Sulfolane (CAS: 126-33-0) Procurement & Selection Manual from HiSiaddi

Target Audience of This Manual

Procurement Engineers, Process Engineers, Production Supervisors, Foreign Trade Compliance Specialists

Table of Contents

I. Universal Basic Physicochemical Benchmarks (Applicable to All Grades)

Chemical Name: Tetrahydrothiophene 1,1-dioxide

Molecular Formula: $C_4H_8O_2S$; Molecular Weight: 120.17

Melting Point: 27.4°C (crystallizes below this temperature; heat tracing at 30–40°C required throughout handling)

Normal Boiling Point: 285°C; Maximum Safe Operating Temperature: 220°C; Thermal decomposition releases SO_2 above 230°C

Closed Cup Flash Point: 166°C; Not classified as flammable hazardous chemical; Low toxicity; Strong polar aprotic solvent

Miscibility Characteristics: Miscible infinitely with water, alcohols, ketones and aromatics; Virtually insoluble in alkanes

Core Drawbacks: Rapid oxidation to sulfonic acids under simultaneous conditions of oxygen, high temperature and water content, leading to carbon steel corrosion; Crystallization at low temperatures causes pipeline blockages

II. Technical Index Comparison for Four Product Grades (Core Selection Basis)

Unified Grade Definition

1. General Industrial Grade (Aromatic Extraction, Natural Gas Desulfurization, Printing & Dyeing)

2. Polymer & Pharmaceutical High-Purity Grade (PEEK/PI, Pharmaceutical Intermediates)
3. Laboratory AR Reagent Grade (Chromatography, R&D Small-Scale Trials)
4. Ultra-High-Purity Electronic Lithium Battery Grade (High-Voltage Electrolytes, Semiconductor Cleaning)

Test Item	General Industrial Grade	Polymer & Pharmaceutical Grade	AR Reagent Grade	Electronic Lithium Battery Grade
GC Purity (Dry Basis)	≥99.0% (Premium ≥99.5%)	≥99.9%	≥99.9%	≥99.99%
Water Content	≤3000 ppm (0.3%)	≤50 ppm	≤50 ppm	≤10 ppm
Color (APHA)	≤30	≤10	≤10	≤5
Total Acid Value (mgKOH/g)	≤0.3	≤0.1	≤0.08	≤0.03
Sulfolene Impurity	≤500 ppm	≤50 ppm	≤30 ppm	≤1 ppb
Single Metal Ion (Na/Fe/Ca/K)	≤10 ppm	≤3 ppm	≤1 ppm	≤1 ppb
Total Metal Ions	≤20 ppm	≤5 ppm	≤2 ppm	≤10 ppb
Free Sulfur / Sulfides	≤10 ppm	≤2 ppm	≤1 ppm	≤0.5 ppb
Thermal Stability (SO_2 Release)	≤20 mg/kg	≤8 mg/kg	≤5 mg/kg	≤1 mg/kg
Shelf Life (Nitrogen-Sealed Packaging)	12 months	18 months	18 months	24 months

Test Item	General Industrial Grade	Polymer & Pharmaceutical Grade	AR Reagent Grade	Electronic Lithium Battery Grade
Applicable Standards	GB/T23946 Industrial Sulfolane	Enterprise High-Purity Rectification Standard	Analytical Reagent Standard	Internal Standard for Wet Electronic Chemicals

III. Industry-Specific Targeted Selection Schemes (Including Risk Warnings)

1) Petrochemical Industry (Aromatic Extraction, Natural Gas MDEA Desulfurization)

Recommended Grade: Premium Industrial Grade (≥99.5%, Water ≤0.3%)

Applicable Processes

- BTX Extraction Units for Reformed Gasoline / Cracked Gasoline
- Sulfolane-MDEA Composite Desulfurization & Decarbonization Systems

Selection Constraints

1. No strict control over metal content; ppm-level metal ions impose no adverse impact on processes
2. Systems tolerate 0.5%–2.5% water content; deep dehydration is unnecessary
3. Optimal budget with the lowest per-ton procurement cost

Risks of Downgrading to Standard 99.0% Industrial Grade

Elevated sulfolene impurities form colloids via long-term high-temperature polymerization, causing frequent filter clogging, 50% higher solvent consumption, and a 70% shortened heat exchanger pickling cycle.

