

SAFETY DATA SHEET

Version 6.4
Revision Date 04/14/2022
Print Date 06/01/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

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

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 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)**

Eye irritation (Category 2A), H319

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

Short-term (acute) aquatic hazard (Category 1), H400

Long-term (chronic) aquatic hazard (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.
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

SECTION 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

Component	Classification	Concentration
5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine		
	Eye Irrit. 2A; Aquatic Acute 1; Aquatic Chronic 1; H319, H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	<= 100 %

Xylene		
	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 3; H226, H332, H312, H315, H319, H335, H373, H304, H401, H412	>= 1 - < 5 %

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.

In case of skin contact

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

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

Water 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

Nitrogen oxides (NO_x)

Combustible.

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

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. 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: Avoid inhalation of dusts. 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

Storage stability

Recommended storage temperature

2 - 8 °C

Storage class

Storage class (TRGS 510): 13: Non Combustible Solids

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

Component	CAS-No.	Value	Control parameters	Basis
Xylene	1330-20-7	PEL	100 ppm 435 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)
		STEL	150 ppm 655 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
		TWA	100 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		
		STEL	150 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Xylene	1330-20-7	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

Change contaminated clothing. Wash hands 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

Handle with impervious gloves.

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 EN374 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: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatrill® L

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:KCL 741 Dermatril® L

Body Protection

protective clothing

Respiratory protection

required when dusts 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: solid Color: white, to, yellow
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point: ca.204 °C (ca.399 °F) at 1,013.25 hPa - (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) Vapor pressure	< 0.1 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	1.26 g/cm ³ at 20 °C (68 °F) - OECD Test Guideline 109
Relative density	No data available
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) Autoignition temperature	No data available

- q) Decomposition temperature ca.204 °C (ca.399 °F) -
r) Viscosity 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

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Aluminum, Alkali metals, 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

Acute toxicity estimate Oral - 2,522 mg/kg
(Calculation method)

LD50 Oral - Rat - female - > 2,000 mg/kg (5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)
(OECD Test Guideline 423)

Acute toxicity estimate Inhalation - 4 h - > 200 mg/l - vapor(Calculation method)

Acute toxicity estimate Dermal - > 5,000 mg/kg
(Calculation method)

Skin corrosion/irritation

Skin - reconstructed human epidermis (RhE) (5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)
Result: No irritation

(OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - Human (5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)

Result: Causes serious eye irritation.

(OECD Test Guideline 492)

Eyes - Bovine cornea (5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)

Result: non-corrosive - 4 h

(OECD Test Guideline 437)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse (5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)

Result: negative

(OECD Test Guideline 429)

Remarks: (in analogy to similar products)

The value is given in analogy to the following substances: 5'-O-(4,4'-dimethoxytriphenylmethyl)thymidine

Germ cell mutagenicity

Test Type: Ames test

(5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

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

No data available

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

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 0.61 mg/l - 48 h (5'-O-(4,4'-dimethoxytriphenylmethyl)-N ⁴ -benzoyl-2'-desoxycytidine) (OECD Test Guideline 202)
Toxicity to algae	static test NOEC - Pseudokirchneriella subcapitata (green algae) - >= 0.12 mg/l - 72 h (5'-O-(4,4'-dimethoxytriphenylmethyl)-N ⁴ -benzoyl-2'-desoxycytidine) (OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d (5'-O-(4,4'-dimethoxytriphenylmethyl)-N ⁴ -benzoyl-2'-desoxycytidine) Result: 0 % - Not biodegradable (OECD Test Guideline 301B)
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12.3 Bioaccumulative potential

No data available

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

No data available

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 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. (5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)
Marine pollutant : yes

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Marine pollutant : no

IATA

UN number: 3077 Class: 9

Packing group: III

Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (5'-O-(4,4'-dimethoxytriphenylmethyl)-N⁴-benzoyl-2'-desoxycytidine)

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. Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

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:

	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

No components are subject to the Massachusetts Right to Know Act.

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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