*According to Regulation (EC) No 1907/2006*

# 1,4-Dioxane

**Version number:** 2
**Issued:** 2023-08-16

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

### 1.1. Product identifier

***Trade name***
1,4-Dioxane

***CAS number***
123-91-1

***EC number***
204-661-8

***Synonyms***
1,4-Dioxane 1,4-Dioxacyclohexane

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

***Relevant identified uses***
Research and development.

***Not suitable for use in***
Not suitable for human consumption or veterinary purposes.

### 1.3. Details of the supplier of the safety data sheet

***Supplier***
Molekula Group

Street address
Molekula Ltd, Lingfield Way, Darlington,
DL1 4XX Darlington
United Kingdom

Telephone
+44 (0) 3302 000 333

Email
info@molekula.com

Web site
www.molekula.com

***Contact person***
Kevin Banks

***Email address***
+44 (0) 7769276927

### 1.4. Emergency telephone number

***Poison center/Additional emergency number***
0344 892 0111 - National Poisons Information Service (Newcastle Centre)

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

*Classification according to Regulation (EC) No 1272/2008*

***Classification***

Flammable gases, hazard Category 2
Carcinogenicity, hazard category 2
Serious eye damage, hazard category 1
Specific Target Organ Toxicity — Single exposure, hazard category 3

***Hazard statements***

H225, H319, H335, H351

***Supplemental hazard statements***

EUH019, EUH066

### 2.2. Label elements

*Labelling according to Regulation (EC) No 1272/2008*

***Hazard pictograms***

***Signal word***

Danger

***Hazard statements***

H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H351 Suspected of causing cancer.

***Supplemental hazard statements***

EUH019 May form explosive peroxides.
EUH066 Repeated exposure may cause skin dryness or cracking.

***Precautionary statements***

P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P261 Avoid breathing dust/fumes/gas/mist/vapours/spray.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313 IF exposed or concerned: Get medical advice/attention.
P337 + P313 If eye irritation persists: Get medical advice/attention.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.
P501 Dispose of contents/container to local regulations.

### 2.3. Other hazards

No data available

## SECTION 3: Composition/information on ingredients

### 3.2. Mixtures

| Chemical name | CAS No.<br>EC No.<br>REACH No.<br>Index No. | Concentration | Classification | H-phrase<br>M factor acute<br>M factor chronic | Note |
|---|---|---|---|---|---|
| 1,4-dioxane | 123-91-1<br>204-661-8<br>01-2119462837-26<br>603-024-00-5 | 100% | Flam. Liq. 2, Eye Irrit. 2, STOT SE 3 - resp. tract irrit., Carc. 1B | H225, H319, H335, H350<br>-<br>- | D |

***Molecular weight***

88.11

***Substance additional information***

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel.  NEVER MAKE AN UNCONSCIOUS PERSON VOMIT OR DRINK FLUIDS!

***Inhalation***

IF INHALED: Remove person to fresh air and keep comfortable for breathing. In case of persistent throat irritation or coughing: Seek medical attention and bring these instructions.

***Skin contact***
IF ON SKIN: Wash with plenty of water. Continue to rinse for at least 15 minutes and seek medical attention. Get medical advice/attention if you feel unwell.

***Eye contact***
Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

***Ingestion***
IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. Get medical advice/attention if you feel unwell.

***Information for doctors***
First aiders/ medical personnel need to protect themselves.

**4.2. Most important symptoms and effects, both acute and delayed**
The severity of the symptoms described will vary dependant of the concentration and the length of exposure.

***Inhalation***
Single exposure may cause the following adverse effects: Upper respiratory irritation. Difficulty in breathing.

***Skin contact***
Single exposure may cause the following adverse effects: Severe skin irritation.

***Eye contact***
Single exposure may cause the following adverse effects: Severe irritation.

***Ingestion***
Single exposure may cause the following adverse effects: Severe abdominal pain. Nausea, vomiting.

**4.3. Indication of any immediate medical attention and special treatment needed**
Treat symptomatically. No special treatment requirement.

