

Bis(2-ethylhexyl) sebacate

sc-239352

Material Safety Data Sheet



The Power to Question

Hazard Alert Code Key: **EXTREME** **HIGH** **MODERATE** **LOW**

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

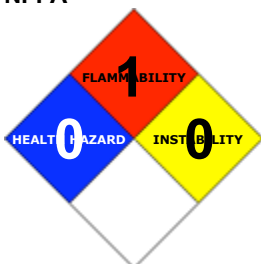
PRODUCT NAME

Bis(2-ethylhexyl) sebacate

STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA



SUPPLIER

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EMERGENCY:

ChemWatch

Within the US & Canada: 877-715-9305

Outside the US & Canada: +800 2436 2255

(1-800-CHEMCALL) or call +613 9573 3112

SYNONYMS

C26-H50-O4, C8H17OCOCH2CH2COOC8H17, di(2-ethylhexyl)sebacate, bis(2-ethylhexyl)sebacate, "sebacic acid, bis(2-ethylhexyl)ester", "octyl sebacate", "1-hexanol, 2-ethyl-, sebacate", "decanedioic acid, bis(2-ethylhexyl) ester", "Bisoflex DOS", "Monoplex DOS", "Octoil S", "PX 438", "Stafllex DOS"

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	2		
Body Contact:	0		Min/Nil=0 Low=1
Reactivity:	1		Moderate=2
Chronic:	2		High=3 Extreme=4

CANADIAN WHMIS SYMBOLS

None

EMERGENCY OVERVIEW

RISK

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

- Accidental ingestion of the material may be damaging to the health of the individual.

EYE

- Although the liquid is not thought to be an irritant, direct contact with the eye may produce transient discomfort characterized by tearing or conjunctival redness (as with windburn).

SKIN

- The liquid may be miscible with fats or oils and may degrease the skin, producing a skin reaction described as non-allergic contact dermatitis.

The material is unlikely to produce an irritant dermatitis as described in EC Directives .

- Open cuts, abraded or irritated skin should not be exposed to this material.

- Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.

Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

- The material is not thought to produce either adverse health effects or irritation of the respiratory tract following inhalation (as classified using animal models).

Nevertheless, adverse effects have been produced following exposure of animals by at least one other route and good hygiene practice requires that exposure be kept to a minimum and that suitable control measures be used in an occupational setting.

- Not normally a hazard due to non-volatile nature of product.

CHRONIC HEALTH EFFECTS

- Long-term exposure to the product is not thought to produce chronic effects adverse to the health (as classified using animal models); nevertheless exposure by all routes should be minimized as a matter of course.

Exposure to the material may cause concerns for humans owing to possible developmental toxic effects, on the basis that similar materials tested in appropriate animal studies provide some suspicion of developmental toxicity in the absence of signs of marked maternal toxicity, or at around the same dose levels as other toxic effects but which are not a secondary non-specific consequence of other toxic effects.

2-Ethylhexanoic acid (2-EHA) its esters and its salts are of concern to human health because of their potential to induce carcinogenicity, liver toxicity and developmental/reproductive toxicity. 2-EHA is of low acute oral and dermal toxicity, is a mild skin irritant and a severe eye irritant. It is not mutagenic in Ames test, but is capable of inducing chromosome aberration and sister chromatid exchanges in vitro, liver toxicity and liver tumours after repeated dose treatment. In addition, 2-EHA acid has been associated with reproductive and developmental toxicity in experimental animals.

2-EHA is quickly resorbed orally, dermally and following inhalation and almost fully excreted mainly in urine. As in the case of fatty acids, degradation mainly takes place by means of peroxisomal beta-oxidation.

