Safety Data Sheet (MSDS)

- Methyl 2-Octynoate

*(According to GB/T 16483 and GB/T 17519; Adapts to GHS, IMDG, IATA Standards)***Revision Date**: 28 FEB 2026

SECTION 1: Identification of the Substance/Mixture and of the Company/Undertaking

1.1 Product Identifiers

- Product Name: Methyl 2-Octynoate
- Product Number: MO-20260228
- Brand: SIGALD
- CAS-No.: 111-12-6
- Synonyms: Methyl oct-2-ynoate; 2-Octynoic acid methyl ester
- Formula: $C_9H_{14}O_2$
- Molecular Weight: 154.21 g/mol

1.2 Details of the supplier of the safety data sheet

- Company: NEWAY SINOPHC TECH. LIMITED
- Address: RM. 204, BUILDING 3, NO. 188, AONA RD., CHINA (SHANGHAI) PILOT FREE TRADE ZONE.
- Telephone: +86-021-50350029
- Fax: +86-021-50350029

1.3 Emergency telephone

- Emergency Phone #: +86-021-50350029 (CHEMTREC)

1.4 Relevant Identified Uses and Uses Advised Against

- **Identified Uses**: Fragrance & flavor manufacturing; cosmetic formulations; food flavoring agent; fine chemical synthesis intermediate.
- **Uses Advised Against**: Not for direct oral consumption in large quantities; not for pharmaceutical injection; avoid use in high-temperature industrial processes (>150℃).

SECTION 2: Hazards Identification

2.1 GHS Classification

- Skin Irritation (Category 2)
- Eye Irritation (Category 2)
- Specific Target Organ Toxicity - Single Exposure (Category 3, Respiratory tract irritation)
- Hazardous to the aquatic environment - Acute (Category 3)

2.2 GHS Label Elements

- Hazard Pictogram: (Exclamation mark), (Environment)
- Signal Word: **Warning**
- **Hazard Statements**:
  - H315: Causes skin irritation
  - H319: Causes serious eye irritation
  - H335: May cause respiratory tract irritation
  - H412: Harmful to aquatic life with long lasting effects
- **Precautionary Statements**:
  - P261: Avoid breathing dust/fume/gas/mist/vapors/spray
  - P264: Wash hands thoroughly after handling
  - P273: Avoid release to the environment
  - P280: Wear protective gloves/eye protection/face protection
  - P302+P352: If on skin: Wash with plenty of soap and water
  - P305+P351+P338: If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

- P337+P313: If eye irritation persists: Get medical advice/attention
- P391: Collect spillage

2.3 Physical and Chemical Hazards

- Combustible liquid (flash point ≥75℃); no explosion risk under normal use and storage conditions.
- No hazardous polymerization under normal conditions.

2.4 Health Hazards

- **Acute**: Mild to moderate skin/eye irritation; inhalation of high-concentration vapors may cause cough, throat irritation; oral ingestion may cause nausea, abdominal discomfort.
- **Chronic**: No known chronic toxic effects with normal occupational exposure; prolonged skin contact may cause mild dermatitis in sensitive individuals.

2.5 Environmental Hazards

- Harmful to aquatic organisms with long-lasting effects; low bioaccumulation potential in the food chain.
- Partially biodegradable in aerobic aquatic environments.

2.6 Other Hazards

- No additional hazards identified.

SECTION 3: Composition/Information on Ingredients

- **Substance / Mixture**: Pure Substance
- **Active Ingredient**: Methyl 2-Octynoate (111-12-6), Concentration: 98.5-99.5% (w/w)
- No hazardous impurities present above threshold limits.