## SECTION 5: Firefighting measures

**5.1. Extinguishing media**

***Suitable extinguishing media***
In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

***Unsuitable extinguishing media***
No specific fire fighting procedure given.

### 5.2. Special hazards arising from the substance or mixture

Specific hazards:
Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.
Carbon dioxide (CO2). Carbon monoxide (CO).
Corrosive vapours.

### 5.3. Advice for firefighters

***Special protective equipment for fire-fighters***

Evacuate area. Avoid breathing gas, fume, vapours or spray. Cool containers exposed to heat with water spray and remove container, 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. Provide adequate ventilation. Avoid contact with skin and eyes. Prevent the build up of electrostatic charge. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. 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 and reuse, if possible. Dispose of large amounts of spillage/waste according to agreement with local authorities.

### 6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

***Preventive handling precautions***

Dispose of contents/container as hazardous waste. Provide adequate ventilation. Use non-sparking tools. Do not handle until all safety precautions have been read and understood. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Protect from moisture. For precautions see section 2.2.

***General hygiene***

Observe good chemical hygiene practices. Do not eat, drink or smoke when using this product. Wash skin thoroughly after handling. Remove contaminated clothing and launder thoroughly before re-use.

### 7.2. Conditions for safe storage, including any incompatibilities

Store at ambient temperature. Store in a dry place. Store in a closed container. Ground container and transfer equipment to eliminate static electric sparks. Use explosion-proof electrical, ventilating and lighting equipment. Keep in original container. Protect from sunlight. Store in a well-ventilated place. Keep container tightly closed.

Incompatible materials:
oxidising agents halogens Reducing Agents. Water.

### 7.3. Specific end use(s)

No specific usage precautions noted.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

***Exposure limits***

TWA 20ppm 73 mg/m3 UK. EH40. WEL = Workplace Exposure Limit.
TWA 20ppm 73mg/m3 Europe Directive:  2009/161/EU

*DNEL/DMEL*

| Product/Substance name (CAS No./EC No.) | Type | Exposure | Value | Population | Effects |
|---|---|---|---|---|---|
| 1,4-dioxane (123-91-1/204-661-8) | DNEL | Chronic (long term) Inhalation | 144 mg/m³ | Workers | Systemic |
| 1,4-dioxane (123-91-1/204-661-8) | DNEL | Chronic (long term) Inhalation | 73 mg/kg bw/day | Workers | Systemic |
| 1,4-dioxane (123-91-1/204-661-8) | DNEL | Chronic (long term) Dermal | 21 mg/m³ | Workers | Systemic |

*PNEC/PEC*

| Product/Substance name (CAS No./EC No.) | Type | Environmental compartment | Value |
|---|---|---|---|
| 1,4-dioxane (123-91-1/204-661-8) | PNEC | Soil | 0.153 mg/kg |
| 1,4-dioxane (123-91-1/204-661-8) | PNEC | Marine water | 0.67 mg/l |
| 1,4-dioxane (123-91-1/204-661-8) | PNEC | Freshwater | 10 mg/l |
| 1,4-dioxane (123-91-1/204-661-8) | PNEC | Sediment (freshwater) | 37 mg/kg |
| 1,4-dioxane (123-91-1/204-661-8) | PNEC | Sewage Treatment Plant | 2700 mg/l |

| Product/Substance name (CAS No./EC No.) | Type | Environmental compartment | Value |
|---|---|---|---|
| 1,4-dioxane (123-91-1/204-661-8) | PNEC | Intermittent releases | 10 mg/l |

### 8.2. Exposure controls

***Eye / face protection***
Wear eye protection.

***Hand protection***
Wear protective gloves. Recommended gloves: Butyl rubber.
Glove Thickness: 0.7mm
Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