Various studies on reproduction toxicity have produced indications of an embryotoxic effect of 2-EHA. After oral administration, NOAEL values for maternal toxicity and foetotoxic effects of 2-EHA were determined in rabbits at 25 and >250 mg/kg body weight/day and in rats at 250 and 100 mg/kg body weight/day. The foetotoxic findings in rats were based on a reduced skeleton ossification at the next higher dose (250 mg/kg body weight/day). No teratogenic effects were observed in this study. In comparison with the structural isomer valproic acid, a known human teratogen, 2-EHA does have similar reprotoxic effects at maternal toxic doses in animal experiments but a far lower potency

Following sub-chronic oral administration of 2-EHA, critical effects like liver changes (higher relative liver weight, histological changes in hepatocytes) were observed in rats and mice and histological renal tubule results were observed in mice. Furthermore, statistically significant, higher cholesterol values were found in all treated male rats (61, 303 and 917 mg/kg body weight/day) and in male and female mice in the middle and high dose groups (885-3139 mg/kg body weight/day). In rats the maximum dose with no adverse effect (NOAEL) was 61 mg/kg body weight/day

In bacterial test systems, mutagenicity studies produced negative findings. In test systems

with mammalian cells, by contrast, the findings were weakly positive. Cytogenetic and SCE studies involving CHO cells were positive, one SCE test in human lymphocytes was questionably positive and one experiment concerning tritium-thymidine incorporation into the DNA of mouse lymphocytes was negative. Furthermore, An unpublished micronucleus study on the bone marrow of CD-1 mice was conducted in compliance with OECD Guideline 474. No significant increase in the micronuclei was observed at doses of 400, 800 or 1,600 mg/kg body weight (Inveresk Research International Ltd, 1994). Furthermore, in vitro and in vivo genotoxicity data (micronucleus test, dominant lethal test) are available for 2-ethylhexanol which is rapidly and quantitatively converted into 2-EHA in metabolism studies. This data do not indicate any genotoxic potential which means that such an effect of 2-EHA is not likely either. As 2-EHA can induce both DNA synthesis and inhibition of intercellular communication in hepatic cells, a tumour-promoting potential in rodents, comparable to that of other peroxisome proliferators, cannot be ruled out. The carcinogenic effect of peroxisome proliferators in rodents (e.g. of di(2-ethylhexyl)phthalate, DEHP) is not deemed to be relevant for humans.

Calcium/zinc and barium/zinc salts of 2-EHA are used as thermo-stabilisers for PVC, together with co-stabilisers like polyols or epoxy compounds, in order to capture the hydrochloride cleaved during the thermal loading of PVC; in addition various salts are used in other food and beverage containers as plasticisers. The migration of 2-EHA from the sealing compounds in the metal lids. has been demonstrated in food contamination. The potential for human exposure to 2-EHA therefore is significant.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
dioctyl sebacate	122-62-3	> 99

Section 4 - FIRST AID MEASURES

SWALLOWED

· If swallowed do NOT induce vomiting. · If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.

EYE

■ If this product comes in contact with the eyes: · Wash out immediately with fresh running water. · Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.

SKIN

■ If skin or hair contact occurs: · Flush skin and hair with running water (and soap if available). · Seek medical attention in event of irritation.

INHALED

· If fumes or combustion products are inhaled remove from contaminated area. · Other measures are usually unnecessary.

NOTES TO PHYSICIAN

■ Treat symptomatically.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Negligible
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	0.92
Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA

· Foam.
· Dry chemical powder.

FIRE FIGHTING

· Alert Emergency Responders and tell them location and nature of hazard.
· Wear full body protective clothing with breathing apparatus.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

· Combustible.
· Slight fire hazard when exposed to heat or flame.
Combustion products include: carbon dioxide (CO₂), other pyrolysis products typical of burning organic material.
May emit poisonous fumes.

FIRE INCOMPATIBILITY

■ Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids, chlorine bleaches, pool chlorine etc. as ignition may result.

PERSONAL PROTECTION

Glasses:
Chemical goggles.
Gloves:
Respirator:
Type A Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

■ Slippery when spilt.
· Remove all ignition sources.
· Clean up all spills immediately.

MAJOR SPILLS

■ Slippery when spilt.
Moderate hazard.
· Clear area of personnel and move upwind.
· Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.

RECOMMENDED STORAGE METHODS

- Glass container.
- Metal can or drum
- Packing as recommended by manufacturer.

STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.
- No smoking, naked lights or ignition sources.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.
- Protect containers against physical damage and check regularly for leaks.
- Observe manufacturer's storing and handling recommendations.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

The following materials had no OELs on our records

- dioctyl sebacate: CAS:122-62-3

PERSONAL PROTECTION



RESPIRATOR

- type a filter of sufficient capacity.