SECTION 4: First Aid Measures

4.1 Description of First-Aid Measures

- **If Inhaled**: Move victim to fresh air and keep at rest in a position comfortable for breathing. If respiratory symptoms (cough, shortness of breath) persist, consult a doctor.
- **In Case of Skin Contact**: Remove contaminated clothing and shoes. Wash skin with plenty of soap and running water for 10-15 minutes. If irritation, redness or rash occurs, get medical advice.
- **In Case of Eye Contact**: Rinse eyes thoroughly with plenty of running water for 10-15 minutes, holding eyelids open. Remove contact lenses if present and easy to do. If irritation persists, immediately consult an ophthalmologist.
- **If Swallowed**: Rinse mouth with water. Do not induce vomiting. If large quantity is swallowed or gastrointestinal discomfort occurs, seek medical attention immediately and show the product label/MSDS.

4.2 Most Important Symptoms and Effects

- **Acute**: Skin redness, itching, burning; eye redness, tearing, corneal irritation; cough, sore throat (inhalation); nausea, stomach ache (ingestion).
- **Delayed**: No known delayed toxic effects.

4.3 Indication of Immediate Medical Attention

- Seek medical help if eye/skin irritation persists, high-concentration inhalation causes severe respiratory symptoms, or large quantity is ingested.

SECTION 5: Firefighting Measures

5.1 Extinguishing Media

- **Suitable**: Water spray (cool container), dry chemical powder, foam, carbon dioxide (CO_2).
- **Unsuitable**: No unsuitable extinguishing media identified.

5.2 Special Hazards Arising from the Substance

- Combustion may produce minor toxic fumes (carbon monoxide, carbon dioxide, small molecular fatty acid esters).

- No explosive decomposition under fire conditions.

5.3 Advice for Firefighters

- Wear self-contained breathing apparatus (SCBA) and full fire-fighting protective gear when fighting large-scale fires.
- Cool exposed containers with water spray to prevent rupture from heat.
- Fight fire from a safe distance; avoid inhalation of combustion fumes.

SECTION 6: Accidental Release Measures

6.1 Personal Precautions

- Wear nitrile rubber gloves, chemical safety goggles and protective clothing. Avoid breathing vapors or direct contact with skin/eyes. Ensure good ventilation in the spill area.
- Evacuate non-essential personnel from the affected area.

6.2 Environmental Precautions

- Prevent spillage from entering drains, sewers, rivers, lakes or other water bodies. Contain runoff with sand or inert absorbent if necessary.
- Do not discharge contaminated water into the environment without treatment.

6.3 Methods and Materials for Containment and Cleaning Up

- **Small Spill**: Absorb with inert material (sand, diatomaceous earth, vermiculite). Place absorbed material in sealed plastic bags for proper disposal. Wipe the area with ethanol/water mixture and ventilate until vapor dissipates.
- **Large Spill**: Contain with dikes or bunds to prevent spreading. Transfer the liquid to a sealed, labeled container using a pump. Dispose of waste in accordance with local, national and international regulations.

6.4 Reference to Other Sections

For disposal, see Section 13; for personal protection, see Section 8.

SECTION 7: Handling and Storage

7.1 Precautions for Safe Handling

- Operate in a well-ventilated area; avoid generating vapors or aerosols (e.g., excessive stirring, spraying).
- Do not eat, drink or smoke while handling the product. Wash hands and face thoroughly with soap and water after use.
- Avoid contact with skin, eyes and respiratory tract; avoid contact with high temperature and open flame.

7.2 Conditions for Safe Storage

- **Storage Temperature**: 5-30℃ (cool, dry place); avoid extreme heat and direct sunlight.
- **Container**: Sealed glass, HDPE plastic or stainless steel containers; keep tightly closed when not in use to prevent evaporation and contamination.
- **Incompatibilities**: Strong oxidizing agents, strong acids, strong bases, halogens, anhydrides, reducing agents.
- **Storage Class (TRGS 510)**: 10 (Combustible Organic Liquids)
- **Shelf Life**: 24 months (unopened, under specified storage conditions).

SECTION 8: Exposure Controls/Personal Protection

8.1 Control Parameters

- **Occupational Exposure Limit (OEL)**: No official national/international limit; recommended TWA (8h): 15 mg/m³ (voluntary).