***Other skin protection***
Wash skin thoroughly after handling.

***Respiratory protection***
Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

***Environmental exposure controls***
Avoid discharge into drains.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

***Physical state***
Liquid

***Colour***
Colourless.

***Odour***
No data available

***Melting point / freezing point***
11.8 °C

***Boiling point or initial boiling point and boiling range***
100 - 102 °C

***Flammability***
No data available

***Lower and upper explosion limit***
Upper explosion limit: 22 %(V) Lower explosion limit: 2 %(V)

***Flash point***
11 °C
**Method**
CC (Closed cup).

***Auto-ignition temperature***
190.55 °C

***Decomposition temperature***
No data available

***pH***
6 - 8

***Kinematic viscosity***
1.27 mm2/s

***Viscosity, dynamic***
1.2 mPa.s

***Solubility***
1000 g/l

***Partition coefficient n-octanol/water***
log Pow: -0.42

***Vapour pressure***
36 hPa

***Density and/or relative density***
1.034 g/cm³

***Relative vapour density***
3.04

***Particle characteristics***
No data available

**9.2. Other information**
No data available

## SECTION 10: Stability and reactivity

**10.1. Reactivity**
Vapours may form explosive mixture with air at room temperature.

### 10.2. Chemical stability

Stable under the prescribed storage conditions.

### 10.3. Possibility of hazardous reactions

Risk of explosion with:
triethylaluminium
lithium aluminium hydride.
TRIETHYLAMINE
Boranes
silver perchlorate
Oxygen.
Nitric acid with perchloric acid.
Raney-nickel with Hydrogen.

Risk of ignition or formation of inflammable gases or vapours with: fire-promoting substances

Exothermic reaction with:
oxidising agents Acids.
sulfur trioxide

### 10.4. Conditions to avoid

Heating. Sources of ignition

### 10.5. Incompatible materials

Strong oxidising agents.

### 10.6. Hazardous decomposition products

Peroxides See section 5.

## SECTION 11: Toxicological information

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

***Acute toxicity***

| Product / Substance name<br>CAS / EC no. | Dose descriptor | Value / Dose | Exposure route | Test animals |
|---|---|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | LD50 | 5,150 mg/kg | Oral | Rat |
| 1,4-dioxane<br>123-91-1 / 204-661-8 | LD50 | 7,378 mg/kg | - | Rabbit |

***Skin corrosion/irritation***

| Product / Substance name<br>CAS / EC no. | Result | Duration of exposure | Species |
|---|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | No skin irritation. | 20 hours | Rabbit |

***Serious eye damage/irritation***

| Product / Substance name<br>CAS / EC no. | Result | Species |
|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | Causes eye irritation. | Rabbit |

***Respiratory or skin sensitisation***

| Product / Substance name<br>CAS / EC no. | Result | Species | Method / Guideline |
|---|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | Negative. | Guinea Pig | Maximization Test |

***Germ cell mutagenicity***

| Product / Substance name<br>CAS / EC no. | Result | Exposure route | Metabolic activation / Exposure | Species | Method / Guideline |
|---|---|---|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | Negative. | - | with and without metabolic activation | Salmonella typhimurium | Ames test |
| 1,4-dioxane<br>123-91-1 / 204-661-8 | Negative. | - | with and without metabolic activation | Chinese Hamster cells: Ovary | In vitro mammalian cell gene mutation test. |
| 1,4-dioxane<br>123-91-1 / 204-661-8 | Negative. | - | with and without metabolic activation | Chinese Hamster cells: Ovary | Chromosome aberration: In Vitro Test |
| 1,4-dioxane<br>123-91-1 / 204-661-8 | Negative. | Oral | - | Rat Liver. | unscheduled DNA synthesis assay |

***Carcinogenicity***

| Product / Substance name<br>CAS / EC no. | Other |
|---|---|
| 1,4-dioxane | Potentially carcinogenic to humans. |

| Product / Substance name<br>CAS / EC no. | Other |
|---|---|
| 123-91-1 / 204-661-8 | |

***STOT-single exposure***

| Product / Substance name<br>CAS / EC no. | Result |
|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | May cause respiratory irritation. |

***Aspiration hazard***

Based on available data, the classification criteria are not met.

