

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.14

Revision Date 05.09.2024

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Dibutyl phthalate-3,4,5,6-d₄

Product Number : 34169

Brand : Sigma-Aldrich

Index-No. : 607-318-00-4

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration or the annual tonnage does not require a registration.

CAS-No. : 93952-11-5

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Scientific research and development

1.3

CHEMIKART

1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Reproductive toxicity, (Category 1B)	H360FD: May damage fertility. May damage the unborn child.
Short-term (acute) aquatic hazard, (Category 1)	H400: Very toxic to aquatic life.
Long-term (chronic) aquatic hazard, (Category 2)	H411: Toxic to aquatic life with long lasting effects.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H360FD	May damage fertility. May damage the unborn child.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P391	Collect spillage.
P405	Store locked up.
Supplemental Hazard Statements	none
	Restricted to professional users.

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word	Danger
Hazard Statements	
H360FD	May damage fertility. May damage the unborn child.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P405	Store locked up.
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

This substance/mixture contains components considered to have endocrine disrupting properties for environment , according to REACH Article 57(f), Commission Regulation (EU) 2018/605 or Commission Delegated Regulation (EU) 2017/2100.

Toxicological information:

This substance/mixture contains components considered to have endocrine disrupting properties affecting human health, according to REACH Article 57(f), Commission Regulation (EU) 2018/605 or Commission Delegated Regulation (EU) 2017/2100.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Di-n-butyl phthalate-d4
Di-n-butyl phthalate-d4

Formula : C₁₆D₄H₁₈O₄
Molecular weight : 282,37 g/mol
CAS-No. : 93952-11-5
EC-No. : 685-197-7
Index-No. : 607-318-00-4

Component		Classification	Concentration
Dibutyl phthalate-3,4,5,6-d4 Included in the Candidate List of Substances of Very High Concern (SVHC) according to Regulation (EC) No. 1907/2006 (REACH)			
CAS-No.	93952-11-5	Repr. 1B; Aquatic Acute 1; Aquatic Chronic 2; H360FD, H400, H411 M-Factor - Aquatic Acute: 1	<= 100 %
EC-No.	685-197-7		

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage**7.1 Precautions for safe handling****Advice on safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities**Storage conditions**

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 60 min

Material tested: KCL 741 Dermatril® L

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- a) Physical state liquid

b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	Melting point/ range: -35 °C - lit.
e) Initial boiling point and boiling range	340 °C - lit.
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	No data available
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient: n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	No data available
Relative density	No data available
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .
Stable

10.3 Possibility of hazardous reactions

Violent reactions possible with:
Strong oxidizing agents
Chlorine
Bases
nitrates
acids

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 6.279 mg/kg
(OECD Test Guideline 401)

Remarks: The value is given in analogy to the following substances: dibutyl phthalate
LC50 Inhalation - Rat - male and female - 4 h - $\geq$ 15,68 mg/l - aerosol

Remarks: (ECHA)

The value is given in analogy to the following substances: dibutyl phthalate
LD50 Dermal - Rabbit - $>$ 21.000 mg/kg

Remarks: (RTECS)

The value is given in analogy to the following substances: dibutyl phthalate

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: dibutyl phthalate

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h
(OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: dibutyl phthalate

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative
(OECD Test Guideline 406)

Remarks: The value is given in analogy to the following substances: dibutyl phthalate

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

The value is given in analogy to the following substances: dibutyl phthalate

Test Type: Micronucleus test
Species: Mouse

Application Route: Oral

Result: negative
Remarks: (ECHA)

The value is given in analogy to the following substances: dibutyl phthalate

Carcinogenicity

No data available

Reproductive toxicity

May damage the unborn child.
May damage fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment

This substance/mixture contains components considered to have endocrine disrupting properties affecting human health, according to REACH Article 57(f), Commission Regulation (EU) 2018/605 or Commission Delegated Regulation (EU) 2017/2100.

Components:

Dibutyl phthalate-3,4,5,6-d4:

Assessment

The substance is considered to have endocrine disrupting properties according to REACH Article 57(f) for human health.

