

Diethyl Sebacate

1 Nonproprietary Names

USP–NF: Diethyl Sebacate

2 Synonyms

Bisoflex DES; decanedioic acid, diethyl ester; DES; diethyl 1,10-decanedioate; diethyl 1,8-octanededicarboxylate; ethyl sebacate; *DES-SP*; sebacic acid, diethyl ester; *Stelliesters DES*.

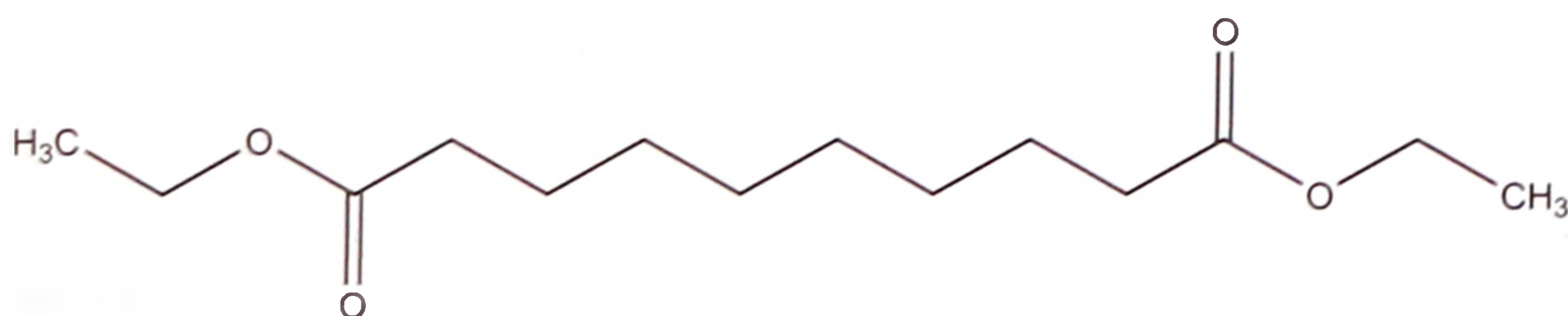
3 Chemical Name and CAS Registry Number

Diethyl decanedioate [110-40-7]

4 Empirical Formula and Molecular Weight

C₁₄H₂₆O₄ 258.35

5 Structural Formula



6 Functional Category

Emollient; penetration enhancer.

7 Applications in Pharmaceutical Formulation or Technology

Diethyl sebacate is used as an emollient in topical creams, emulsions, and solutions. It has been shown to aid skin penetration of various anti-inflammatory,^(1,2) antifungal,⁽³⁾ and local anesthetic⁽⁴⁾ drugs, at concentrations of up to 24%.

Diethyl sebacate is also used as a flavoring agent in foods.⁽⁵⁾

8 Description

Diethyl sebacate is a colorless or yellowish liquid with a characteristic fruity odor.

9 Pharmacopeial Specifications

See Table I.

Table I: Pharmacopeial specifications for diethyl sebacate.

Test	USP 40–NF 35 S1
Identification	+
Residue on ignition	≤0.10%
Heavy metals	≤20 ppm
Specific gravity	0.958–0.968
Refractive index	1.435–1.437
Acid value	≤0.5
Iodine value	≤0.5
Assay	98.0%–100.5%

10 Typical Properties

Boiling point 307–312°C (with some decomposition)

Flash point > 93°C (closed cup); 113°C (open cup)

Melting point 1–3°C

Partition coefficient Log *P* (octanol : water) = 3.8–4.3 (calculated)

Refractive index *n*_D²⁰ = 1.435

Solubility Miscible with alcohol, ether, hydrocarbons, fixed oils and fats; soluble 1 in 700 cold water, 1 in 50 boiling water.

Specific Gravity 0.960–0.965 at 20°C

Surface tension 33.2 mN/m at 20°C

Viscosity (dynamic) 6.1 mPa s (6.1 cP) at 20°C

11 Stability and Storage Conditions

Diethyl sebacate is stable to hydrolysis at room temperature and does not tend to go rancid.

Store in tightly closed containers in a cool, well-ventilated area. Protect from light. Keep away from heat and sources of ignition.

12 Incompatibilities

Diethyl sebacate is incompatible with oxidizing agents and alkalis.

13 Method of Manufacture

Diethyl sebacate is prepared by the esterification of sebacic acid and ethanol in the presence of sulfuric acid.

14 Safety

Diethyl sebacate is mildly toxic by ingestion and a skin irritant. It may cause irritation to the eyes and mucous membranes. Contact dermatitis due to diethyl sebacate has been reported.^(6,7)

LD₅₀ (guinea pig, oral): 7.28 g/kg⁽⁸⁾

LD₅₀ (rat, oral): 14.47 g/kg

15 Handling Precautions

Observe normal precautions appropriate to the circumstances and quantity of the material handled. When heated, diethyl sebacate emits acrid smoke and irritating fumes. Wear suitable protective clothing. Avoid contact with skin and eyes.

16 Regulatory Status

GRAS listed. Included in the FDA Inactive Ingredients Database (topical; emulsions, creams, solutions). Diethyl sebacate is listed as a food additive in the EAFUS list compiled by the FDA.

17 Related Substances

Dibutyl sebacate.

18 Comments

Diethyl sebacate has been used in PEG-poly(amine-co-ester) block copolymer micelles as a novel anticancer drug delivery system.⁽⁹⁾

A specification for diethyl sebacate is included in the *Food Chemicals Codex* (FCC)⁽⁵⁾ and in the *Japanese Pharmaceutical Excipients* (JPE);⁽¹⁰⁾ see Table II.

The EINECS number for diethyl sebacate is 203-764-5. The PubChem Compound ID (CID) is 8049.

19 Specific References

- 1 Fukuyasu H, *et al.* *In vivo* activity and metabolic fate of 2-(2,3,3-triiodoallyl tetrazole (ME1401), a novel antifungal agent. *Drugs Exp Clin Res* 1989; 15: 335–347.