

CAFFEINE

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

Formula	C ₈ H ₁₀ N ₄ O ₂
Mol. wt.	194.0804 g/mol
InChIKey	RYYVLZVUVIJVGH-UHFFFAOYSA-N

1. MOLECULAR STRUCTURE 2D



2. HAZARD IDENTIFICATION (GHS)

Signal word: WARNING

Hazard pictograms:



Irritant

Hazard statements (H)

- H360: May damage fertility or the unborn child [Danger Reproductive toxicity]

Precautionary statements (P)

- P203, P261, P264, P270, P271, P280, P301+P316, P304+P340, P317, P318, P321, P330, P405, and P501

3. NFPA 704 SYSTEM

NFPA 704 data not available.

4. ACUTE TOXICITY

LD50 data not available.

5. RELEVANT PHYSICAL AND CHEMICAL PROPERTIES

Property	Value	Unit	Source
Boiling point	352 °F at 760 mmHg (sublimes) (NTP, 1992)	—	pubchem_pugview

Density	1.23 at 64 °F (NTP, 1992) - Denser than water; will sink	—	pubchem_pugview
LogP (experimental)	log Kow = -0.07	—	pubchem_pugview
Melting point	460 °F (NTP, 1992)	—	pubchem_pugview
Vapor pressure	0.00000001 [mmHg]	—	pubchem_pugview
Water solubility	10 to 50 mg/mL at 73 °F (NTP, 1992)	—	pubchem_pugview

IMPORTANT LEGAL DISCLAIMER

This document is an INFORMATIONAL SAFETY PROPERTIES SUMMARY automatically generated from PubChem data (National Institutes of Health, USA). It is NOT an official Safety Data Sheet (SDS) and does not comply with GHS, OSHA HazCom, REACH (EU), or any equivalent national regulation. It must NOT be used as the sole reference document in industrial settings, professional laboratories, or for occupational risk assessment. Always consult the official SDS from the compound supplier and applicable local regulations before handling.

Official SDS sources:

- Sigma-Aldrich (Merck): <https://www.sigmaaldrich.com/search#q=CAFFEINE>
- Fisher Scientific: <https://www.fishersci.com/us/en/catalog/search/sds?query=CAFFEINE>
- PubChem (source data): <https://pubchem.ncbi.nlm.nih.gov/#query=CAFFEINE>
- GESTIS (database): <https://gestis-database.dguv.de/>

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