

MATERIAL SAFETY DATA SHEET

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

Product name : **5'-O-DMT-2'-deoxyguanosine (N-iBu)**
CAS-No. : 68892-41-1
Catalog : **CGIDDB-1103**
Synonyms : N2-Isobutyryl-5'-O-(4,4'-dimethoxytrityl)-2'-deoxyguanosine

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SECTION 2: HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008
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 Label elements
Labelling according Regulation (EC) No 1272/2008
Pictogram



Signal word none
Hazard statement(s)
H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)
P273 Avoid release to the environment.
P391 Collect spillage.
P501 Dispose of contents/ container to an approved waste disposal plant.

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.

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances
Synonyms : iBu-DMT-dG
Formula : C35H37N5O7
Molecular weight : 639,7 g/mol
CAS-No. : 68892-41-1
EC-No. : 272-615-4

Component	Classification	Concentration
5'-O-[Bis(4-methoxyphenyl)benzyl]-2'-deoxy-N-(2-methyl-1-oxopropyl)guanosine	Aquatic Chronic 2; H411	<= 100 %

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
Consult a physician. Show this safety data sheet to the doctor in attendance.
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
Flush eyes with water as a precaution.

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

SECTION 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
Carbon oxides, Nitrogen oxides (NO_x)
- 5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.
- 5.4 Further information
No data available

SECTION 6: ACCIDENTAL RELEASE MEASURES

- 6.1 Personal precautions, protective equipment and emergency procedures
Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. 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.

SECTION 7: HANDLING AND STORAGE

- 7.1 Precautions for safe handling
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. Store in cool place. Recommended storage temperature -20 °C

- 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

Components with workplace control parameters

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

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. 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.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | | |
|----|---|----------------------------|
| a) | Appearance | Form: powder Colour: white |
| b) | Odour | No data available |
| c) | Odour Threshold | No data available |
| d) | pH | No data available |
| e) | Melting point/freezing point | No data available |
| f) | Initial boiling point and boiling range | |
| | Melting point/range: 150 °C - dec. | 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 at 20 °C - OECD Test Guideline 104
- l) Vapour density No data available
- m) Relative density 1,28 g/cm³ at 20 °C - OECD Test Guideline 109
- n) Water solubility ca.2,4 g/l at 20 °C - OECD Test Guideline 105
- o) Partition coefficient: n-octanol/water log Pow: 2,98 at 20 °C - (calculated) - Bioaccumulation is not expected.
- p) Auto-ignition temperature No data available
- q) Decomposition temperature No data available
- 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

SECTION 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
Strong oxidizing agents
- 10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO_x)
Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: TOXICOLOGICAL INFORMATION

- 11.1 Information on toxicological effects
- Acute toxicity
LD50 Oral - Rat - female - > 2.000 mg/kg (OECD Test Guideline 423)
- Skin corrosion/irritation
Skin - reconstructed human epidermis (RhE)
Result: No skin irritation - 60 min
(OECD Test Guideline 439)
- Serious eye damage/eye irritation
Eyes - In vitro study
Result: No eye irritation - 6 h
(OECD Test Guideline 492)
- Respiratory or skin sensitisation
Germ cell mutagenicity
Ames test

Salmonella typhimurium

Result: negative

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.

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

Additional Information

RTECS: Not available

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

SECTION 12: ECOLOGICAL INFORMATION

12.1 Toxicity

No data available

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - 8,29 mg/l - 48 h (OECD Test Guideline 202)

static test NOEC - Daphnia magna (Water flea) - 5,35 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae

static test NOEC - Pseudokirchneriella subcapitata (green algae) - \geq 4,92 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 4,7 % - Not biodegradable (OECD Test Guideline 301B)

12.3 Bioaccumulative potential

No bioaccumulation is to be expected ($\log P_{ow} \leq 4$).

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 Other adverse effects

Toxic to aquatic life with long lasting effects. No data available

SECTION 13: DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

Dissolve or mix the material with a combustible solvent and burn in a chemical

incinerator equipped with an afterburner and scrubber. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. Contaminated packaging
Dispose of as unused product.

SECTION 14: TRANSPORT INFORMATION

- 14.1 UN number
ADR/RID: 3077 IMDG: 3077 IATA: 3077
- 14.2 UN proper shipping name
ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (5'-O-[Bis(4-methoxyphenyl)benzyl]-2'-deoxy-N-(2-methyl-1-oxopropyl)guanosine)
- IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (5'-O-[Bis(4-methoxyphenyl)benzyl]-2'-deoxy-N-(2-methyl-1-oxopropyl)guanosine)
- IATA: Environmentally hazardous substance, solid, n.o.s. (5'-O-[Bis(4-methoxyphenyl)benzyl]-2'-deoxy-N-(2-methyl-1-oxopropyl)guanosine)
- 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

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 safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.
- 15.2 Chemical safety assessment
For this product a chemical safety assessment was not carried out

SECTION 16. OTHER 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. ChemGenes (I) Pvt. Ltd. shall not be held liable for any damage resulting from handling or from contact with the above product.

-----End of MSDS-----