EYE

- Safety glasses with side shields
- Chemical goggles.

HANDS/FEET

- Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include: such as:
 - frequency and duration of contact,
 - chemical resistance of glove material,
 - glove thickness and
 - dexterity

Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).

- When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.
- When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.
- Contaminated gloves should be replaced.

Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

Wear chemical protective gloves, eg. PVC.

OTHER

- Overalls.
- P.V.C. apron.
- Barrier cream.
- Skin cleansing cream.
- Eye wash unit.

ENGINEERING CONTROLS

- General exhaust is adequate under normal operating conditions. If risk of overexposure exists, wear an approved respirator.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Liquid.

Does not mix with water.

Floats on water.

State	Liquid	Molecular Weight	426.76
Melting Range (°F)	-80	Viscosity	Not available
Boiling Range (°F)	711	Solubility in water (g/L)	Immiscible
Flash Point (°F)	419 (OCP)	pH (1% solution)	Not applicable.
Decomposition Temp (°F)	Not available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	500	Vapour Pressure (mmHG)	Negligible
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	0.92
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	14.8
Volatile Component (%vol)	Negligible	Evaporation Rate	Not available

APPEARANCE

Colourless to pale straw coloured liquid with practically no odour; does not mix with water. Partly compatible with cellulose acetate and cellulose acetate butyrate; compatible with ethyl cellulose, polystyrene, polyethylene, vinyl chloride and vinyl chloride acetate.

In general, the short-chain alkyl (e.g., methyl, isopropyl, and butyl) diesters are generally more water soluble, less lipophilic and relatively more volatile than the corresponding long-chain alkyl (C7-C 13 alcohol) diesters. Long chain diesters have molecular weight of greater than 350, have high boiling points (~300 C) and are expected to be relatively non-volatile, lipophilic (log Kow > 7) and extremely water-insoluble.

Material	Value
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Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.

STORAGE INCOMPATIBILITY

- Avoid reaction with oxidizing agents.

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

dioctyl sebacate

TOXICITY AND IRRITATION

DIOCTYL SEBACATE:

- unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

TOXICITY	IRRITATION
Oral (rat) LD50: 12800 mg/kg	Nil Reported
Oral (mouse) LD50: 1280 mg/kg [Manufacturer]	

- For Group B aliphatic esters of mono-alcohols and diacids (diesters)

According to a classification scheme described by the American Chemistry Council's Aliphatic Esters Panel, Group B substances are comprised of aliphatic esters derived from linear diacids and monofunctional alcohols. The diacids include maleic (C4), adipic (C6), azelaic (C9) and sebacic (C10) acid. The monofunctional alcohols most common in the diesters are in the C8 to C13 carbon range, although methyl, isopropyl and butyl occur in some diesters.

Due to the physicochemical properties of the diesters (e.g., viscosity, pour point), they have widespread applications as lubricants, solvents, and plasticisers. The linear diacid portion of the diester contributes to the good viscosity index while branching in the alcohol portion provides good pour point characteristics. Because diesters have good polarity characteristics, they are useful as solvents.

Acute toxicity: Most of the diesters in Group B are higher alkyl (>C8) adipates, azelates and sebacates and these diesters generally have a low order of toxicity. Oral rat LD50 values ranged from >2 g/kg to >64 g/kg.

Metabolism of the diesters in animals is expected to lead to the generation of corresponding diacids: namely, maleic, adipic, azelaic and sebacic acid and the corresponding linear or branched alcohol (e.g., 2-ethylhexyl, 1-methylheptyl, isooctyl, isononyl, isodecyl, tridecyl alcohols). These diacids and alcohols can further be metabolized and conjugated to products that are excreted in the urine. The diacids

and alcohols have a low order of toxicity

Repeated Dose Toxicity. Data on repeated dose toxicity have been reported for diisononyl adipate and tridecyl adipate. In 90-day toxicity studies, rats were administered diisononyl adipate (CAS 33703-08-1) in the diet at levels equivalent to 0,50, 150 and 500 mg/kg/day. The NOAEL was 500 mg/kg/day. Feeding studies were also carried out in beagle dogs for 13 weeks at dietary concentrations of 0,0.3, 1 and 3% (increased to 6% at week 9). The NOAEL was determined to be 1% in the diet or approximately 274 mg/kg/day. In another 13-week study, ditridecyl adipate was well tolerated in rats given dermal doses of 800 and 2000 mg/kg/day.