Repeated dose toxicity - Rat - male and female - Oral - 90 d - NOAEL (No observed adverse effect level) - 152 mg/kg - LOAEL (Lowest observed adverse effect level) - 752 mg/kg

Remarks: Subchronic toxicity

The value is given in analogy to the following substances: dibutyl phthalate

Nausea, Dizziness, Headache

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Systemic effects:

Dizziness
Headache
conjunctivitis
somnolence

hallucinations
Coma
Symptoms may be delayed.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	static test LC50 - <i>Lepomis macrochirus</i> (Bluegill sunfish) - ca. 0,48 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: dibutyl phthalate
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - ca. 2,99 mg/l - 48 h (US-EPA) Remarks: The value is given in analogy to the following substances: dibutyl phthalate
Toxicity to algae	static test EC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - 0,75 mg/l - 10 d (US-EPA) Remarks: The value is given in analogy to the following substances: dibutyl phthalate static test NOEC - <i>Pseudokirchneriella subcapitata</i> (green algae) - 0,39 mg/l - 10 d (US-EPA) Remarks: The value is given in analogy to the following substances: dibutyl phthalate
Toxicity to bacteria	EC50 - <i>Tetrahymena pyriformis</i> - 2,2 mg/l - 24 h Remarks: (ECHA) The value is given in analogy to the following substances: dibutyl phthalate
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - <i>Oncorhynchus mykiss</i> (rainbow trout) - 0,1 mg/l - 99 d (US-EPA) Remarks: The value is given in analogy to the following substances: dibutyl phthalate
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	flow-through test NOEC - <i>Daphnia magna</i> (Water flea) - 0,158 mg/l - 21 d (OECD Test Guideline 211) Remarks: The value is given in analogy to the following substances: Bis(2-ethylhexyl) phthalate

12.2 Persistence and degradability

Biodegradability Result: 81 % - Readily biodegradable.
(Regulation (EC) No. 440/2008, Annex, C.4-C)
Remarks: The value is given in analogy to the following substances:
dibutyl phthalate

12.3 Bioaccumulative potential

Bioaccumulation Pimephales promelas (fathead minnow) - 11 d
- 0,0348 mg/l(Dibutyl phthalate-3,4,5,6-d4)

Bioconcentration factor (BCF): 2.165
Remarks: Does not bioaccumulate.
The value is given in analogy to the following substances: dibutyl
phthalate

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment : This substance/mixture contains components considered to have endocrine disrupting properties for environment , according to REACH Article 57(f), Commission Regulation (EU) 2018/605 or Commission Delegated Regulation (EU) 2017/2100.

Components:

Dibutyl phthalate-3,4,5,6-d4:

Assessment : The substance is considered to have endocrine disrupting properties according to REACH Article 57(f) for the environment.

12.7 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 3082

IMDG: 3082

IATA: 3082

14.2 UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Dibutyl phthalate-3,4,5,6-d4)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Dibutyl phthalate-3,4,5,6-d4)

IATA: Environmentally hazardous substance, liquid, n.o.s. (Dibutyl phthalate-3,4,5,6-d4)

14.3 Transport hazard class(es)

ADR/RID: 9

IMDG: 9

IATA: 9

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: yes

14.6 Special precautions for user

Tunnel restriction code : (-)

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

Authorisations and/or restrictions on use

REACH - Candidate List of Substances of Very High Concern for Authorisation (Article 59) : Dibutyl phthalate-3,4,5,6-d4

This product contains a substance listed on Annex XIV of the REACH Regulation (EC) Nr. 1907/2006.

Listed substance / Sunset Date : Dibutyl phthalate-3,4,5,6-d4 / 21.02.2015

After the sunset date the use of this substance requires either an authorization or can only be used for exempted uses, e.g. use in scientific research and development which includes routine analytics or use as intermediate.

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII) : Dibutyl phthalate-3,4,5,6-d4

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards E1 ENVIRONMENTAL HAZARDS

involving dangerous substances.

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements

H360FD	May damage fertility. May damage the unborn child.
H400	Very toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Details in analogy to the undeuterated compound.

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