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Technical Data Sheet (TDS)

- Methyl Octanoate 甲基辛酸盐

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1. Product Overview

- **Product Name**: Methyl Octanoate (甲基辛酸盐)
- **English Name**: Methyl Octanoate; Methyl caprylate; Octanoic acid methyl ester
- **CAS Number**: 111-11-5
- **Molecular Formula**: $C_9H_{18}O_2$
- **Molecular Weight**: 158.24 g/mol
- **Form**: Colorless transparent liquid with a fresh, sweet fruity aroma (citrus, coconut & pineapple note)
- **Grade**: Food Grade / Flavor & Fragrance Grade / Industrial Grade / Cosmetic Grade

Methyl Octanoate is a high-purity fatty acid methyl ester, naturally present in various fruits and essential oils. It complies with EU REACH, US FDA GRAS, FEMA and Chinese national food/cosmetic safety standards. As a classic aroma ingredient in the flavor & fragrance industry, it also serves as an important organic synthesis intermediate and plasticizer raw material for chemical manufacturing. The product features pure fruity aroma, excellent thermal stability and compatibility, with stable performance and wide application prospects in food, cosmetic and fine chemical fields.

2. Technical Specifications (Complies with Flavor/Food/Industrial Standard)

Item	Specification
Appearance	Colorless clear liquid, characteristic fruity aroma
Assay (Methyl Octanoate)	≥ 99.0%
Refractive Index (n_{20}^{D})	1.415 ~ 1.419
Relative Density (25/25℃)	0.870 ~ 0.874 g/cm³
Boiling Point	192 ~ 194℃
Flash Point (Closed Cup)	≥ 80℃
Acid Value (as KOH)	≤ 0.5 mg KOH/g
Water Content	≤ 0.1%
Heavy Metals (Pb)	≤ 5 ppm
Heavy Metals (As)	≤ 1 ppm
Ethanol Solubility (1:5, 95% EtOH)	Clear, no turbidity
Total Bacterial Count (Food/Cosmetic Grade)	≤ 100 CFU/mL
E. coli (Food/Cosmetic Grade)	Negative
Temperature Stability	Stable at 0 ~ 50℃ (purity/aroma retention ≥ 99%)
pH Stability	Stable at pH 5.0 ~ 8.0 (no hydrolysis)
Storage Stability	24 months unopened (under specified conditions), no discoloration/odor change

3. Product Advantages

1. **High Purity & Pure Aroma**: Assay ≥99.0%, no off-flavor, pure fresh fruity note, excellent blending and fragrance fixing effect in flavor/fragrance formulations.
2. **Excellent Stability**: Good thermal and chemical stability, no easy hydrolysis/decomposition under normal use conditions, no secondary reaction in organic synthesis.
3. **Wide Compatibility**: Miscible with ethanol, ether, vegetable oil, ester and most organic solvents, compatible with various flavor/fragrance raw materials and cosmetic bases.
4. **Multi-grade Compliance**: Food grade meets FEMA 2724, FDA GRAS; cosmetic/industrial grade complies with EU REACH and Chinese chemical product standards, low toxicity and safe use.
5. **Natural Source Traceable**: Exists in natural fruits (pineapple, coconut, orange) and essential oils, suitable for natural flavor formulation requirements.

6. **Versatile Application**: Dual properties of aroma ingredient and chemical intermediate, suitable for flavor & fragrance, organic synthesis, plasticizer and cosmetic industries.

4. Application Fields

- **Food & Beverage Industry**: Flavoring agent for candy, pastry, ice cream, beverage, dairy products and canned food; used to prepare citrus, coconut, pineapple and tropical fruit flavors, also as a fragrance fixative.
- **Cosmetic & Personal Care**: Fragrance ingredient for perfume, lotion, cream, shampoo, body wash and candle; enhances the fresh fruity note of cosmetic and daily chemical formulations.
- **Flavor & Fragrance Industry**: Core raw material for synthetic fruit essential oils; blending ingredient for daily chemical and fine fragrances, improving aroma layering.
- **Organic Synthesis**: Key intermediate for synthesizing pharmaceuticals, pesticides, plasticizers and surfactant; reaction solvent for esterification and transesterification reactions.
- **Other Fields**: Plasticizer additive for polyvinyl chloride (PVC); raw material for biodiesel and lubricating oil production.

5. Usage Methods

Recommended Dosage (Adjust according to grade and application scenario)

- **Food & Beverage**: 0.001 ~ 0.05% of total formulation (beverage/dairy); 0.01 ~ 0.1% (candy/pastry); follow FEMA maximum use level.
- **Cosmetic & Fragrance**: 0.1 ~ 3.0% of total formulation (perfume/candle); 0.05 ~ 1.0% (shampoo/body wash).
- **Flavor & Fragrance**: 4 ~ 18% of total essence formulation (as aroma ingredient/fragrance fixative).
- **Organic Synthesis**: 10 ~ 50% of total reaction system (as intermediate/solvent), adjust according to reaction process.

Key Application Tips

1. **Mixing & Addition**: At room temperature, can be directly mixed with organic solvents/oil-based formulations; dilute with ethanol/propylene glycol for water-based formulations to avoid phase separation.
2. **Compatibility Note**: Stable in neutral/weak acidic/weak alkaline systems (pH 5.0 ~ 8.0); avoid strong acidic/strong alkaline (pH <3.0 or pH >9.0) high-temperature environments to prevent hydrolysis.
3. **Fragrance Blending**: Blends well with linalool, limonene, ethyl acetate and fruit aldehydes to enhance the fresh and sweet fruity note of formulations.
4. **Industrial Use**: For organic synthesis, control reaction temperature below 180℃ to avoid slight volatilization and ensure reaction efficiency.

6. Packaging & Storage

Packaging Specifications (Sealed Food/Industrial Grade Packaging)

- 500 mL brown glass bottle (inner) + carton (outer) (laboratory/R&D/small-batch use)
- 25 kg HDPE plastic drum (cosmetic/industrial grade use)
- 200 kg galvanized iron drum (flavor/food grade bulk use)
- 1000 kg IBC tote (large-scale chemical manufacturing/flavor production use)
- Custom packaging available (100g/250g small glass bottle for flavor formulation).

7. Safety & Protection

1. The product is low-toxic and slightly irritating; a small number of sensitive individuals may have mild skin/eye irritation after direct contact; avoid prolonged contact and inhalation of high-concentration vapor.
2. **Recommended PPE**: Wear nitrile rubber gloves and safety glasses for large-scale handling/pouring; a dust/mist mask is optional for operation in poor ventilation; no special PPE for small-batch formulation.