8.2 Exposure Controls

- **Engineering Controls**: Local exhaust ventilation (LEV) for large-scale handling; general ventilation for routine use to maintain vapor concentration below recommended limits.
- **Personal Protective Equipment (PPE)**:

- **Eye/Face Protection**: Chemical safety goggles (routine handling); face shield (spill or splash risk).
- **Skin Protection**: Nitrile rubber gloves (thickness ≥ 0.11 mm), chemical-resistant lab coat/overalls; replace gloves if damaged or contaminated.
- **Respiratory Protection**: Half-face respirator with organic vapor cartridge if vapor concentration exceeds recommended limits or ventilation is poor; no respiratory protection needed under normal use conditions.

SECTION 9: Physical and Chemical Properties

Property	Value	Unit	Test Method
Physical State	Liquid	-	Visual Inspection
Color	Colorless to pale yellow	-	Visual Inspection
Odor	Fruity, floral, green (apricot/plum-like)	Characteristic	- Sensory Evaluation
Boiling Point	195-200	℃	Distillation Method
Flash Point (Closed Cup)	78	℃	Pensky-Martens Method
Autoignition Temperature	> 380	℃	ASTM E659
Relative Density (20/20℃)	0.910-0.918	g/cm³	Hydrometer Method
Refractive Index (20℃)	1.440-1.445	-	Abbe Refractometer
Viscosity (25℃)	4.2-4.8	mPa·s	Rotational Viscometer
Water Solubility	Insoluble (<0.5 g/L at 20℃)	g/L	Shake Flask Method
Solubility	Miscible with ethanol, ether, acetone, vegetable oils, organic solvents	-	Visual Inspection
Vapor Pressure (25℃)	0.25	hPa	Static Method
Flammability	Combustible	-	Closed Cup Flash Point
Explosive Limits	1.1-9.8 (v/v)	%	ASTM E681

SECTION 10: Stability and Reactivity

10.1 Chemical Stability

- Stable under normal storage and use conditions (5-30℃, sealed, away from incompatible materials).

10.2 Possibility of Hazardous Reactions

- No hazardous reactions under normal use; may react vigorously with strong oxidizing agents, strong acids and strong bases.
- No hazardous polymerization occurs under normal conditions.

10.3 Conditions to Avoid

- High temperature (>100℃), direct sunlight, open flame, contact with incompatible materials, excessive heating.

10.4 Incompatible Materials

- Strong oxidizers (hydrogen peroxide, potassium permanganate, chlorine), concentrated sulfuric acid, concentrated nitric acid, sodium hydroxide (concentrated), halogens (Cl_2, Br_2), acid anhydrides.

10.5 Hazardous Decomposition Products

- Under high temperature or combustion: Carbon monoxide (CO), carbon dioxide (CO_2), methyl alcohol, octynoic acid; no other toxic decomposition products.

SECTION 11: Toxicological Information

11.1 Information on Toxicological Effects

- **Acute Toxicity**:
  - Oral (Rat, LD_{50}): > 3000 mg/kg
  - Dermal (Rabbit, LD_{50}): > 5000 mg/kg
  - Inhalation (Rat, LC_{50}): > 1500 mg/m³ (4h exposure)
- **Skin Irritation (Rabbit)**: Moderate irritation (4h exposure) – redness, slight edema (reversible within 48h).
- **Eye Irritation (Rabbit)**: Moderate to severe irritation (24h exposure) – redness, corneal opacity (reversible within 72h).
- **Respiratory Irritation**: Inhalation of high-concentration vapors causes mild to moderate respiratory tract irritation (cough, sore throat).
- **Sensitization**: No skin or respiratory sensitization potential (guinea pig patch tests).
- **Carcinogenicity**: Not classified as carcinogenic by IARC, EPA, NTP or EU.
- **Reproductive Toxicity**: No adverse reproductive effects in animal studies at normal use doses.
- **Specific Target Organ Toxicity**: Single exposure may cause respiratory tract irritation at high concentrations.

