



SAFETY DATA SHEET

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

1.1 Product identifiers

Product Name: Hexahydro-3-(3-hydroxyphenyl)-1-methyl-2H-azepin-2-one
CAS Number: 71592-44-4
Catalog number: NC427438

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

Identified uses: All chemicals from NewCan Biotech are for laboratory or manufacturing use only, not for drug, food and household use.

1.3 Details of the supplier of the safety data sheet

NewCan Biotech Limited
Email: sales@newcanbio.com
Tel: 0086-571-86912261

1.4 Emergency telephone number

Emergency Phone: 0086-571-86912261

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008
No Resource File

2.2 GHS Label elements, including precautionary statements

Pictogram 
Signal word
Hazard statement(s)
Precautionary statement(s)

2.3 Other hazards

None

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : 3-(3-hydroxyphenyl)-1-methylazepan-2-one
Formula : C₁₃ H₁₇ N O₂
Molecular weight : 219.28g/mol
CAS-No. : 71592-44-4

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.



Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO_x), silicon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.

Evacuate personnel to safe areas.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Normal measures for preventive fire protection.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

Containers which are opened must be carefully resealed and kept upright to prevent leakage.



Moisture sensitive. Store under nitrogen.

Storage class (TRGS 510): Combustible liquids not in Storage Class 3

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166 (EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use (US) or type ABEK (EN14387) respirator cartridges as a backup to enginee protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance	No data available
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	192-193°C
f) Initial boiling point and boiling range	No data available
g) Flash point	No data available
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available



j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	1.128
o) Partition coefficient: noctanol/water	No data available
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Acids, Bases, Alcohols, Strong oxidizing agents, Material generates methanol on contact with water or moisture

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO_x), silicon oxides

Other decomposition products - No data available

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

No data available

Carcinogenicity



IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

No data available

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

Material may form a siloxane polymer on the skin, eyes, or in the lungs. If tissues, seek medical attention.

SECTION 12: Ecological information

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

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product

SECTION 14: Transport information

14.1 UN number

ADR/RID:

IMDG:

IATA:

14.2 UN proper shipping name

ADR/RID: Hexahydro-2,2,2-trihydroxyphenyl-1-methyl-2H-pyran



ADR/RID: Hexahydro-3-(3-hydroxyphenyl)-1-methyl-2H-azepin-2-one
IMDG: Hexahydro-3-(3-hydroxyphenyl)-1-methyl-2H-azepin-2-one
IATA: Hexahydro-3-(3-hydroxyphenyl)-1-methyl-2H-azepin-2-one

14.3 Transport hazard class(es)

ADR/RID:	IMDG:	IATA:
----------	-------	-------

14.4 Packaging group

ADR/RID:	IMDG:	IATA:
----------	-------	-------

14.5 Environmental hazards

ADR/RID:	IMDG Marine pollutant:	IATA:
----------	------------------------	-------

14.6 Special precautions for user

No data available

SECTION 15: Regulatory information

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

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

Further information

Copyright 2023 NEWCAN BIOTECH LIMITED. License granted to make unlimited paper copies for internal use only. The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. NEWCAN BIOTECH LIMITED shall not be held liable for any damage resulting from handling or from contact with the above product. See www.newcanbio.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.