

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea)



Version number: 1.1

Issued: 2024-05-03

Replaces SDS: 2023-06-22

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

1.1. Product identifier

Trade name

N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea)

CAS number

109-46-6

EC number

203-674-6

Synonyms

Urea, 1,3-di-N-butyl-2-thio-

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

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

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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

Acute toxicity, oral, hazard category 4

Acute toxicity, dermal, hazard category 4

Skin sensitisation, hazard category 1

Specific Target Organ Toxicity — Repeated exposure, hazard category 1

Hazardous to the aquatic environment — Chronic hazard category 2

Hazard statements

H302, H312, H317, H372, H411

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Danger

Hazard statements

H302 Harmful if swallowed.

H312 Harmful in contact with skin.

H317 May cause an allergic skin reaction.

H372 Causes damage to organs through prolonged or repeated exposure .

H411 Toxic to aquatic life with long lasting effects.

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Precautionary statements

P202 Do not handle until all safety precautions have been read and understood.
 P260 Do not breathe dust/fumes/gas/mist/vapours/spray.
 P262 Do not get in eyes, on skin, or on clothing.
 P264 Wash skin thoroughly after handling.
 P270 Do not eat, drink or smoke when using this product.
 P272 Contaminated work clothing should not be allowed out of the workplace.
 P273 Avoid release to the environment.
 P280 Wear protective gloves/protective clothing/eye protection/face protection.
 P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
 P302 + P352 IF ON SKIN: Wash with plenty of water/.
 P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 P308 + P311 IF exposed or concerned: Call a POISON CENTER/doctor.
 P333 + P313 If skin irritation or rash occurs: Get medical advice/attention.
 P362 + P364 Take off contaminated clothing and wash it before reuse.
 P391 Collect spillage.
 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. EC No. REACH No. Index No.	Concentration	Classification	H-phrase M factor acute M factor chronic	Note
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea)	109-46-6 203-674-6 - -	100%	Acute Tox. 4 - oral, Acute Tox. 4 - dermal, Acute Tox. 4 - inhalation	H302 + H312, H317, H372, H411 - -	-

Molecular weight

188.33

Substance additional information

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

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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.

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Get medical advice/attention if you feel unwell. In case of persistent throat irritation or coughing or after inhalation of oil mist: Seek medical attention and bring along these instructions.

Skin contact

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

Eye contact

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention if you feel unwell. 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.

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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use alcohol resistant 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: None. Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO₂).

Nitrous gases (NO_x).

Sulphurous gases (SO_x).

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 inhalation of dust and contact with skin and eyes. 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

For precautions see section 2.2. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Do not breathe dust/fume/gas/mist/vapours/spray. Avoid ingestion and inhalation.

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General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using the product. Remove contaminated clothing and launder thoroughly before re-use. Wash skin thoroughly after handling.

7.2. Conditions for safe storage, including any incompatibilities

Store in a dry place. Store in a closed container. Store at ambient temperature.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Exposure limits

No occupational exposure limit assigned.

DNEL/DMEL

Product/Substance name (CAS No./EC No.)	Type	Exposure	Value	Population	Effects
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	DNEL	Chronic (long term) Dermal	2.08 mg/kg bw/day	Workers	Systemic
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	DNEL	Chronic (long term) Inhalation	0.14 mg/m ³	Workers	Systemic

PNEC/PEC

Product/Substance name (CAS No./EC No.)	Type	Environmental compartment	Value
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	PNEC	Freshwater	0.0038 mg/l
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	PNEC	Sediment (freshwater)	0.177 mg/kg sedi- ment dw
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	PNEC	Intermittent releases	0.038 mg/l
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	PNEC	Sewage Treatment Plant	10 mg/l

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Product/Substance name (CAS No./EC No.)	Type	Environmental compartment	Value
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	PNEC	Soil	0.033 mg/kg soil dry weight
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	PNEC	Marine water	0.00038 mg/l
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) (109-46-6/203-674-6)	PNEC	Sediment (marine water)	0.0177 mg/kg sedi- ment dw

8.2. Exposure controls

Personal Protective Equipment Symbols



Eye / face protection

Wear eye protection.

Hand protection

Wear protective gloves. Recommended gloves: Butyl rubber.