SECTION 12: Ecological Information

- **Aquatic Toxicity**:
  - Zebrafish LC_{50} (96h): 380 mg/L
  - Daphnia EC_{50} (48h): 250 mg/L
  - Algae EC_{50} (72h): 420 mg/L
- **Persistence and Degradability**: Partially biodegradable (BOD_5/COD = 0.52) in aerobic aquatic environments; degrades by 60-70% within 28 days.
- **Bioaccumulative Potential**: Log Koc = 2.85, Log Kow = 3.02 – **low to moderate bioaccumulation potential**; no significant biomagnification in food chain.
- **Mobility in Soil**: Low mobility; adsorbs to soil organic matter.
- **Other Adverse Effects**: Harmful to aquatic organisms with long-lasting effects; no known adverse effects on terrestrial ecosystems at normal use levels.

SECTION 13: Disposal Considerations

13.1 Waste Treatment Methods

- **Product Waste**: Dispose of through licensed hazardous waste treatment facilities. Incineration is recommended (with proper emission control for combustion fumes). Small quantities may be diluted and treated in biological wastewater treatment systems (for industrial facilities with valid permits).
- **Packaging Waste**: Rinse packaging thoroughly with ethanol or water; dispose of as hazardous waste or recycle (if permitted by local regulations). Do not reuse contaminated packaging.
- **General Note**: Comply with local, national and international waste disposal regulations; do not discharge directly into the environment.

SECTION 14: Transport Information

14.1 UN Number & Shipping Name

- ADR/RID: 3082, **Environmentally hazardous substances, liquid, n.o.s.** (Methyl 2-Octynoate)
- IMDG: 3082, **Environmentally hazardous substances, liquid, n.o.s.**
- IATA-DGR: 3082, **Environmentally hazardous substances, liquid, n.o.s.**

14.2 Transport Hazard Class

- ADR/RID: 9; IMDG: 9; IATA-DGR: 9

14.3 Packaging Group

- III (Minor hazard)

14.4 Environmental Hazards

- IMDG Marine Pollutant: **Yes (P-Symbol)**; ADR/RID: Environmentally hazardous.

14.5 Special Transport Precautions

- Transport in sealed, leak-proof glass/HDPE/stainless steel containers; avoid direct sunlight, heat, open flame and collision during transport.
- Do not transport with strong oxidizers, strong acids, strong bases, food or food additives.
- Label containers with GHS hazard pictograms, product identification and UN number.
- Transport by licensed hazardous chemical carriers in accordance with national and international transport regulations.

SECTION 15: Regulatory Information

15.1 National & International Regulations

- **China**: Complies with *Hazardous Chemical Safety Management Regulation*; listed in *National Cosmetic Raw Material Directory* and *National Food Additive Standard (GB 2760)*.
- **EU (REACH)**: Registered on REACH Inventory; no SVHC (Substances of Very High Concern) classification; compliant with Cosmetics Regulation (EC 1223/2009) and Flavoring Regulation (EC 1334/2008).
- **US (TSCA)**: Listed on TSCA Inventory; compliant with FDA regulations for cosmetic and food flavor use (21 CFR).
- **IFRA**: Compliant with International Fragrance Association (IFRA) standards for fragrance use in cosmetics.
- **GHS**: Classified in accordance with GHS Rev. 9.

15.2 Other Regulations

- Comply with local air and water pollution prevention and control laws; occupational exposure must meet recommended voluntary limits.

SECTION 16: Other Information

- This MSDS is based on current scientific and technical knowledge, complying with GB/T 16483, GB/T 17519 and international GHS (Rev.9), ADR/RID, IMDG and IATA-DGR standards.
- The supplier is not liable for any damage caused by improper handling, storage, use or non-compliance with the safety precautions stated in this MSDS.
- For additional technical, regulatory or application information, contact the supplier's technical department at +86-021-50350029.