

SAFETY DATA SHEET

Version 5.11
Revision Date 08/20/2018
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1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : *N*⁴-Benzoyl-5'-O-(4,4'-dimethoxytrityl)-2'-deoxycytidine

Product Number : 258504

Brand : Aldrich

CAS-No. : 67219-55-0

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
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Eye irritation (Category 2A), H319

Specific target organ toxicity - repeated exposure, Inhalation (Category 2), Central nervous system, Liver, Kidney, H373

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (Category 1), H410

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

Warning

Hazard statement(s)

H319

Causes serious eye irritation.

H373

May cause damage to organs (Central nervous system, Liver, Kidney) through prolonged or repeated exposure if inhaled.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P260

Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.

P264

Wash skin thoroughly after handling.

P273

Avoid release to the environment.

P280

Wear eye protection/ face protection.

| | |
|--------------------|--|
| P305 + P351 + P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P314 | Get medical advice/ attention if you feel unwell. |
| P337 + P313 | If eye irritation persists: Get medical advice/ attention. |
| P391 | Collect spillage. |
| P501 | Dispose of contents/ container to an approved waste disposal plant. |

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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

| | |
|------------------|---|
| Synonyms | : Bz-DMT-dC |
| Formula | : C ₃₇ H ₃₅ N ₃ O ₇ |
| Molecular weight | : 633.69 g/mol |
| CAS-No. | : 67219-55-0 |
| EC-No. | : 266-605-9 |

Hazardous components

| Component | Classification | Concentration |
|---|---|---------------|
| N-benzoyl-5'-O-(p,p'-dimethoxytrityl)-2'-deoxycytidine | | |
| | Eye Irrit. 2A; Aquatic Acute 1; Aquatic Chronic 1; H319, H410 | 90 - 100 % |
| Xylene | | |
| | Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; H226, H304, H315, H332, H335, H373, H401 | 1 - 5 % |

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature 2 - 8 °C

Storage class (TRGS 510): 6.1D: Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

| Component | CAS-No. | Value | Control parameters | Basis |
|-----------|-----------|--|----------------------|---|
| Xylene | 1330-20-7 | STEL | 150 ppm 655 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | C | 300 ppm | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | PEL | 100 ppm 435 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | TWA | 100 ppm 435 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | Remarks | The value in mg/m3 is approximate. | | |
| | | TWA | 100 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen | | |
| | | STEL | 150 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen | | |

Hazardous components without workplace control parameters

Biological occupational exposure limits

| Component | CAS-No. | Parameters | Value | Biological specimen | Basis |
|-----------|---------|--|-------------------|---------------------|---|
| | - | Methylhippuric acids | 1.5g/g creatinine | Urine | ACGIH - Biological Exposure Indices (BEI) |
| | Remarks | End of shift (As soon as possible after exposure ceases) | | | |

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES**9.1 Information on basic physical and chemical properties**

| | |
|---|--|
| a) Appearance | Form: solid Colour: white, to, yellow |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point: ca.204 °C (399 °F) at 1,013.25 hPa (760.00 mmHg) - (decomposition) |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | No data available |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | The product is not flammable. - Test N.1: Test method for readily combustible solids |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapour pressure | < 0.1 hPa (< 0.1 mmHg) at 20 °C (68 °F) - OECD Test Guideline 104 |
| l) Vapour density | No data available |
| m) Relative density | 1.26 g/cm ³ at 20 °C (68 °F) - OECD Test Guideline 109 |
| n) Water solubility | 0.0001 g/l at 20 °C (68 °F) - OECD Test Guideline 105 |
| o) Partition coefficient: n-octanol/water | log Pow: 5.3 at 20 °C (68 °F) - (calculated) - Potential bioaccumulation |
| p) Auto-ignition temperature | No data available |
| q) Decomposition temperature | ca.204 °C (399 °F) - |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY**10.1 Reactivity**

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Aluminum, Alkali metals, Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Skin corrosion/irritation

Serious eye damage/eye irritation

Respiratory or skin sensitisation

Germ cell mutagenicity

Carcinogenicity

IARC: No component 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 component 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

Specific target organ toxicity - single exposure

Specific target organ toxicity - repeated exposure

Aspiration hazard

Additional Information

RTECS: Not available

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence (Xylene)

12. ECOLOGICAL INFORMATION

12.1 Toxicity

12.2 Persistence and degradability

12.3 Bioaccumulative potential

12.4 Mobility in soil

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

UN number: 3077 Class: 9 Packing group: III EMS-No: F-A, S-F
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (N-benzoyl-5'-O-(p,p'-dimethoxytrityl)-2'-deoxycytidine)
Marine pollutant:yes

IATA

UN number: 3077 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (N-benzoyl-5'-O-(p,p'-dimethoxytrityl)-2'-deoxycytidine)

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.

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:

| | CAS-No. | Revision Date |
|--------|-----------|---------------|
| Xylene | 1330-20-7 | 1993-04-24 |

SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

:
Reportable Quantity F003 lbs

Massachusetts Right To Know Components

| | CAS-No. | Revision Date |
|--------|-----------|---------------|
| Xylene | 1330-20-7 | 1993-04-24 |

Pennsylvania Right To Know Components

| | CAS-No. | Revision Date |
|--|------------|---------------|
| N-benzoyl-5'-O-(p,p'-dimethoxytrityl)-2'-deoxycytidine | 67219-55-0 | 2009-07-17 |
| Xylene | 1330-20-7 | 1993-04-24 |

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

| | |
|-----------------|---|
| Acute Tox. | Acute toxicity |
| Aquatic Acute | Acute aquatic toxicity |
| Aquatic Chronic | Chronic aquatic toxicity |
| Asp. Tox. | Aspiration hazard |
| Eye Irrit. | Eye irritation |
| Flam. Liq. | Flammable liquids |
| H226 | Flammable liquid and vapour. |
| H304 | May be fatal if swallowed and enters airways. |

| | |
|-------------|--|
| H315 | Causes skin irritation. |
| H319 | Causes serious eye irritation. |
| H332 | Harmful if inhaled. |
| H335 | May cause respiratory irritation. |
| H373 | May cause damage to organs (/\$/*_2ORG_REP_INH/\$/) through prolonged or repeated exposure if inhaled. |
| H400 | Very toxic to aquatic life. |
| H401 | Toxic to aquatic life. |
| H410 | Very toxic to aquatic life with long lasting effects. |
| Skin Irrit. | Skin irritation |
| STOT RE | Specific target organ toxicity - repeated exposure |

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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