

Safety Data Sheet

#90023219 · 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
Isophorone diisocyanate (IPDI)	4098-71-9	OCNC6H7(CH3)3CH2NCO	10	16 Oct 2026

SECTION 1

Identification

1.1 Product identifier

Product name	Isophorone diisocyanate (IPDI)
CAS number	4098-71-9
EC / EINECS number	223-861-6
Chemical formula	OCNC6H7(CH3)3CH2NCO
Molecular weight	222.28
SMILES	O=C=NCC1(C)CC(N=C=O)CC(C)(C)C1

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

Research and development, laboratory chemicals, manufacture of substances; not suitable for human consumption or veterinary purposes.

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

Skin Irrit. 2, H315
 Skin Sens. 1, H317
 Eye Irrit. 2, H319
 Acute Tox. 1 (inhalation), H330
 Resp. Sens. 1, H334
 STOT SE 3 (respiratory tract irritation), H335
 Aquatic Chronic 2, H411

2.2 Label elements



DANGER

CODE	HAZARD STATEMENT
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H317	May cause an allergic skin reaction
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H319	Causes serious eye irritation
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H330	Fatal if inhaled
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H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled
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H335	May cause respiratory irritation
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H411	Toxic to aquatic life with long lasting effects
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CODE	PRECAUTIONARY STATEMENT
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P260	Do not breathe dust/fume/gas/mist/vapours/spray
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P273	Avoid release to the environment
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P280	Wear protective gloves/protective clothing/eye protection/face protection
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P302+352	IF ON SKIN: Wash with soap and water
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P305+351+338	IF IN EYES: Rinse with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing
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P308+313	IF exposed or concerned: Get medical advice/attention
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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	Isophorone diisocyanate (IPDI)
CAS number	4098-71-9
EC number	223-861-6
Concentration / purity	c. 100%
Classification according to Regulation (EC) No 1272/2008	Skin Irrit. 2, H315 Skin Sens. 1, H317 Eye Irrit. 2, H319 Acute Tox. 1 (inhalation), H330 Resp. Sens. 1, H334 STOT SE 3 (respiratory tract irritation), H335 Aquatic Chronic 2, H411
Hazard statements	H317, H319, H330, H334, H335, H411
Acute toxicity estimate (ATE)	<i>No data available</i>
Impurities / stabilising additives	<i>Not applicable</i>

SECTION 4

First-aid measures**4.1 Description of first aid measures**

Inhalation	Remove person to fresh air and keep comfortable for breathing; immediately call a poison center/doctor; give artificial respiration if breathing stops (no mouth-to-mouth) and oxygen if breathing is difficult.
Skin contact	Immediately remove all contaminated clothing, rinse skin with water or shower, immediately call a poison center/doctor and transfer to hospital.
Eye contact	Remove contact lenses if present and rinse eyes with water for at least 15 minutes; seek medical attention.
Ingestion	Give water to drink (two glasses at most) and seek medical advice immediately; induce vomiting only in exceptional cases if no medical care within one hour and person is fully conscious; give activated charcoal; do not attempt to neutralise.

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

Inhalation may cause difficulty breathing, unconsciousness, possibly death; skin contact may cause unconsciousness, possibly death; severe eye irritation; ingestion may cause severe abdominal pain and internal injury.

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically; no special treatment required.

SECTION 5

Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media Carbon dioxide or dry powder.

Unsuitable extinguishing media Foam; water.

5.2 Special hazards arising from the substance or mixture

Toxic and combustible; combustion may liberate carbon monoxide, carbon dioxide, nitrous gases and other toxic gases; vapours are heavier than air and forms explosive mixtures with air on intense heating.

5.3 Advice for firefighters

Evacuate area, avoid breathing gas/fumes/vapours, cool heat-exposed containers with water spray and remove them if no risk is involved.

SECTION 6

Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid breathing dust/fume/gas/mist/vapours/spray, ensure adequate ventilation, avoid contact with skin and eyes and avoid dust formation; see section 8 for PPE.

6.2 Environmental precautions

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

6.3 Methods and material for containment and cleaning up

Absorb spillage with suitable absorbent material, collect with shovel or broom and reuse if possible; dispose of large amounts according to local authorities.

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

Work under hood, keep containers tightly closed, wear protective clothing, gloves, eye and face protection; avoid contact with skin and eyes and do not breathe dust/fume/gas/mist/vapours/spray.