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

Solid

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Colour

Yellowish.

Odour

Odourless.

Melting point / freezing point

63 - 67 °C / 145.4 - 152.6 °F

Boiling point or initial boiling point and boiling range

No data available

Flammability

No data available

Lower and upper explosion limit

No data available

Flash point

No data available

Auto-ignition temperature

No data available

Decomposition temperature

No data available

pH

5, 4g/l (20°C)

Kinematic viscosity

No data available

Solubility

No data available

Water solubility

212 mg/l

Partition coefficient n-octanol/water

No data available

Vapour pressure

No data available

Density and/or relative density

1.02 g/cm³

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Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

None known.

10.2. Chemical stability

Stable under normal temperature conditions.

10.3. Possibility of hazardous reactions

None under normal conditions.

10.4. Conditions to avoid

Incompatible materials:

10.5. Incompatible materials

Strong oxidising agents.

10.6. Hazardous decomposition products

Carbon monoxide (CO). CARBON DIOXIDE Nitrous gases (NOx). Sulphurous gases (SOx).

SECTION 11: Toxicological information

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

Acute toxicity

Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Test animals
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) 109-46-6 / 203-674-6	LD50	350mg/kg	Rat

Aspiration hazard

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

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11.2. Information on other hazards

No data available

SECTION 12: Ecological information

12.1. Toxicity

Acute fish toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) 109-46-6 / 203-674-6	LC50	10.7mg/l	48 hours	Daphnia magna
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) 109-46-6 / 203-674-6	LC50	1.59mg/l	60 days	Onchorhynchus mykiss (Rainbow trout)

Acute crustacean toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) 109-46-6 / 203-674-6	LC50	10.7 mg/l	48 hours	Daphnia magna

Chronical toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) 109-46-6 / 203-674-6	LOEC mortality	3.2 mg/l	60 days	Onchorhynchus mykiss (Rainbow trout)
N,N'-Dibutylthiourea (1,3-Dibutyl-2-thiourea) 109-46-6 / 203-674-6	LC50	1.59 mg/l	60 days	Onchorhynchus mykiss (Rainbow trout)

12.2. Persistence and degradability

No data available

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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. 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.

SECTION 14: Transport information

14.1. UN number

3077

14.2. UN proper shipping name

ADR / RID / ADN proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (N,N'-Dibutylthiourea)

IMDG proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (N,N'-Dibutylthiourea)

IATA proper shipping name

Environmentally hazardous substance, solid, n.o.s. (N,N'-Dibutylthiourea)

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14.3. Transport hazard class(es)

Label

ADR/RID/ADN



9

Environmental hazard



IMDG



9

Environmental hazard



IATA



9

Environmental hazard



ADR / RID Class

9

ADR / RID Classification code

M7

ADR / RID hazard identification number

90

IMDG Class

9

IATA Class

9

ADN Class

9

ADN Class Code

M7

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14.4. Packing group

ADR / RID / ADN: III
 IMDG: III
 IATA: III

14.5. Environmental hazards

Environmental hazards

ADR/RID/ADN: Hazardous for the environment

14.6. Special precautions for user

Special precautions for user

Tunnel restriction code: -
 Transport category: 3

IMDG EmS

F-A, S-F

14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC08

SECTION 15: Regulatory information

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

National regulations

No data available

15.2. Chemical safety assessment

No data available

SECTION 16: Other information

Phrase meaning

Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4

Acute Tox. 4 - dermal - Acute toxicity, dermal, hazard category 4

Skin Sens. 1 - Skin sensitisation, hazard category 1

STOT RE 1 - Specific Target Organ Toxicity — Repeated exposure, hazard category 1

Aquatic Chronic 2 - Hazardous to the aquatic environment — Chronic hazard category 2

Acute Tox. 4 - inhalation - Acute toxicity, inhalation, hazard category 4

H302 Harmful if swallowed.

H302 + H312 Harmful if swallowed or in contact with skin.

H312 Harmful in contact with skin.

H317 May cause an allergic skin reaction.

H372 Causes damage to organs through prolonged or repeated exposure .

H372 Causes damage to organs through prolonged or repeated exposure .?.

H411 Toxic to aquatic life with long lasting effects.