Prohibited Grades: Polymer Grade / Electronic Grade

Cost surges by 40%–120% with no process benefits, drastically increasing production costs.

2) High-Temperature Engineering Plastic Polymerization (PEEK/PI, Polyethersulfone, Aramid)

Recommended Grade: Polymer & Pharmaceutical Grade (99.9%, Water ≤50 ppm, Single Metal ≤3 ppm)

Applicable Processes

PEEK high-temperature polycondensation, polyimide synthesis, aramid spinning dope production

Hard Selection Red Lines

1. Water content exceeding 50 ppm directly reduces polymer molecular weight and renders mechanical properties non-compliant
2. Iron/sodium metal ions catalyze monomer oxidation, leading to batch viscosity fluctuations

Risks of Downgrading to Standard Industrial Grade

Sharp rise in by-products, unstable resin melt index, excessive residual solvent in finished goods, and non-compliance with EU REACH testing for export products.

Optional Upgrade: AR Reagent Grade for small-batch R&D sampling; Electronic Grade is strictly forbidden for mass production due to excessive premium pricing.

3) Pharmaceutical & Pesticide Fine Chemical Intermediate Synthesis (EU/US Pharmacopoeia Export)

Recommended Grade: Anhydrous Polymer & Pharmaceutical Grade

Core Selection Logic

1. Low impurities and low unsaturated contaminants reduce by-product formation
2. Low residual solvent post rectification recovery, complying with ICH residual solvent limits
3. Free of high-concern SVHC impurities for REACH compliance

Industrial Grade Prohibition: Excessive impurities cause heavy metal and unknown contaminant overages in finished goods, blocking exports to EU and US markets.

4) Lithium Battery High-Voltage Electrolytes & Semiconductor Wafer Cleaning

Mandatory Grade: Electronic Lithium Battery Grade (99.99%, Water ≤10 ppm, Metal Ions ≤1 ppb)

Hard Selection Thresholds (Automatic Rejection Criteria)

1. Water above 10 ppm hydrolyzes lithium salts to generate HF, resulting in cell swelling
2. Trace heavy metals catalyze continuous electrolyte decomposition, causing catastrophic decline in cycle life
3. Production requires nitrogen-sealed filling under oxygen-free conditions and rectification in dust-free workshops

Fatal Risks of Downgrading to Polymer / Industrial Grade

Cell defect rate rises by over 90%; capacity retention falls below 60% after 500 cycles for 4.4V high-voltage systems.

5) Laboratory R&D, Gas Chromatography Stationary Phases, Small-Scale Synthesis

Recommended Grade: AR Analytical Reagent Grade
Advantages: High batch stability and low impurities for repeatable experimental data; only suitable for small trials, with excessive procurement costs for mass production.
6) Printing & Dyeing, Extractive Distillation, Heat Transfer Media
Recommended Grade: Standard 99.0% Industrial Grade
No strict limits on metal or water content, delivering the highest cost performance.
IV. Automatic Rejection Procurement Criteria (Mandatory Inspection Upon Arrival)
Shipments failing any single item below shall be rejected outright with no conditional acceptance allowed:

1. Industrial Grade: Purity ＜99.0%, Acid Value ＞0.5 mgKOH/g, Color ＞50 APHA
2. Polymer / Pharmaceutical Grade: Water ＞80 ppm, Sulfolene ＞100 ppm, Single Metal Ion ＞5 ppm
3. Electronic Grade: Water ＞15 ppm, Any Single Metal Ion ＞5 ppb, Color ＞10 APHA

Supplementary Priority Screening Factors (Preferred Suppliers for Large-Volume Procurement)

1. Capable of providing full third-party SGS test reports
2. Equipped with multi-stage vacuum rectification and molecular sieve deep dehydration production lines
3. Nitrogen-blanketed storage tanks and heat-traced closed filling facilities
4. Able to supply REACH registration certificates and SDS safety data sheets
5. Offers free sample testing for small-lot submissions