7.2 Conditions for safe storage, including any incompatibilities

Storage temperature Ambient

Conditions for safe storage (incompatibilities) Store at room temperature in a dry place in a closed container under inert gas; moisture sensitive; storage class 6.1A (toxic).

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) UK EH40 WEL: TWA 0.02 mg/m³; STEL 0.07 mg/m³.

DNEC/PNEC data DNEL workers inhalation (local) chronic 45 µg/m³ and acute 45 µg/m³; PNEC freshwater 27 µg/l, intermittent freshwater 270 µg/l, marine water 400 ng/L, intermittent marine 40 µg/l, STP 10.6 mg/l, sediment freshwater 98.51 mg/kg dw, sediment marine 1.46 mg/kg dw, soil 19.8 mg/kg dw.

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 Butyl rubber gloves, thickness 0.7 mm, breakthrough time 8 hours; use gloves with long sleeves.

Respiratory protection Self-contained breathing apparatus
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 Use gloves with long sleeves; wash skin thoroughly after handling.

Environmental exposure controls Avoid discharge into drains.

SECTION 9

Physical & chemical properties**9.1 Information on basic physical and chemical properties**

Appearance / physical state Liquid
DERIVED FROM: LITERATURE

Colour Colourless
DERIVED FROM: LITERATURE

Odour Pungent
DERIVED FROM: LITERATURE

Melting / freezing point -60 °C
DERIVED FROM: LITERATURE

Boiling point 153 - 159 °C
DERIVED FROM: LITERATURE

Flammability *No data available*

Lower and upper explosion limit 0.7 - 4.5 %
DERIVED FROM: LITERATURE

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) 1.049 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

Forms explosive mixtures with air on intense heating.

10.2 Chemical stability

Not applicable

10.3 Possibility of hazardous reactions

Violent reactions possible with amides, amines, oxidising agents, ammonia, alkali hydroxides, alcohols, glycols, phenols, water and mercaptans (thiols).

10.4 Conditions to avoid

Not applicable

10.5 Incompatible materials

Not applicable

10.6 Hazardous decomposition products

Not applicable

SECTION 11

Toxicological information

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

Acute toxicity (LD50 / LC50) LD50 oral rat 4,814 mg/kg; LC50 inhalation rat 0.135 mg/l (4 h); LD50 dermal rat > 7,000 mg/kg.

Skin corrosion / irritation *Not applicable*

Eye corrosion / irritation	Irritating to eyes (rabbit); classification criteria not met based on available data.
Respiratory / skin sensitisation	Causes sensitisation (guinea pig maximization test). May cause an allergic skin reaction. May cause sensitisation by inhalation.
Carcinogenicity	<i>Not applicable</i>
Mutagenicity	<i>Not applicable</i>
Reproductive toxicity	<i>Not applicable</i>
STOT (single / repeated exposure)	Single exposure: May cause respiratory irritation
Aspiration hazard	<i>Not applicable</i>

11.2 Information on other hazards

Not applicable

SECTION 12

Ecological information

12.1 Toxicity

LC50 fish (Cyprinus carpio) >208 mg/l/96h; EC50 algae (Desmodesmus subspicatus) >70 mg/l/72h, NOEC 4.4 mg/l/72h; EC50 Daphnia magna 27 mg/l/48h; EC50 activated sludge 263 mg/l/3h.

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 contents/container in accordance with local/regional/national/international regulations.

SECTION 14

Transport information**14.1 UN number or ID number**

UN2290

14.2 UN proper shipping name

ISOPHORONE DIISOCYANATE

14.3 Transport hazard class(es)

6.1

**14.4 Packing group**

III

14.5 Environmental hazards*Not applicable***14.6 Special precautions for user**

Special precautions for user Tunnel restriction code: E; Transport category: 2; IMDG EmS F-A, S-A; IBC Instruction: IBC03.

Transport category 2

Tunnel code (E)

Packing instruction (ADR) P001

Packing instruction (IMDG) P001

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)**

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.

REACH code Y110

ECHA notification *Not applicable*

15.2 Chemical safety assessment

Not applicable

SECTION 16

Other information

Revision notes / other information

Version 2.1, issued 2026-02-03, replaces SDS dated 2024-08-30; full texts of hazard classes and H-statements (H315, H317, H319, H330, H334, H335, H411) listed.

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.