### 11.2. Information on other hazards

No data available

## SECTION 12: Ecological information

### 12.1. Toxicity

***Acute algae toxicity***

| Product / Substance name<br>CAS / EC no. | Measurement type | Value / Result | Duration of exposure | Species |
|---|---|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | ErC50 | >1000 mg/l | 72 hours | Pseudokirchneriella subcapitata |

***Acute crustacean toxicity***

| Product / Substance name<br>CAS / EC no. | Measurement type | Value / Result | Duration of exposure | Species |
|---|---|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | EC50 | >1000 mg/l | 48 hours | Daphnia magna |

***Chronical toxicity***

| Product / Substance name<br>CAS / EC no. | Measurement type | Value / Result | Duration of exposure | Species |
|---|---|---|---|---|
| 1,4-dioxane | NOEC | 1000 mg/l | 21 days | Daphnia magna |

| Product / Substance name<br>CAS / EC no. | Measurement type | Value / Result | Duration of exposure | Species |
|---|---|---|---|---|
| 123-91-1 / 204-661-8 | | | | |
| 1,4-dioxane<br>123-91-1 / 204-661-8 | NOEC | 103 mg/l | 32 days | Pimephales promelas (Fat-head Minnow) |

### 12.2. Persistence and degradability

***Persistence and degradability***

| Product / Substance name<br>CAS / EC no. | Type of test | Duration | Result | Degradation |
|---|---|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | aerobic | 29 days | <10% | The product is not readily biodegradable. |

### 12.3. Bioaccumulative potential

***Bioaccumulative potential***

| Product / Substance name<br>CAS / EC no. | Bioconcentration factor (BCF) | Result | Species |
|---|---|---|---|
| 1,4-dioxane<br>123-91-1 / 204-661-8 | 0.3-0.7 | 10 mg/l | Cyprinus carpio (Common carp) |

### 12.4. Mobility in soil

No data available

### 12.5. Results of PBT and vPvB assessment

No data available

### 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

***Disposal considerations***

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

*According to Regulation (EC) No 1907/2006*

# 1,4-Dioxane

**Version number:** 2
**Issued:** 2023-08-16

## SECTION 14: Transport information

### 14.1. UN number

1165

### 14.2. UN proper shipping name

***ADR / RID / ADN proper shipping name***

DIOXANE

***IMDG proper shipping name***

DIOXANE

***IATA proper shipping name***

Dioxane

### 14.3. Transport hazard class(es)

***Label***

ADR/RID/ADN


*3*

IMDG


*3*

IATA


*3*

***ADR / RID Class***

3

***ADR / RID Classification code***

F1

***ADR / RID hazard identification number***

33

***IMDG Class***

3

***IATA Class***
3

***ADN Class***
3

***ADN Class Code***
F1

**14.4. Packing group**
ADR / RID / ADN: II
IMDG: II
IATA: II

**14.5. Environmental hazards**
***IMDG EmS***
F-E, S-D

**14.6. Special precautions for user**
Tunnel restriction code: D/E
Transport category: 2

**14.7. Maritime transport in bulk according to IMO instruments**
IBC Instruction: IBC02

## SECTION 15: Regulatory information

**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**
***EU regulations***
This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

***National regulations***
No data available

**15.2. Chemical safety assessment**
No data available

## SECTION 16: Other information

***Phrase meaning***

Flam. Gas 2 - Flammable gases, hazard Category 2
Carc. 2 - Carcinogenicity, hazard category 2
Eye Dam. 1 - Serious eye damage, hazard category 1
STOT SE 3 - Specific Target Organ Toxicity — Single exposure, hazard category 3
Flam. Liq. 2 - Flammable liquids, hazard category 2
Eye Irrit. 2 - Eye irritation, hazard category 2
STOT SE 3 - resp. tract irrit. - Specific Target Organ Toxicity — Single exposure, hazard category 3 - respiratory tract irritation
Carc. 1B - Carcinogenicity, hazard category 1B
H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H350 May cause cancer.
H351 Suspected of causing cancer.
EUH019 May form explosive peroxides.
EUH066 Repeated exposure may cause skin dryness or cracking.