For adipic acid di-C7-9 branched and linear alkyl ester (CAS 685 15-75-3), rats were fed 0,0. 1,0.5 and 2.5% of the test substance in the diet. No significant signs of toxicity were observed in male and female rats administered the test material in the diet at concentrations up to 2.5% for a period of 13 weeks. The NOAEL was 2.5% for both sexes (males -1300 mg/kg; females -1800 mg/kg). In the 90-day dietary studies with 2-ethylhexyl adipate (CAS 103-23-1), the NOAEL was -300 mg/kg/day in rats and -230 mg/kg/day in mice. The LOAEL was -600 mg/kg/day in rats and -460 mg/kg/day in mice. Hepatic hypertrophy and increased peroxisomal enzyme activity occurred in rats and mice; however, there were no adverse effects on the liver.

Reproductive toxicity: Di-2-ethylhexyl adipate (DEHA)(CAS 103-23-1) has been evaluated for reproductive effects in a one-generation study. Test diets, up to 1080 mg/kg/day, were fed continuously throughout the study (18-19 weeks of exposure). No effects were seen on male or female fertility. However, at the highest dose, there was a reduction in body weight in the dams, and reduction in offspring body weight, total litter weight and litter size. The NOAEL and LOAEL for this study was 170 and 1080 mg/kg/day, respectively. In 13-week dermal studies with ditridecyl adipate, there was no sperm morphological changes observed in male rats treated at levels of 2000 mg/kg. Increases in organ weight of the epididymides and uterus were observed at dermal exposure to 2000 mg/kg but not at 800 mg/kg. In a 19-week oral feeding study with sebacic acid, bis(2-ethylhexyl) ester (CAS 122-62-3), no adverse reproductive effects were reported for this material. Dibutyl maleate has been evaluated in an OECD reproductive/developmental toxicity screening test (oral gavage) and no adverse effects on reproduction were reported.

Since these four materials cover the carbon number range of C12-C32 for the diesters and because of the chemical similarity of the alkyl diesters, the available reproductive toxicity data should be sufficient for read-across assessment of most of the other diesters in Group B.

Developmental toxicity: No evidence of developmental toxicity was observed at dose levels of 1000 and 4000 mg/kg/day after oral gavage of adipic acid, di-C7-9 branched and linear alkyl ester (CAS 685 15-75-3). Slight maternal toxicity (reduced body weight) and embryotoxicity (reduced foetal weight) was observed at the highest dose (7000 mg/kg/day). The NOAEL for maternal and developmental toxicity was 4000 mg/kg/day. No adverse developmental effects were reported for dibutyl maleate in an OECD reproductive/developmental screening study

The developmental toxicity has also been evaluated for adipic acid, bis(2-ethylhexyl) ester (CAS 103-23-1) by dietary exposure. Pregnant rats administered 2-ethylhexyl adipate in the diet throughout gestation showed reduced body weight at dietary equivalent doses of 1080 mg/kg/day. At 1080 mg/kg/day, implantation fetal loss was evident; however, no gross, skeletal or visceral abnormalities were observed. LOAEL was 1080 mg/kg/day and NOAEL was 170 mg/kg/day (developmental toxicity). The developmental toxicity data from these three studies provide sufficient data for the read-across assessment of most of the other diesters in Group B due to their chemical structural similarities.

