

# Safety Data Sheet

## SECTION 1: Identification of the substance and of the company

### 1.1 Product identifier

NAME: 1,4-Dioxane-2,2,3,3,5,5,6,6-d8

PRODUCT CODE: AS-75447

CAS No: 17647-74-4

Synonyms/Tradenames:

IUPAC Name: 1,4-Dioxane-2,2,3,3,5,5,6,6-d8

MDL No: MFCD00044239

EINECS No:

REACH No: A REACH registration number is not available for this substance as the substance or its uses are exempted from registration. The annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

Identified Use: Research and Development

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

Key Organics Limited

Highfield Road Industrial Estate  
Camelford  
Cornwall PL32 9RA UKTel: +44(0)1840 212171  
Fax: +44(0)1840 213712  
Email: enquiries@keyorganics.net

### 1.4 Emergency telephone number

+44(0)1840 212137 between the hours 9am to 5pm Monday to Friday.

## SECTION 2: Hazard Identification

### 2.1 GHS Classification of the substance or mixture

(Classification according to Regulation (EC) No 1272/2008 [EU-GHS/CLP])

Flammable liquids (Category 2)

Acute toxicity, oral (Category 4)

Serious eye damage/eye irritation (Category 2A)

Specific target organ toxicity, single exposure; Respiratory tract irritation (Category 3)

Skin corrosion/irritation (Category 2)

Acute toxicity, inhalation (Category 4)

Carcinogenicity (Category 1B)

### 2.2 Label elements

(Labelling according to Regulation (EC) No 1272/2008 [EU-GHS/CLP])

Signal Word: Danger



#### Hazard Statements:

H225 Highly flammable liquid and vapour.

H302 Harmful if swallowed.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H350	May cause cancer.

**Precautionary Phrases:**

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P240	Ground/bond container and receiving equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
P264	Wash hands thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell. Rinse mouth.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of water. Call a POISON CENTRE/Doctor if you feel unwell.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P308 + P313	IF exposed or concerned: Get medical advice/attention.
P332 + P313	If skin irritation occurs: Get medical advice/attention.
P337 + P313	If eye irritation persists: Get medical advice/attention.
P362	Take off contaminated clothing and wash before reuse.
P402 + P404	Store in a dry place. Store in a closed container.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store it locked up.
P501	Dispose of contents/container to an approved waste disposal plant.

**2.3 Other Hazards**

Test for peroxide formation periodically and before distillation.

**SECTION 3: Composition/Information on ingredients****3.1 Substances**

AS-75447: 17647-74-4 1,4-Dioxane-2,2,3,3,5,5,6,6-d8  
MF: C4D8O2 MW: 96.1550

**3.2 Mixtures**

Not relevant.

**SECTION 4: First Aid Measures****4.1 Description of the first aid measures**

Skin Contact	Remove any contaminated clothing and shoes. Wash with plenty of soap and water.If skin irritation occurs: Get medical advice/attention.
Eye Contact	Hold eyelids open and rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation or visual changes persists: Get medical advice/attention.
Ingestion	Do not induce vomiting. If victim is conscious and alert, give 1-2 glasses of water to wash out mouth thoroughly. Do not give anything by mouth to an unconscious person. Get medical advice/attention. Do not leave victim unattended.

**Inhalation**

If respiratory irritation or distress occurs, remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical advice/attention if respiratory irritation or distress continues.

**4.2 Most important symptoms and effect, both acute and delayed**

To the best of our knowledge the acute and delayed symptoms and effects of this substance are not fully known.

**4.3 Indication of any immediate medical attention and special treatment needed**

Call a POISON CENTRE or doctor/physician if you feel unwell.  
No additional measures required.

**SECTION 5: Firefighting Measures****5.1 Extinguishing media****Suitable:**

Carbon Dioxide  
Dry Chemical Powder  
AFFF  
Water

**Unsuitable:**

Do not use water with a full water jet.

**5.2 Special hazards arising from the substance or mixture**

In combustion toxic fumes may form.

**5.3 Advice for fire fighters**

Wear protective clothing to prevent contact with skin and eyes.  
Wear self-contained breathing apparatus.

**SECTION 6: Accidental Release Measures****6.1 Personal precautions, protective equipment and emergency procedures.**

Refer to section 8 of SDS for personal protection details.

**6.2 Environmental precautions.**

Do not discharge into rivers and drains.

**6.3 Methods and materials for containment and cleaning up**

Mix with sand or vermiculite, transfer to suitable container and arrange disposal by approved disposal specialists.

**SECTION 7: Handling and Storage****7.1 Precautions for safe handling****Safe handling:**

Do not store, use, and/or consume foods, beverages, tobacco products or cosmetics in areas where this material is stored.  
Wash hands and face carefully before eating, drinking, using tobacco or applying cosmetics in areas where this material is stored.  
Handle in BS approved adequately ventilated fume cupboard.  
Wash exposed skin promptly to remove accidental splashes of contact with this material.  
Remove and thoroughly wash any clothing if spillage occurs.

