

Bis(1-butylpentyl) adipate

sc-252438

Material Safety Data Sheet



The Power to Question

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

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

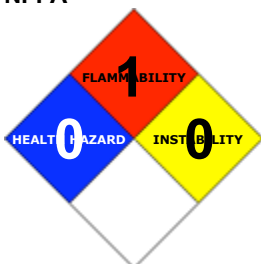
PRODUCT NAME

Bis(1-butylpentyl) adipate

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

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SYNONYMS

C24-H64-O4, "adipic acid di-5-nonyl ester", di(5-nonyl)adipate

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

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

CANADIAN WHMIS SYMBOLS

None

EMERGENCY OVERVIEW

RISK

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

- The material has NOT been classified as "harmful by ingestion". This is because of the lack of corroborating animal or human evidence.

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 material is not thought to produce adverse health effects or skin irritation following contact (as classified using animal models). Nevertheless, good hygiene practice requires that exposure be kept to a minimum and that suitable gloves be used in an occupational setting.

- 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 adverse health effects or irritation of the respiratory tract (as classified using animal models). Nevertheless, good hygiene practice requires that exposure be kept to a minimum and that suitable control measures be used in an occupational setting.

- Inhalation of vapours may cause drowsiness and dizziness.

This may be accompanied by narcosis, reduced alertness, loss of reflexes, lack of coordination and vertigo.

- There is some evidence to suggest that the material can cause respiratory irritation in some persons.

The body's response to such irritation can cause further lung damage.

- The material has NOT been classified as "harmful by inhalation".

This is because of the lack of corroborating animal or human evidence.

- Inhalation hazard is increased at higher temperatures.

- Inhalation of high concentrations of gas/vapor causes lung irritation with coughing and nausea, central nervous depression with headache and dizziness, slowing of reflexes, fatigue and inco-ordination.

CHRONIC HEALTH EFFECTS

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
bis(1-butylpentyl)adipate	77916-77-9	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

· Immediately give a glass of water. · First aid is not generally required. If in doubt, contact a Poisons Information Center or a doctor.

EYE

■ If this product comes in contact with eyes: · Wash out immediately with water. · If irritation continues, seek medical attention.

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):	Not available
Upper Explosive Limit (%):	Not available.

Specific Gravity (water=1):	0.910
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.
May emit corrosive 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

- Remove all ignition sources.
- Clean up all spills immediately.

MAJOR SPILLS

- 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

- 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

- bis(1-butylpentyl)adipate: CAS:77916-77-9

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.

- Neoprene gloves.

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. Local exhaust ventilation may be required in special circumstances.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Liquid.

Does not mix with water.

Floats on water.

State	Liquid	Molecular Weight	398.63
Melting Range (°F)	Not available	Viscosity	Not Available
Boiling Range (°F)	352- 356 (0.2 mm)	Solubility in water (g/L)	Partly miscible
Flash Point (°F)	230	pH (1% solution)	Not applicable
Decomposition Temp (°F)	Not available.	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapour Pressure (mmHG)	Not available
Upper Explosive Limit (%)	Not available.	Specific Gravity (water=1)	0.910
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	>1
Volatile Component (%vol)	Not available	Evaporation Rate	Not available

APPEARANCE

Liquid; does not mix well with water.

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

bis(1-butylpentyl)adipate

TOXICITY AND IRRITATION

BIS(1-BUTYLPENTYL)ADIPATE:

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

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

According to a classification scheme described by the American Chemistry Council' 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, 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, ditiidecyl ester (CAS 16958-92-2) was negative in the micronucleus assay. Adipic acid bis(2- ethylhexyl) ester (CAS 103-23-l), 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. No significant acute toxicological data identified in literature search.

Section 12 - ECOLOGICAL INFORMATION

No data

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
bis(1-butylpentyl)adipate	LOW	No Data Available	LOW	LOW

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

No data for bis(1-butylpentyl)adipate (CAS: , 77916-77-9)

Section 16 - OTHER INFORMATION

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■ 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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