

Product Name: Xanthine monosodium salt monohydrate, 96+% (dry basis),
 Thermo Scientific

Catalog Number: J23465.22

CAS Number: 1196-43-6

IUPAC Name: sodium 2,6-dioxo-2,3,6,9-tetrahydro-1H-purin-9-ide

Molecular Formula: C₅H₃N₄NaO₂

Molecular Weight: 174.10

InChI Key: HKDXLLDCXWUUKY-UHFFFAOYSA-M

SMILES: [Na+].O=C1NC2=C(N=C[N-]2)C(=O)N1

Synonym: sodium 2,6-dioxo-3,9-dihydro-1H-purin-9-ide

Product Specification

Form: White to off-white crystalline powder

Comment: Reference Constants: I_{max} (pH 10, NRC): 277 nm

Comment: Reference Constants: ε_{max} (pH 10, NRC): 9.3 x 10³

Identification (FTIR): Conforms

Assay (UV/vis): ≥ 96.0% (dry basis)

Water Content (Karl Fischer Titration): ≤ 12.0%

Spectral Ratio: (pH 10.0): A₂₈₀/A₂₆₀: 1.71 ± 0.05

Comment: Reference Constants: ε₂₆₀ (pH 10, DBR): 5.2 x 10³

Spectral Ratio: (pH 10.0): A₂₅₀/A₂₆₀: 1.29 ± 0.06

Date Of Print: 05/26/2025

Product Specifications are subject to amendment and may change over time. Data contained is accurate as of the date printed.