

Safety Data Sheet

#12068825 · Full 16-section SDS

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

PRODUCT	CAS NUMBER	FORMULA	VERSION	REVISION DATE
5-Iodo-2'-deoxycytidine	611-53-0	C9H12IN3O4	10	01 Sep 2026

SECTION 1

Identification

1.1 Product identifier

Product name 5-Iodo-2'-deoxycytidine

CAS number 611-53-0

EC / EINECS number 210-269-8

Chemical formula C9H12IN3O4

Molecular weight 353.12

SMILES C1[C@@H]([C@H](O[C@H]1N2C=C(C(=NC2=O)N)I)CO)O

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

For research use only, laboratory use, manufacture of chemicals. Not for human or animal use

1.3 Details of the supplier of the safety data sheet

Molekula Limited
1 Millennium Way, Newton Aycliffe
Durham, DL5 6JW, United Kingdom
info@molekula.com · +44 (0) 3302 000333

1.4 Emergency telephone number

0344 892 0111 — National Poisons Information Service (NPIS) (United Kingdom — for healthcare professionals (via TOXBASE))

SECTION 2

Hazard identification

2.1 Classification of the substance or mixture

Acute Tox. 4; H302

2.2 Label elements



WARNING

CODE	HAZARD STATEMENT
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H302	Harmful if swallowed
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CODE	PRECAUTIONARY STATEMENT
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P264	Wash thoroughly after handling
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P280	Wear protective gloves/protective clothing/eye protection/face protection
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P301+P330+P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting
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P501	Dispose of contents/container to an approved waste disposal plant
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2.3 Other hazards

Does not meet PBT or vPvB criteria under REACH Annex XIII. This product does not contain any known or suspected Endocrine disruptors.

SECTION 3

Composition / information on ingredients

3.1 Substances

Name	5-Iodo-2'-deoxycytidine
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CAS number	611-53-0
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EC number	210-269-8
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Concentration / purity	c. 100% 5-Iodo-2'-deoxycytidine (CAS:611-53-0): H302
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Classification according to Regulation (EC) No 1272/2008	Acute Tox. 4; H302
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Hazard statements	H302
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Acute toxicity estimate (ATE)	No data available
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Impurities / stabilising additives	None
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SECTION 4

First-aid measures

4.1 Description of first aid measures

Inhalation	Move to fresh air. Get medical attention if any discomfort continues.
Skin contact	Rinse skin with water. If skin irritation or rash occurs: get medical advice/attention.
Eye contact	Remove contact lenses if present. Rinse eyes with water. If eye irritation persists: get medical advice/attention.
Ingestion	Rinse mouth. Do NOT induce vomiting. Get medical advice/attention if you feel unwell.

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel. First aiders/ medical personnel need to protect themselves.

4.2 Most important symptoms and effects, both acute and delayed

See Section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5

Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media	For this substance/mixture no limitations of extinguishing agents are given.
Unsuitable extinguishing media	None known

5.2 Special hazards arising from the substance or mixture

Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Hydrogen iodide.

5.3 Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6

Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid breathing dust/fume/gas/mist/vapours/spray. Provide adequate ventilation. For personal protection, see section 8.

6.2 Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

6.3 Methods and material for containment and cleaning up

Collect spillage with shovel, broom or the like.

6.4 Reference to other sections

For specific precautions, see Section 8 and Section 13.

SECTION 7

Handling & storage

7.1 Precautions for safe handling

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Wash contaminated skin thoroughly after handling. Do not eat, drink or smoke when using this product. Remove contaminated clothing and laundry thoroughly before re-use.

7.2 Conditions for safe storage, including any incompatibilities

Storage temperature -15 to -20 °C

Conditions for safe storage (incompatibilities) Store in a dry place. Store in a closed container.

7.3 Specific end use(s)

See Section 1.2.

SECTION 8

Exposure controls / personal protection

8.1 Control parameters

Occupational exposure limits (OEL / WEL) *Not applicable*

DNEC/PNEC data *Not applicable*

8.2 Exposure controls

Eye / face protection Safety glasses
Wear eye/face protection as recommended. All eye/face protection should comply with EN ISO 16321-1:2022.

