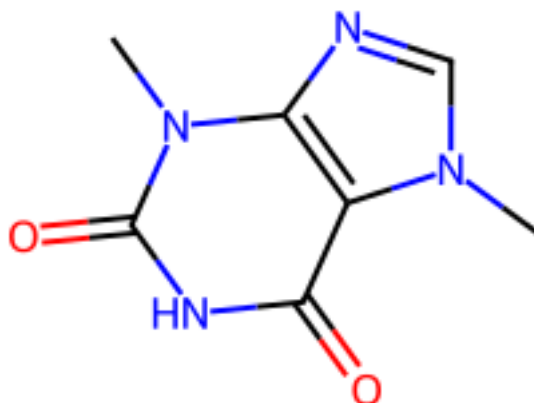


THEOBROMINE

3,7-dimethylpurine-2,6-dione

Formula	C ₇ H ₈ N ₄ O ₂
Mol. wt.	180.0647 g/mol
InChIKey	YAPQBXQYLJRXSA-UHFFFAOYSA-N

1. MOLECULAR STRUCTURE 2D



2. HAZARD IDENTIFICATION (GHS)

Signal word: WARNING

Hazard pictograms:



Irritant

Hazard statements (H)

- H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation]

Precautionary statements (P)

- P203, P260, P264, P270, P280, P301+P317, P308+P316, P318, P321, P330, P405, and P501 (click each P-code to see the statement)

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
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Boiling point	Sublimes at 554-563 °F (NTP, 1992)	—	pubchem_pugview
Density	1.522 g/cu cm at 20 °C; relative density: 1.522 at 20 °C	—	pubchem_pugview
LogP (experimental)	log Kow = -0.78	—	pubchem_pugview
Melting point	675 °F (NTP, 1992)	—	pubchem_pugview
Water solubility	less than 1 mg/mL at 64 °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=THEOBROMINE>
- Fisher Scientific: <https://www.fishersci.com/us/en/catalog/search/sds?query=THEOBROMINE>
- PubChem (source data): <https://pubchem.ncbi.nlm.nih.gov/#query=THEOBROMINE>
- GESTIS (database): <https://gestis-database.dguv.de/>

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