V. Matching Selection for Supporting Equipment, Seals & Packaging (Aligned with Product Grades)
1) Storage & Packaging Selection

- Industrial Grade: IBC Totes / Q235 carbon steel nitrogen-blanketed storage tanks (system acid value controlled below 0.3)
- Polymer / Pharmaceutical Grade: 316L stainless steel drums, PTFE-lined IBC totes
- Electronic Lithium Battery Grade: High-purity 316L + PVDF piping, Kalrez perfluorinated seals, dust-free vacuum nitrogen-sealed drums

2) Gasket & Seal Selection

- General Industrial Facilities: Grade A compatible FKM fluoroelastomer

- High-Temperature Polymer / Electronic Operations: Kalrez perfluoroelastomer, PTFE encapsulated gaskets
- Strictly Prohibited for Long-Term High-Temperature Service: NBR, PU, EPDM

3) Conveyance Piping

- Industrial Use: 304 stainless steel
- High-Purity / Electronic Use: 316L + PVDF/PTFE lined piping

VI. Compliance Selection Guidelines (Mandatory for Exports)

1. EU REACH
   All sulfolane grades hold complete REACH registration with no SVHC high-concern substance restrictions; full registration certificates must be provided for pharmaceutical and electronic grades.
2. RoHS (Lithium Battery / Semiconductor Applications)
   Only Electronic Grade meets RoHS heavy metal residual controls; Industrial Grade fails electronic export compliance requirements.
3. Pharmaceutical Exports (ICH Q3C)
   Only Polymer & Pharmaceutical Grade is permitted for API synthesis; Industrial Grade contains excessive impurities and fails pharmacopoeia solvent standards.
4. Domestic Hazardous Chemical Transport
   Sulfolane is not classified as a hazardous chemical and may be shipped via standard chemical trucks; vehicles must be insulated during winter transport to prevent crystallization and valve blockages.

VII. Common Selection Pitfalls & Substitution Logic

Pitfall 1: Substituting Industrial Grade for Polymer Grade in PEEK Production
Consequences: Unstable molecular weight, non-compliant finished mechanical properties, excess residual contaminants failing export testing
Solution: Standardize procurement of Polymer Grade with batch-by-batch water and metal ion testing

Pitfall 2: Using Polymer Grade for Lithium Battery Electrolytes
Consequences: Cell swelling, poor cycle life, full batch scrapping
Solution: Mandate exclusive Electronic Grade procurement with full water and metal testing upon delivery

Pitfall 3: Low-Cost Low-Purity Industrial Grade for Aromatic Extraction
Consequences: Solvent discoloration rate doubles, annual make-up solvent consumption rises by 100%, increasing overall total cost
Optimization: Source Premium 99.5% Industrial Grade for lower long-term total cost of ownership

Solvent Substitution Logic (When Sulfolane Supply Is Unavailable)

1. Aromatic Extraction Alternative: NMP (Lower selectivity, requiring higher solvent-to-oil ratio)
2. High-Temperature Polymerization Alternative: Diphenyl Sulfone (High melting point, high viscosity requiring extensive process modification)
3. No Low-Cost Perfect Substitute for Lithium Battery Electrolytes; Electronic Grade Sulfolane is mandatory

VIII. One-Page Quick Reference Selection Card (Printable for Workshop & Procurement Teams)

Application Scenario → Recommended Grade → Core Controlled Indicators

1. Aromatic Extraction, Natural Gas Desulfurization → Premium 99.5% Industrial Grade
   Controls: Acid Value, Color, Sulfolene; 0.5–3% water permitted
2. PEEK/PI Polymerization, Mass-Produced Pharmaceutical Intermediates → Polymer & Pharmaceutical Grade (99.9%)
   Controls: Water ≤50 ppm, Metal Ions, Unsaturated Impurities
3. Laboratory Small Trials, Chromatography Analysis → AR Reagent Grade (99.9%)
   Controls: Low impurities, consistent batch performance
4. High-Voltage Lithium Battery Electrolytes, Semiconductor Cleaning → Electronic Lithium Battery Grade (99.99%)
   Controls: Water ≤10 ppm, Single Metal Ion ≤1 ppb, Color ≤5 APHA
