

Safety Data Sheet

according to UK REACH Regulation

(+)-McN 5652 Thiobutyrate

Revision date: 23.05.2022

Product code: 4360

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

(+) -McN 5652 Thiobutyrate

Further trade names

Butanethioic acid, S-[4-(1,2,3,5,6,10b-hexahydropyrrolo[2,1-a]isoquinolin-6-yl)phenyl] ester, trans-(+), (2R,3R)-2,3-dihydroxybutanedioate

Synonyms:

Thiobutyric acid S-[4-(1,2,3,5,6,10b-hexahydro-pyrrolo[2,1-a]isoquinolin-6-yl)-phenyl] ester; compound with 2,3-dihydroxy-succinic acid; S-Bu-McN-5652 tartrate

CAS No: 167548-65-4

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

Precursor for (+)-[11C]McN 5652

1.3. Details of the supplier of the safety data sheet

Company name:	ABX advanced biochemical compounds	
	Biomedizinische Forschungsreagenzien GmbH	
Street:	Heinrich-Gläser-Straße 10-14	
Place:	01454 Radeberg	
Telephone:	+49 3528 4041 60	Telefax: +49 3528 4041 65
e-mail:	info@abx.de	
Contact person:	Dr. Christoph Meyer	Telephone: +49 3528 4041 8732
e-mail:	meyer@abx.de	
Internet:	http://www.abx.de	

1.4. Emergency telephone number:

+49 3528 4041 60

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****GB CLP Regulation**

This substance is not classified as hazardous in accordance with GB CLP Regulation.

2.2. Label elements**2.3. Other hazards**

Warning - substance not yet tested completely.

SECTION 3: Composition/information on ingredients**3.1. Substances****Chemical characterization**

Butanethioic acid, S-[4-(1,2,3,5,6,10b-hexahydropyrrolo[2,1-a]isoquinolin-6-yl)phenyl] ester, trans-(+), (2R,3R)-2,3-dihydroxybutanedioate

Sum formula: C₂₂H₂₅NOS x C₄H₆O₆

Molecular weight: 501.59

Hazardous components

none (according to UK REACH Regulation)

SECTION 4: First aid measures

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4.1. Description of first aid measures**After inhalation**

Provide fresh air.

After contact with skin

After contact with skin, wash immediately with: Water. Change contaminated clothing.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water.

After ingestion

Rinse mouth immediately and drink plenty of water. Medical treatment necessary.

SECTION 5: Firefighting measures**5.1. Extinguishing media****Suitable extinguishing media**Water spray. Foam. Extinguishing powder. Carbon dioxide (CO₂).**5.2. Special hazards arising from the substance or mixture**In case of fire may be liberated: Carbon dioxide (CO₂). Carbon monoxide Nitrogen oxides (NO_x). Sulfur oxides.**5.3. Advice for firefighters**

In case of fire: Wear self-contained breathing apparatus.

Additional information

Contaminated fire-fighting water must be collected separately. Do not allow to enter into surface water or drains.

SECTION 6: Accidental release measures**6.1. Personal precautions, protective equipment and emergency procedures****General advice**

Wear personal protection equipment. Provide adequate ventilation. Avoid dust formation.

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up**Other information**

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal.

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

Do not breathe dust. If handled uncovered, arrangements with local exhaust ventilation have to be used.

Advice on general occupational hygiene

Change contaminated clothing. Wash hands before breaks and after work. When using do not eat or drink.

Protect skin by using skin protective cream.

Further information on handling

When using do not eat, drink, smoke, sniff.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container dry. Keep container tightly closed.

Further information on storage conditions

storage temperature:

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of °C: -25

up to °C: -15

Protect against: Light.

Store under (Gas): argon. Nitrogen.

SECTION 8: Exposure controls/personal protection**8.1. Control parameters****Additional advice on limit values**

To date, no national critical limit values exist.

8.2. Exposure controls**Individual protection measures, such as personal protective equipment****Eye/face protection**

Eye protection: Tightly sealed safety glasses.

Hand protection

Tested protective gloves are to be worn: Single-use gloves. NBR (Nitrile rubber).

Skin protection

Body protection: Lab apron. Chemical resistant safety shoes.

Respiratory protection

With correct and proper use, and under normal conditions, breathing protection is not required.

SECTION 9: Physical and chemical properties**9.1. Information on basic physical and chemical properties**

Physical state:

solid

Colour:

colourless, whitish

Changes in the physical state

Melting point/freezing point:

118 - 125 °C

Solubility in other solvents

Chloroform. dimethylsulphoxide (DMSO). Ethanol

SECTION 10: Stability and reactivity**10.4. Conditions to avoid**

Light.

10.6. Hazardous decomposition productsCarbon dioxide. Carbon monoxide. Nitrogen oxides (NO_x). Sulfur oxides.**SECTION 11: Toxicological information****11.1. Information on hazard classes as defined in GB CLP Regulation****Carcinogenic/mutagenic/toxic effects for reproduction**

No information available.

Further information

Toxicological data are not available.

SECTION 12: Ecological information**12.5. Results of PBT and vPvB assessment**

This substance does not meet the PBT/vPvB criteria of UK REACH.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

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Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Do not allow to enter into surface water or drains. Dispose of waste according to applicable legislation.

List of Wastes Code - residues/unused products

160508 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and discarded chemicals; discarded organic chemicals consisting of or containing hazardous substances; hazardous waste

List of Wastes Code - used product

160508 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and discarded chemicals; discarded organic chemicals consisting of or containing hazardous substances; hazardous waste

List of Wastes Code - contaminated packaging

150110 WASTE PACKAGING; ABSORBENTS, WIPING CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); packaging containing residues of or contaminated by hazardous substances; hazardous waste

Contaminated packaging

Non-contaminated packages may be recycled. Handle contaminated packages in the same way as the substance itself.

SECTION 14: Transport information**Other applicable information**

No dangerous good in sense of these transport regulations.

SECTION 15: Regulatory information**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****National regulatory information**

Water hazard class (D): 3 - highly hazardous to water

SECTION 16: Other information