHA, NIST and others).

Scientific citations (9)

Deng H, Wang L, Liu P et al.. *Caffeine and taurine: a systematic review and network meta-analysis of their individual and combined effects on physical capacity, cognitive function, and physiological markers.*. Journal of the International Society of Sports Nutrition (2025). DOI: 10.1080/15502783.2025.2566371

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Marcus GM, Hu FB, van Dam RM et al.. *Caffeine and Cardiovascular Disease: A Scientific Statement From the American Heart Association.*. Circulation (2026). DOI: 10.1161/CIR.0000000000001454

Eichenwald E, Corwin M, McEntire B et al.. *Intermittent hypoxia and caffeine in infants born preterm: the ICAF Randomized Clinical Trial.*. Archives of disease in childhood. Fetal and neonatal edition (2026). DOI: 10.1136/archdischild-2025-329230

Razazan R, Hemmatinafar M, Imanian B et al.. *Performance-enhancing effects of caffeine and L-Theanine among Iranian elite wrestlers: a focus on cognitive and specific physical performance.*. Journal of the International Society of Sports Nutrition (2025). DOI: 10.1080/15502783.2025.2564238

Nawarathna GS, Ariyasinghe DI, Dassanayake TL. *High-dose L-theanine-caffeine combination improves neurobehavioural and neurophysiological measures of selective attention in acutely sleep-deprived young adults: a double-blind, placebo-controlled crossover study.*. The British journal of nutrition (2025). DOI: 10.1017/S0007114525104169

Full text of H statements

H302	Harmful if swallowed

Full text of P statements

P264	Wash thoroughly after handling
P270	Do not eat, drink or smoke when using this product
P301+P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P330	Rinse mouth
P501	Dispose of contents/container to an approved waste collection point

Abbreviations

ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service
CLP	Classification, Labelling and Packaging (Reg. (EC) 1272/2008)
CMR	Carcinogenic, Mutagenic, toxic to Reproduction
DNEL	Derived No-Effect Level
EC	European Community number
EPI	Personal protective equipment
GHS	Globally Harmonized System
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods Code
SDS	Safety Data Sheet
LC50	Lethal Concentration, 50%
LD50	Lethal Dose, 50%
NDS	Maximum admissible concentration (workplace, PL)
NDSCh	Short-term exposure limit (PL)
OEL	Occupational Exposure Limit
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals (Reg. (EC) 1907/2006)
STOT	Specific Target Organ Toxicity
SVHC	Substance of Very High Concern
TPSA	Topological Polar Surface Area
vPvB	very Persistent and very Bioaccumulative

Version history

v13 (26.10.2026)	Based on ECHA harmonised classification (Annex VI to CLP, ATP 23).

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References

[1] EP and Council. Reg.(EC) No 1907/2006 (REACH). Art.31, Annex II. OJ EU L 396/2006. URL: https://eur-lex.europa.eu/eli/reg/2006/1907/oj Accessed: 2026-10-26.

[2] European Commission. Reg.(EU) 2020/878 — amending Annex II REACH. OJ EU L 203/2020. From 01.01.2023. URL: https://eur-lex.europa.eu/eli/reg/2020/878/oj Accessed: 2026-10-26.

[3] EP and Council. Reg.(EC) 1272/2008 (CLP) + ATP 23. OJ EU L 353/2008. (2026-07-07) URL: https://eur-lex.europa.eu/eli/reg/2008/1272/oj Accessed: 2026-10-26.

[4] United Nations. GHS Rev.9. ST/SG/AC.10/30/Rev.9. New York and Geneva: United Nations, 2021. URL: https://unece.org/transport/dangerous-goods/ghs-rev9-2021 Accessed: 2026-10-26.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-10-26.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-10-26.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/2519

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=58-08-2

[9] O'Neil, M.J., ed. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 15th ed. Cambridge: Royal Society of Chemistry, 2013.

[10] ECHA. European Chemicals Agency — harmonised classification inventory (CLP Annex VI). URL: https://echa.europa.eu

[11] Adamson, R.H. "The acute lethal dose 50 (LD50) of caffeine in albino rats." Regulatory Toxicology and Pharmacology 80 (2016): 274–276. URL: https://doi.org/10.1016/j.yrtph.2016.07.011

[12] ECHA. REACH Registration Dossier (registered substance, acute toxicity study record). Helsinki: European Chemicals Agency. URL: https://echa.europa.eu/registration-dossier

[13] European Commission. Decision 2000/532/EC establishing a list of wastes (European Waste Catalogue). OJ EU L 226/3. URL: https://eur-lex.europa.eu/eli/dec/2000/532/oj

[14] European Chemicals Agency (ECHA). Guidance on the Compilation of Safety Data Sheets. Version 4.0. Helsinki: European Chemicals Agency, 2020. URL: https://echa.europa.eu/documents/10162/2324906/sds_en.pdf

[15] Urben, P.G., ed. Bretherick's Handbook of Reactive Chemical Hazards. 8th ed. Oxford: Academic Press.

[16] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.

[17] ECHA. Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB Assessment. Helsinki: European Chemicals Agency. URL: https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment

[18] European Parliament and Council. Regulation (EC) No 1907/2006 (REACH), Annex XIII — Criteria for the identification of PBT and vPvB substances. OJ EU L 396/2006 (consolidated). URL: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:02006R1907-20140410

[19] U.S. EPA. ECOTOX Knowledgebase. Washington, DC: U.S. Environmental Protection Agency. URL: https://cfpub.epa.gov/ecotox/

[20] MRiPS Regulation of 12.06.2018 — NDS/NDN. Journal of Laws 2024 item 1017. URL: https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20240001017 Accessed: 2026-10-26.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=58-08-2

NFPA 704 (supplementary information — NFPA/USA system; not a required element of an EU safety data sheet under REACH Annex II)



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