

Paraxanthine

1,7-dimethyl-3H-purine-2,6-dione | CAS 611-59-6

Product identification

Product name	Paraxanthine
Chemical name	1,7-dimethyl-3H-purine-2,6-dione
CAS number	611-59-6
PubChem CID	4687
Molecular formula	C7H8N4O2
Molecular weight	180.16 g/mol
InChIKey	—
Canonical / reference SMILES	—
Material type	Chemical reference material / technical compound

Material description

Paraxanthine is a dimethylxanthine derivative supplied by Rexar as a chemical reference material / technical compound. The identity data support laboratory identification, documentation and analytical comparison.

Intended use

For laboratory, analytical, chemical and method-development applications. Not for human or animal consumption. Not intended for food, supplement, cosmetic, medical, diagnostic or therapeutic use.

Reference characteristics

Structural class	Dimethylxanthine derivative
Typical physical form	Solid / powder
Storage guidance	Keep tightly closed, dry and protected from light; follow lot-specific supplier storage information.

Analytical use and traceability

Lot-specific purity, water content, residual solvents and analytical acceptance criteria must be taken from applicable supplier documentation or a certificate of analysis; they are not inferred by this datasheet.

Safety note

PubChem provides an LCSS record for paraxanthine. Use applicable supplier/batch classification and normal laboratory controls. Consult the applicable Safety Data Sheet before handling.

Identity verification note

Identity verified against PubChem CID 4687: CAS 611-59-6, C7H8N4O2 and 180.16 g/mol.

Document control

Document	Rexar Technical Compound Datasheet
Revision	10 September 2026

Status	Reference information; not a certificate of analysis
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Disclaimer

This document is provided for chemical identification and laboratory reference purposes. It does not certify batch purity or replace lot-specific analytical documentation. Users remain responsible for suitability, regulatory status and safe handling.