Dibutyl adipate

sc-223934

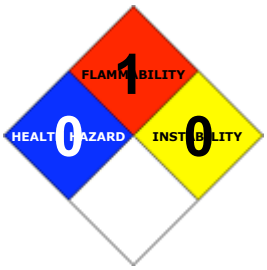
Material Safety Data Sheet

Hazard Alert Code Key:	EXTREME	HIGH	MODERATE	LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME
Dibutyl adipate

STATEMENT OF HAZARDOUS NATURE
CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA


SUPPLIER
Santa Cruz Biotechnology, Inc.
2145 Delaware Avenue
Santa Cruz, California 95060
800.457.3801 or 831.457.3800

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
C14-H26-O4, [-CH2CH2CO2(CH2)3CH3]2, "adipic acid, dibutyl ester", "butyl adipate", "di-n-butyl adipate", "dibutyl adipinate", "dibutyl hexanedioate", "experimental tick repellent 3, 3PS", "hexanedioic acid, dibutyl ester"

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	2		
Body Contact:	2		
Reactivity:	1		
Chronic:	0		

Min/Nil=0
Low=1
Moderate=2
High=3
Extreme=4

CANADIAN WHMIS SYMBOLS
None

EMERGENCY OVERVIEW
RISK
POTENTIAL HEALTH EFFECTS
ACUTE HEALTH EFFECTS

SWALLOWED
■ Although ingestion is not thought to produce harmful effects, the material may still be damaging to the health of the individual following ingestion, especially where pre-existing organ (e.
g.
■ Swallowing of the liquid may cause aspiration into the lungs with the risk of chemical pneumonitis; serious consequences may result. (ICSC13733).

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 .
■ Repeated exposure may cause skin cracking, flaking or drying following normal handling and use.
■ Skin contact with the material may damage the health of the individual; systemic effects may result following absorption.
■ 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 respiratory irritation (as classified using animal models).
Nevertheless inhalation of vapors, fumes or aerosols, especially for prolonged periods, may produce respiratory discomfort and occasionally, distress.
■ Inhalation of vapours may cause drowsiness and dizziness.
This may be accompanied by narcosis, reduced alertness, loss of reflexes, lack of coordination and vertigo.
■ Inhalation of aerosols (mists, fumes), generated by the material during the course of normal handling, may be damaging to the health of the individual.
■ Inhalation hazard is increased at higher temperatures.
■ The main effects of simple esters are irritation, stupor and insensibility.
Headache, drowsiness, dizziness, coma and behavioral changes may occur.

CHRONIC HEALTH EFFECTS

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
dibutyl adipate	105-99-7	>99

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. · If spontaneous vomiting appears imminent or occurs, hold patient's head down, lower than their hips to help avoid possible aspiration of vomitus.

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 contact occurs: · Immediately remove all contaminated clothing, including footwear · Flush skin and hair with running water (and soap if available).

INHALED
· If fumes or combustion products are inhaled remove from contaminated area. · Lay patient down. Keep warm and rested.

NOTES TO PHYSICIAN
■ Treat symptomatically.
Any material aspirated during vomiting may produce lung injury. Therefore emesis should not be induced mechanically or pharmacologically.
for simple esters:
----------BASIC TREATMENT

· Establish a patent airway with suction where necessary.
· Watch for signs of respiratory insufficiency and assist ventilation as necessary.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Not available
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	0.962

Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA
· Alcohol stable 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 (CO_2), 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:
Safety 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
· 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
• dibutyl adipate: CAS:105-99-7

PERSONAL PROTECTION




RESPIRATOR
•Type A Filter of sufficient capacity. (AS/NZS 1716 & 1715, EN 143:2000 & 149:2001, ANSI Z88 or national equivalent)

EYE
· Safety glasses with side shields
· Chemical goggles.

HANDS/FEET
■ Wear chemical protective gloves, eg. PVC.
For esters:
· Do NOT use natural rubber, butyl rubber, EPDM or polystyrene-containing materials.
Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include:
· 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, AS/NZS 2161.1 or national equivalent).
· 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, AS/NZS 2161.10.1 or national equivalent) 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, AS/NZS 2161.10.1 or national equivalent) 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.

