Safety Data Sheet

SECTION 1: Identification of the substance and of the company

1.1 Product identifier

NAME: (3aR,4R,7S,7aS)-2-(((1R,2R)-2-((4-(Benzo[d]isothiazol-3-yl)piperazin-1-yl)methyl)cyclohexyl)methyl)hexahydro-1H-4,7-methanoisoindole-1,3(2H)-dione

PRODUCT CODE:	BS-50765
CAS No:	1318074-25-7
Synonyms/Tradenames:	
IUPAC Name:	(3aR,4R,7S,7aS)-2-(((1R,2R)-2-((4-(Benzo[d]isothiazol-3-yl)piperazin-1-yl)methyl)cyclohexyl)methyl)hexahydro-1H-4,7-methanoisoindole-1,3(2H)-dione
MDL No:	MFCD28404650
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 UK

Tel: +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])

Acute toxicity,inhalation (Category 4)

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)

2.2 Label elements

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

Signal Word: Warning

Hazard Statements:

H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.

Precautionary Phrases:

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 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTRE/Doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
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.
P411	Store at temperatures not exceeding 4°C.
P501	Dispose of contents/container to an approved waste disposal plant.

2.3 Other Hazards

No Information Available

SECTION 3: Composition/Information on ingredients

3.1 Substances

BS-50765: 1318074-25-7 (3aR,4R,7S,7aS)-2-(((1R,2R)-2-((4-(Benzo[d]isothiazol-3-yl)piperazin-1-yl)methyl)cyclohexyl)methyl)hexahydro-1H-4,7-methanoisoindole-1,3(2H)-dione

MF: C28H36N4O2S MW: 492.6800

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 respiatory 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 treament needed

Call a POISON CENTRE or doctor/physican 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 accidential 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:	Store at 4°C
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 diluation/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:	White to Off-white Solid
Molecular formula:	C28H36N4O2S
Molecular weight:	492.68
Odour:	No data available
Odour threshold:	No data available
pH:	No data available
Melting/Boiling point (°C):	
Flash point:	No data available
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:	No data available
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

No unusual reactivity.

10.2 Chemical stability

Stable under normal conditions as stated in section 7.

10.3 Possibility of hazardous reactions

No hazardous reactions known.

10.4 Conditions to avoid

No specific conditions to avoid.

10.5 Incompatible materials

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

10.6 Hazardous decomposition products

In combustion emits toxic fumes.

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:	No data available.
Skin corrosion/irritation:	Causes skin irritation.
Serious eye damage/irritation:	Causes serious eye irritation.
Respiratory or skin sensitisation:	No data available.
Germ cell mutagenicity:	No data available.
Carcinogenicity:	No data available.
Reproductive toxicity:	No data available.
STOT single exposure:	No data available.
STOT repeated exposure:	No data available.
Aspiration hazard:	No data available.
Signs and Symptoms of Exposure:	No data available.

11.2 Additional Information

To the best of our knowledge the acute and chronic toxicity of this substance is not fully known. The substance is for R&D purposes only and has not been fully characterised. The substance should only be handled by suitably trained professionals.

SECTION 12: Ecological Information

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

12.1 Toxicity

No data available.

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

No data available.

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

No data available.

12.6 Other adverse effects

No data available.

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

No data availble

14.2 UN proper shipping name

No data availble

14.3 Transport class(es)

No data availble

14.4 Packaging group

No data availble

14.5 Environmental hazards

Air (ICAO/IATA): No data available

Road (ADR/RID): No data available

Sea (IMDG): No data available

14.6 Special precautions for user

Air (ICAO/IATA): No data available

Road (ADR/RID): No data available

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:

Date of Revision: 28 March 2022

List of abbreviations used within SDS:

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