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
CAS-No.: 93952-11-5

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

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Reproductive toxicity (Category 1B), H360
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 2), H411

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

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word: Danger

Hazard statement(s): May damage fertility or the unborn child.
Precautionary statement(s)
P201 Obtain special instructions before use.
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.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>Di-n-butyl phthalate-d4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C_{16}D_4H_{18}O_4</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>282.37 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>93952-11-5</td>
</tr>
<tr>
<td>Index-No.</td>
<td>607-318-00-4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibutyl phthalate-3,4,5,6-d4</td>
<td>Repr. 1B; Aquatic Acute 1; Aquatic Chronic 2; H360, H400, H411 M-Factor - Aquatic Acute: 10</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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. Chemisorb®). 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

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibutyl phthalate-3,4,5,6-d4</td>
<td>93952-11-5</td>
<td>TWA</td>
<td>5 mg/m3</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>5 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>5 mg/m3</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>5 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

8.2 Exposure controls

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

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 required

Body Protection protective clothing

Respiratory protection required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

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) Appearance Form: liquid
b) Odor No data available
c) Odor Threshold No data available
d) pH No data available
e) Melting point/freezing point Melting point/range: -35 °C (-31 °F) - lit.
f) Initial boiling point and boiling range 340 °C 644 °F - lit.
g) Flash point () No data available
h) Evaporation rate No data available
i) Flammability (solid, gas) No data available
j) Upper/lower flammability or explosive limits No data available
k) Vapor pressure No data available
l) Vapor density No data available
m) Density No data available
n) Relative density No data available
o) Water solubility No data available
p) Partition coefficient: n-octanol/water No data available
q) Autoignition temperature No data available
r) Decomposition temperature No data available
s) Viscosity No data available
s) Explosive properties  No data available

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
No data available

10.4 Conditions to avoid
No information available

10.5 Incompatible materials
Strong oxidizing agents

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)
LC50 Inhalation - Rat - male and female - 4 h - >= 15.68 mg/l - aerosol
Remarks: (ECHA)
LD50 Dermal - Rabbit - > 21,000 mg/kg
Remarks: (RTECS)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation - 72 h
(OECD Test Guideline 405)

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: negative  
(OECD Test Guideline 406)

**Germ cell mutagenicity**
Test Type: Ames test  
Test system: S. typhimurium  
Metabolic activation: with and without metabolic activation  
Result: negative  
Remarks: (ECHA)

Test Type: Micronucleus test  
Species: Mouse  
Application Route: Oral  
Result: negative

**Carcinogenicity**
IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**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**
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  
Nausea, Dizziness, Headache  
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.  
Stomach - Irregularities - Based on Human Evidence  
Stomach - Irregularities - Based on Human Evidence

**SECTION 12: Ecological information**

**12.1 Toxicity**
Toxicity to fish: static test LC50 - Lepomis macrochirus (Bluegill sunfish) - ca. 0.48 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates: static test EC50 - Daphnia magna (Water flea) - ca. 2.99 mg/l - 48 h (US-EPA)

Toxicity to algae:
- static test NOEC - Pseudokirchneriella subcapitata (green algae) - 0.39 mg/l - 10 d (US-EPA)
- static test EC50 - Pseudokirchneriella subcapitata (green algae) - 0.75 mg/l - 10 d (US-EPA)

Toxicity to bacteria: EC50 - Tetrahymena pyriformis - 2.2 mg/l - 24 h
Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates:
- flow-through test NOEC - Oncorhynchus mykiss (rainbow trout) - 0.1 mg/l - 99 d (US-EPA)
- Flow-through test NOEC - Daphnia magna (Water flea) - 0.158 mg/l - 21 d (OECD Test Guideline 211)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: Bis(2-ethylhexyl) phthalate

12.2 Persistence and degradability

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.

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties
No data available

12.7 Other adverse effects
Discharge into the environment must be avoided.
SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)
UN number: 3082  Class: 9  Packing group: III
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Dibutyl phthalate-3,4,5,6-d4)
Reportable Quantity (RQ): 10 lbs
Marine pollutant: yes  Poison Inhalation Hazard: No

IMDG
UN number: 3082  Class: 9  Packing group: III  EMS-No: F-A, S-F
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Dibutyl phthalate-3,4,5,6-d4)
Marine pollutant: yes
Marine pollutant: no

IATA
UN number: 3082  Class: 9  Packing group: III
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Dibutyl phthalate-3,4,5,6-d4)

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

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
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</thead>
<tbody>
<tr>
<td>Dibutyl phthalate-3,4,5,6-d4</td>
<td>93952-11-5</td>
<td>2007-07-01</td>
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</tbody>
</table>

SARA 311/312 Hazards
Chronic Health Hazard

Massachusetts Right To Know Components

<table>
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Pennsylvania Right To Know Components

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California Prop. 65 Components

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<tbody>
<tr>
<td>Dibutyl phthalate-3,4,5,6-d4</td>
<td>93952-11-5</td>
<td>2008-06-17</td>
</tr>
</tbody>
</table>

which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

SECTION 16: Other information

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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