

Theacrine

1,3,7,9-tetramethylpurine-2,6,8-trione | CAS 2309-49-1

Product identification

Product name	Theacrine
Chemical name	1,3,7,9-tetramethylpurine-2,6,8-trione
CAS number	2309-49-1
PubChem CID	2153
Molecular formula	C ₉ H ₁₂ N ₄ O ₃
Molecular weight	224.22 g/mol
Material type	Chemical reference material / technical compound

Material description

Theacrine is a purine alkaloid / methylurate derivative supplied by Rexar as a chemical reference material / technical compound.

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	Purine alkaloid / methylurate derivative
Typical physical form	Solid / powder
Storage guidance	Keep tightly closed, dry and protected from light unless the lot-specific supplier documentation states otherwise.

Analytical use and traceability

Lot-specific purity, hydration state, water content, residual solvents and analytical acceptance criteria must be taken from applicable supplier documentation or a certificate of analysis.

Safety note

Use applicable supplier/batch hazard documentation; no Rexar-specific CLP classification is inferred from identity alone.

Identity verification note

Identity values have been stated only where sufficiently supported. Any unresolved form, hydrate or catalogue-identity issue should be reconciled against the supplier documentation before public product data are changed.

Document control

Document	Rexar Technical Compound Datasheet
Revision	10 September 2026
Status	Reference information; not a certificate of analysis

Disclaimer

This document is provided for chemical identification and laboratory reference purposes. It does not certify batch purity or replace lot-specific analytical documentation.