Skin / hand protection Nitrile gloves

Respiratory protection Dust mask (FFP2/FFP3)
Keep self-contained breathing apparatus readily available for emergency use. Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided. Respiratory equipment: Reusable Air-Purifying Respirator (APR). Filter type: ABEK. Standard: EN 14387.

Other protection *No data available*

Environmental exposure controls *No data available*

SECTION 9

Physical & chemical properties

9.1 Information on basic physical and chemical properties

Appearance / physical state	Solid DERIVED FROM: LITERATURE
Colour	White to off-white DERIVED FROM: LITERATURE
Odour	Odourless DERIVED FROM: LITERATURE
Melting / freezing point	180-185°C DERIVED FROM: LITERATURE
Boiling point	Not applicable
Flammability	No data available
Lower and upper explosion limit	No data available
Flash point	Not applicable
Auto-ignition temperature	Not applicable
Decomposition temperature	No data available
pH	Not applicable
Acidity	Neutral DERIVED FROM: LITERATURE
Kinematic viscosity	No data available
Solubility	Not applicable
Partition coefficient n-octanol/water (log value)	Not applicable
Vapour pressure	Not applicable
Density (g/mL)	1 g/mL DERIVED FROM: LITERATURE
Relative vapour density	No data available
Particle characteristics	No data available

9.2 Other information

No data available

SECTION 10

Stability & reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under the prescribed storage conditions

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat, sparks, flames.

10.5 Incompatible materials

Strong oxidising agents

10.6 Hazardous decomposition products

See section 5

SECTION 11

Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity (LD50 / LC50)	Information on hazard classes as defined in Regulation (EC) No 1272/2008 Acute Toxicity Estimate (ATE): LD50 > 300 mg/kg < 2000 mg/kg.
Skin corrosion / irritation	Based on available data, the classification criteria are not met
Eye corrosion / irritation	Based on available data, the classification criteria are not met
Respiratory / skin sensitisation	Based on available data, the classification criteria are not met
Carcinogenicity	Based on available data, the classification criteria are not met
Mutagenicity	Based on available data, the classification criteria are not met
Reproductive toxicity	Based on available data, the classification criteria are not met
STOT (single / repeated exposure)	Based on available data, the classification criteria are not met
Aspiration hazard	Based on available data, the classification criteria are not met

11.2 Information on other hazards

Not classified

SECTION 12

Ecological information

12.1 Toxicity

Not applicable

12.2 Persistence and degradability

Not applicable

12.3 Bioaccumulative potential

Not applicable

12.4 Mobility in soil

Not applicable

12.5 Results of PBT and vPvB assessment

Not applicable

12.6 Endocrine disrupting properties

See Section 11.2.

12.7 Other adverse effects

No data available

SECTION 13

Disposal considerations

13.1 Waste treatment methods

Dispose of in accordance with local/national regulations

SECTION 14

Transport information

14.1 UN number or ID number

Not applicable

14.2 UN proper shipping name

Not applicable

14.3 Transport hazard class(es)

Not applicable

14.4 Packing group

Not applicable

14.5 Environmental hazards

Not applicable

14.6 Special precautions for user

Special precautions for user *Not applicable*

Transport category *Not applicable*

Tunnel code *Not applicable*

Packing instruction (ADR) *Not applicable*

Packing instruction (IMDG) *Not applicable*

14.7 Maritime transport in bulk according to IMO instruments

No data available

SECTION 15

Regulatory information

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

Substance-specific regulations (e.g. licences) *No data available*

REACH code Y110

ECHA notification *Not applicable*

15.2 Chemical safety assessment

Not applicable

SECTION 16

Other information

Revision notes / other information

Previous SDS ver. 1 published 25th November 2022
Hazard classification and labelling according to Regulation (EC) 1272/2008
All eye/face protection should comply with EN ISO 16321-1:2022
Respiratory equipment: Reusable air-purifying respirator (APR)
Filter Type: ABEK
Standard: EN 14387
National Regulations:
-Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances
Other regulations, limitations and legal regulations:
-Directive 94/33/EC- The protection of young people at work

This Safety Data Sheet was generated automatically from the data Molekula holds against this product, in the 16-section GHS/CLP format. Fields shown as "No data available" carry no recorded value; fields shown as "Not applicable" were assessed as not relevant to this substance. For queries, contact Molekula at info@molekula.com.