**Protection against explosions and fires:**

Undertake normal measures for fire protection.  
Minimal explosion risk.

**7.2 Conditions for safe storage, including any incompatibilities****Managing storage risks:**

Keep container tightly closed, store in cool, well ventilated area.

**Storage controls:**

No special requirements

**Maintaining integrity:**

Keep in tightly closed container in a cool area away from direct sunlight or heat sources.

**Further information about storage conditions:**

Store in well ventilated place. Keep container tightly closed.

**7.3 Specific end use(s)**

The end use(s) have not been fully determined. The substance is supplied for Research and Development purposes only and should be handled by appropriately trained professionals only.

**SECTION 8: Exposure Controls/Personal Protection**

## 8.1 Control parameters

No data available.

## 8.2 Exposure controls

General protective & hygiene measures:

Wear protective gloves/protective clothing/eye protection/face protection. The standard precautionary measures should be adhered to when handling this material. Wash hands during breaks and at the end of handling the material. Remove immediately any contaminated clothing or footwear and either wash thoroughly or dispose of in hazardous waste.

Engineering measures:

Set up hand-wash station and eye station near work area.  
General area dilution/exhaust ventilation.  
Use only in a BS approved fume cupboard or in a well ventilated area.

Eye/face protection:

Safety glasses (NIOSH(US) or EN 166(EU)) and/or full face visor if handling large amounts.

Hand protection:

Suitable protective gloves or gauntlets satisfying EU Directive 89/686/EEC and the standard EN374 derived from it.

Respiratory protection:

Avoid breathing dust, fumes, gas, mist, vapours or sprays. For low level exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABE1P3D (EU EN 143) respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Skin protection:

Protective clothing and gloves or gauntlets.

Other personal protection advice::

No data.

## SECTION 9: Physical and Chemical Properties

### 9.1 Physical and chemical properties

Appearance/form:	
Molecular formula:	C4D8O2
Molecular weight:	96.16
Odour:	No data available
Odour threshold:	No data available
pH:	No data available
Melting/Boiling point (°C):	BP: 99 °C - lit
Flash point:	5 °C - closed cup
Evaporation rate:	No data available
Flammability (solid,gas):	No data available
Upper/lower explosive limits:	No data available
Vapour pressure:	No data available
Vapour density:	No data available
Relative density:	1.129 g/cm3 at 25 °C - lit
Solubility(ies):	No data available
Partition coefficient:	No data available
Auto ignition temperature:	No data available
Decomposition temperature:	No data available
Viscosity:	No data available
Explosive properties:	No data available
Oxidising properties:	No data available

### 9.2 Other information

No other information is available.

## SECTION 10: Stability and Reactivity

### 10.1 Reactivity

Formation of peroxides possible.  
Vapors may form explosive mixture with air.

### 10.2 Chemical stability

Stable under normal conditions as stated in section 7.

### 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:  
Oxidizing agents  
Sulfur trioxide  
acids

### 10.4 Conditions to avoid

Protect against heat, moisture

### 10.5 Incompatible materials

Avoid contact with strong acids, bases, oxidising and reducing agents.

### 10.6 Hazardous decomposition products

Peroxides

## SECTION 11: Toxicology Information

All the data contained in this section is derived from actual test data unless otherwise stated.

### 11.1 Information on toxicology effects

Acute toxicity:	LD50 Oral - Rat - male and female - 5,150 mg/kg (OECD Test Guideline 401) Remarks: The value is given in analogy to the following substances: 1,4-Dioxane Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract, Lung edema LD50 Dermal - Rabbit - 7,378 mg/kg Remarks: (RTECS) The value is given in analogy to the following substances: 1,4-Dioxane
Skin corrosion/irritation:	Causes skin irritation.
Serious eye damage/irritation:	Causes serious eye irritation.
Respiratory or skin sensitisation:	Maximization Test - Guinea pig Result: negative (Regulation (EC) No. 440/2008, Annex, B.6) Remarks: The value is given in analogy to the following substances: 1,4-Dioxane No data available.
Germ cell mutagenicity:	No data available.
Carcinogenicity:	Presumed to have carcinogenic potential for humans
Reproductive toxicity:	No data available.
STOT single exposure:	Inhalation - May cause respiratory irritation.
STOT repeated exposure:	No data available.
Aspiration hazard:	No data available.
Signs and Symptoms of Exposure:	No data available.

### 11.2 Additional Information

Repeated dose toxicity - Rat - male - Oral - 716 Days - NOAEL (No observed adverse effect level) - 9.6 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: 1,4-Dioxane

Nausea, Vomiting, Weakness, Dizziness, Vertigo, Headache, Sweating, loss of appetite, Kidney injury may occur., Liver injury may occur.