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

ENGINEERING CONTROLS
■ Local exhaust ventilation usually required. 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	258.36
Melting Range (°F)	Not available	Viscosity	5.7 cSt@40°C
Boiling Range (°F)	581	Solubility in water (g/L)	Immiscible
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)	0.962
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	>1
Volatile Component (%vol)	Not available	Evaporation Rate	Not available

APPEARANCE
Clear oily liquid; does not mix with water. Essentially odourless. Saponification value = 420-440.

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

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY
· Presence of incompatible materials.
· Product is considered stable.

STORAGE INCOMPATIBILITY
· Esters react with acids to liberate heat along with alcohols and acids.
· Strong oxidizing acids may cause a vigorous reaction with esters that is sufficiently exothermic to ignite the reaction products.

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

Section 11 - TOXICOLOGICAL INFORMATION

dibutyl adipate

TOXICITY AND IRRITATION

DIBUTYL ADIPATE:

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

TOXICITY	IRRITATION
Oral (rat) LD50: 12900 mg/kg	Skin (rabbit):10 mg/24h(open)Mild
Intraperitoneal (rat) LD50: 5244 mg/kg	Skin (rabbit): 500 mg/24h - Mild
Dermal (rabbit) LD50: 20000 mg/kg	Eye (rabbit): 500 mg (open)
	Eye (rabbit): 500 mg/24h - Mild

■ 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, I-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-l) 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,O. 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-l), 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-l) 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-l) 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-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.

The material may be irritating to the eye, with prolonged contact causing inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis.

The material may cause skin irritation after prolonged or repeated exposure and may produce on contact skin redness, swelling, the production of vesicles, scaling and thickening of the skin.

for dibutyl adipate

Repeat dose toxicity: Dibutyl adipate was studied for oral toxicity in rats according to the 28-day repeated dose toxicity test [Japanese TG].

As the study was well controlled and conducted under GLP, it is regarded as a key study. Male and female SD rats were orally administered (gavage) at doses of 0, 20, 140 and 1,000 mg/kg/day. No test substance-related changes were noted in clinical observations, body weight gains, food consumption, and the findings obtained from haematology testing, blood chemical examination, urinalysis, and pathological examination. The NOAELs were considered to be 1,000 mg/kg/day in both sexes.
Reproductive and developmental; toxicity: In a combined repeat dose and reproductive/developmental toxicity screening test, salivation was observed in both sexes given 1,000 mg/kg/day. No test substance-related changes were noted in body weight gains, food consumption, findings obtained from haematology testing, blood chemical examination, urinalysis and pathological examination. For reproductive/developmental end-points, there were no adverse effects of this chemical on copulation, fertility, maintenance of pregnancy, parturition and lactation. In the 1,000 mg/kg group, pup weight on day 0 and 4 of lactation was slightly lower and viability on day 4 of lactation was decreased compared to those of the control group. However, there were no malformations which were considered to be induced by this chemical. Therefore, the NOEL was 300 mg/kg/day for repeated dose toxicity as well as 300 mg/kg/day for reproductive toxicity
Genotoxicity: Although dibutyl adipate showed positive result in chromosomal aberration test in vitro with metabolic activation, no genotoxic effects were observed in bacteria and no chromosomal aberration were observed in vitro without metabolic activation.
Foetotoxicity, specific developmental abnormalities recorded.

Section 12 - ECOLOGICAL INFORMATION

No data

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

dibutyl adipate (CAS: 105-99-7) is found on the following regulatory lists;
"Canada Domestic Substances List (DSL)","US Cosmetic Ingredient Review (CIR) Cosmetic ingredients found safe as used","US EPA Master Testing List - Index I Chemicals Listed","US Toxic Substances Control Act (TSCA) - Chemical Substance Inventory"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

■ Inhalation and/or skin contact may produce health damage*.
■ Repeated exposure potentially causes skin dryness and cracking*.
■ Vapours potentially cause drowsiness and dizziness*.
* (limited evidence).

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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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