Genotoxicity: Adipic acid diisononyl ester and sebacic acid bis(2-ethylhexyl) ester] were shown to be negative in the Ames assay. In addition, diisononyl adipate was negative in the mouse lymphoma assay. Adipic acid, bis(2-ethylhexyl) ester has also been evaluated for mutagenicity and was found to be negative in both the Ames and mouse lymphoma assays. It has also been reported that dibutyl maleate (CAS 105- 76-0) is negative in the Ames assay

Adipic acid, ditridecyl ester (CAS 16958-92-2) was negative in the micronucleus assay. Adipic acid bis(2- ethylhexyl) ester (CAS 103-23-1), also did not cause chromosomal aberrations in the Chinese hamster ovary cell assay or the mouse micronucleus test . Since these two adipates cover the carbon number range of C22-C32 for the diesters, it is unlikely that the substances in Group B are chromosomal mutagens. In addition, dibutyl maleate (C12) has been shown to be negative in the mouse micronucleus test in vivo.

Section 12 - ECOLOGICAL INFORMATION

No data

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
dioctyl sebacate	LOW	No Data Available	LOW	LOW

GESAMP/EHS COMPOSITE LIST - GESAMP Hazard Profiles

Name / EHS TRN A1a A1b A1 A2 B1 B2 C1 C2 C3 D1 D2 D3 E1 E2 E3 Cas No / RTECS No _____
 _____ Fatty 226 278 5 0 (R) 0 NI (0) (0) (1) (1) (1) NI 2 acids, 1 0 linear C12+ saturated with C12+
 unsaturat ed / CAS:122- 62- 3 /

Legend: EHS=EHS Number (EHS=GESAMP Working Group on the Evaluation of the Hazards of Harmful Substances Carried by Ships)
 NRT=Net Register Tonnage, A1a=Bioaccumulation log Pow, A1b=Bioaccumulation BCF, A1=Bioaccumulation, A2=Biodegradation,
 B1=Acuteaquatic toxicity LC/ECIC50 (mg/l), B2=Chronic aquatic toxicity NOEC (mg/l), C1=Acute mammalian oral toxicity LD50 (mg/kg),
 C2=Acute mammalian dermal toxicity LD50 (mg/kg), C3=Acute mammalian inhalation toxicity LC50 (mg/kg), D1=Skin irritation &
 corrosion, D2=Eye irritation& corrosion, D3=Long-term health effects, E1=Tainting, E2=Physical effects on wildlife & benthic habitats,
 E3=Interference with coastal amenities, For column A2: R=Readily biodegradable, NR=Not readily biodegradable. For column D3:
 C=Carcinogen, M=Mutagenic, R=Reprotoxic, S=Sensitising, A=Aspiration hazard, T=Target organ systemic toxicity, L=Lunginjury,
 N=Neurotoxic, I=Immunotoxic. For column E1: NT=Not tainting (tested), T=Tainting test positive. For column E2: Fp=Persistent floater,
 F=Floater, S=Sinking substances. The numerical scales start from 0 (no hazard), while higher numbers reflect increasing hazard.
 (GESAMP/EHS Composite List of Hazard Profiles - Hazard evaluation of substances transported by ships)

Section 13 - DISPOSAL CONSIDERATIONS

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

‡ Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction
- Reuse
- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.

DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.

- Recycle wherever possible or consult manufacturer for recycling options.
- Consult Waste Management Authority for disposal.

Section 14 - TRANSPORTATION INFORMATION

NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: DOT, IATA, IMDG

Section 15 - REGULATORY INFORMATION

dioctyl sebacate (CAS: 122-62-3) is found on the following regulatory lists;

"International Fragrance Association (IFRA) Survey: Transparency List", "OECD Representative List of High Production Volume (HPV) Chemicals", "US DOE Temporary Emergency Exposure Limits (TEELs)", "US EPA High Production Volume Program Chemical List", "US FDA Indirect Food Additives: Adhesives and Components of Coatings - Substances for Use Only as Components of Adhesives - Adhesives", "US Toxic Substances Control Act (TSCA) - Chemical Substance Inventory"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

- Ingestion may produce health damage*.
- May possibly be harmful to the foetus/ embryo*.

* (limited evidence).

Reasonable care has been taken in the preparation of this information, but the author makes no warranty of merchantability or any other warranty, expressed or implied, with respect to this information. The author makes no representations and assumes no liability for any direct, incidental or consequential damages resulting from its use. For additional technical information please call our toxicology department on +800 CHEMCALL.

- Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

A list of reference resources used to assist the committee may be found at:

www.chemwatch.net/references.

- The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

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