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

The substance has delayed effects.

After absorption:

Headache

Dizziness

Nausea

Vomiting

Absorption can result in damage to:

Liver

Kidney

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

## SECTION 12: Ecological Information

All the data contained in this section is derived from actual test data unless otherwise stated.

### 12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 - Daphnia magna (Water flea) - > 1,000 mg/l- 48 h

(OECD Test Guideline 202)

Remarks: The value is given in analogy to the following substances:

1,4-Dioxane

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata (green algae) - >

1,000 mg/l - 72 h

(OECD Test Guideline 201)

Remarks: The value is given in analogy to the following substances:

1,4-Dioxane

Toxicity to fish(Chronic toxicity)

flow-through test NOEC - Pimephales promelas (fathead minnow) - >

103 mg/l - 32 d

Remarks: (ECHA)

The value is given in analogy to the following substances: 1,4-

Dioxane

Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)

NOEC - Daphnia magna (Water flea) - 1,000 mg/l - 21 d

(OECD Test Guideline 211)

Remarks: The value is given in analogy to the following substances:

1,4-Dioxane

### 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 29 d

Result: < 10 % - Not readily biodegradable.

(OECD Test Guideline 301F)

Remarks: The value is given in analogy to the following substances:

1,4-Dioxane

### 12.3 Bioaccumulative potential

Bioaccumulation Cyprinus carpio (Carp) - 10 mg/l(Octadeuterodioxane)

Bioconcentration factor (BCF): 0.3 - 0.7

(OECD Test Guideline 305C)

Remarks: The value is given in analogy to the following substances:

1,4-Dioxane

### 12.4 Mobility in soil

No data available.

### 12.5 Results of PBT and vPvB assessment

No data available.

### 12.6 Other adverse effects

Forms toxic mixtures in water, dilution measures notwithstanding.

Discharge into the environment must be avoided.

## SECTION 13: Disposal Considerations

### 13.1 Waste treatment methods

Disposal considerations:

Consult state, local or national regulations for proper disposal.

Disposal of packaging:

Disposal must be made according to official regulations.

## SECTION 14: Transport Information

### 14.1 UN number

1165

### 14.2 UN proper shipping name

DIOXANE

### 14.3 Transport class(es)

3

### 14.4 Packaging group

II

### 14.5 Environmental hazards

Air (ICAO/IATA): No

Road (ADR/RID): No

Sea (IMDG): No

### 14.6 Special precautions for user

Air (ICAO/IATA): No data available

Road (ADR/RID): Tunnel restriction code : (D/E)

Sea (IMDG): No data available

## SECTION 15: Regulatory Information

### 15.1 Safety, health and environmental regulations

Product is not subject to any additional regulations or provisions. This datasheet complies with the requirements of regulations (EC) No. 1907/2006.

### 15.2 Chemical safety assessment

No chemical safety assessment under Regulation (EC) 1907/2006 is required and has not been carried out.

## SECTION 16: Other Information

Date of Previous SDS: 02 January 2024

Date of Revision: 05 January 2024

List of abbreviations used within SDS:

ADR: Accord European sur le transport des marchandises Dangereuses par Route (European Agreement concerning the international Carriage of Dangerous Goods by road).

RID: Reglement International concernant le transport des marchandises par chemin de fer (Regulations concerning the International transport of Dangerous Goods by Rail).

IMDG: International Maritime Code of Dangerous goods.

IATA: International Air Transport Association.

IATA-DGR: Dangerous Goods Regulations by the International Air Transport Association.

ICAO: International Civil Aviation Organisation.

ICAO-IT: Technical Instructions by the ICAO.

GHS: Globally Harmonised System of Classification and Labelling of Chemicals.

CAS: Chemical Abstracts Service.

IUPAC: International Union for Pure and Applied Chemistry.

MDL: Molecular Design Ltd

EINECS: European Inventory of Existing Commercial Chemical Substances.

EPA: European Protection Agency.

IARC: International Agency on Research on Cancer.

NTP: National Toxicology Program.

OSHA: Occupational Safety and Health Administration.

ACGIH: American Conference of Industrial Hygienists.

## Disclaimer

The information in this Safety Data Sheet is correct to the best of our knowledge at the date of publication. However, the information given should be considered only as a guide. The product listed is for research and development purposes only and not for human or animal use. As such the toxicological, ecological and physiochemical properties have not been fully investigated or determined and the product should be treated with respect and always handled under suitable conditions by suitably qualified personnel. The responsible party shall use this datasheet only in conjunction with other sources of information gathered by them, and should make an independent judgement of suitability, to ensure proper use and protect the health and safety of employees. This Safety Data Sheet is not intended to be a replacement of any statutory assessments required to be completed by the user. This information is furnished without warranty and any use of the product not in conformance with this Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Key Organics Ltd. cannot accept liability for any loss, damage or injury which may result from the use of this product.

## **End of SDS**