

Technical Data Sheet (TDS)

- Methyl 2-Octynoate

Revision Date: 28 FEB 2026 **CAS Number:** 111-12-6 **Formula:** C₉ H₁₄O₂ **Molecular Weight:** 154.21 g/mol

1. Product Overview

Methyl 2-Octynoate is a high-purity synthetic ester with a characteristic **fruity-floral (apricot/plum-like) green odor**, widely used as a key raw material in fragrance, flavor and cosmetic industries. It features excellent odor retention, good chemical stability under normal use conditions, and perfect compatibility with most fragrance and cosmetic ingredients. Compliant with international IFRA, FDA and EU REACH regulations, it is a versatile fine chemical for formulating fruity, floral and green fragrance profiles, and also serves as an intermediate for fine chemical synthesis.

Core Characteristics: High purity (≥98.5%); distinctive fruity-floral odor; long-lasting scent retention; excellent compatibility; multi-industry applicability; compliant with global regulatory standards.

2. Technical Specifications (Complies with IFRA/Food/Cosmetic Industrial Standards)

Item	Specification	Test Method
Appearance	Colorless to pale yellow clear liquid	Visual Inspection
Assay (Purity)	≥ 98.5% (w/w)	Gas Chromatography (GC)
Odor	Characteristic fruity-floral (apricot/plum) green odor	Sensory Evaluation (IFRA Method)
Relative Density (20/20°C)	0.910-0.918 g/cm ³	Hydrometer Method
Refractive Index (20°C)	1.440-1.445	- Abbe Refractometer
Boiling Point	195-200°C	Distillation Method
Flash Point (Closed Cup)	≥ 75°C	Pensky-Martens Method
Water Content	≤ 0.2% (w/w)	Karl Fischer Titration
Acid Value (as KOH)	≤ 1.0 mg/g	KOH Titration
Heavy Metals (Pb)	≤ 5 ppm	Atomic Absorption Spectrometry (AAS)
Residue on Evaporation	≤ 0.1% (w/w)	Gravimetric Method
Viscosity (25°C)	4.2-4.8 mPa·s	Rotational Viscometer
Solubility	Insoluble in water; miscible with ethanol, ether, acetone and vegetable oils	Shake Flask Method

3. Product Advantages

- High Purity & Consistent Odor:** Assay ≥98.5%, low impurity content, consistent physical and odor properties across batches, ensuring stable formulation performance.



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- 2. Distinctive Odor Profile:** Unique fruity-floral green note with apricot/plum characteristics, enhances the depth and layering of fragrance formulations; long-lasting scent retention (8-12h in finished products).
- 3. Excellent Compatibility:** Miscible with all common fragrance raw materials (esters, alcohols, aldehydes, terpenes) and cosmetic bases; no adverse reactions with non-ionic/anionic/cationic surfactants.
- 4. Regulatory Compliance:** Meets IFRA fragrance standards, China GB 2760 (food flavor), EU REACH and US FDA regulations; suitable for global market applications in fragrance, flavor and cosmetics.
- 5. Good Chemical Stability:** Resistant to hydrolysis (pH 5-8); stable at room temperature; no significant degradation in cosmetic/fragrance formulations within shelf life.
- 6. Low Dosage Requirement:** Effective fragrance concentration at 0.05-2.0% (w/w) in formulations; cost-efficient for large-scale production.

4. Application Fields

4.1 Fragrance Industry

- Fine fragrances (perfumes, eau de toilette, cologne): Formulates fruity, floral, green and oriental fragrance profiles.
- Functional fragrances (air fresheners, candles, incense, car fresheners): Adds fruity-green notes to daily fragrance products.
- Household product fragrances (dish soap, laundry detergent): Enhances fruity-floral scents with long-lasting effect.

5. Usage Methods & Dosage

Application Field	Dosage Range	Key Function
Fine Fragrances (Perfume/EDT)	0.5-2.0%	Fragrance raw material, note enhancer
Cosmetic Formulations	0.05-0.5%	Scent additive, fragrance fixative
Household Product Fragrances	0.1-1.0%	Fragrance raw material
Food Flavoring	0.001-0.05%	Fruit flavor enhancer (apricot/plum/peach)
Fine Chemical Synthesis	5.0-30.0%	Synthesis intermediate

6. Packaging & Storage

6.1 Packaging Specifications

- 1 L / 5 L Sealed glass bottles (laboratory/small-scale fragrance/flavor use);
- 25 L HDPE plastic drums (industrial/cosmetic use);
- 200 L stainless steel drums (bulk industrial use);
- **Custom packaging** (100 mL-1000 L) available upon request (food-grade packaging for flavor use).

7. Safety & Handling

- The product is a mild to moderate skin/eye irritant and combustible liquid; avoid direct contact with skin, eyes and respiratory tract, and keep away from open flame and high temperature.
- **Routine Handling:** Wear nitrile rubber gloves and chemical safety goggles; operate in a well-ventilated area.
- **Large-Scale Handling:** Wear a lab coat/protective clothing and a half-face respirator with organic vapor cartridge (if vapor concentration is high).