

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 14.02.2018

Version 7.6

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

1.1 Product identifier

Catalogue No. 820696

Product name 2-Imidazolidinethione for synthesis

REACH Registration Number A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. 96-45-7

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

Identified uses Chemical for synthesis
For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).

1.3 Details of the supplier of the safety data sheet

Company Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0

Responsible Department LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number Please contact the regional company representation in your country.

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SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 4, Oral, H302

Reproductive toxicity, Category 1B, H360D

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

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H360D May damage the unborn child.

H302 Harmful if swallowed.

Precautionary statements

Prevention

P201 Obtain special instructions before use.

Response

P308 + P313 IF exposed or concerned: Get medical advice/ attention.

Restricted to professional users.

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Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H360D May damage the unborn child.

Precautionary statements

P201 Obtain special instructions before use.

P308 + P313 IF exposed or concerned: Get medical advice/ attention.

Index-No. 613-039-00-9

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	C ₃ H ₆ N ₂ S (Hill)
Index-No.	613-039-00-9
EC-No.	202-506-9
Molar mass	102,16 g/mol

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

CAS-No.	Registration number	Classification
Imidazolidine-2-thione (≤ 100 %)		
96-45-7	*)	

Acute toxicity, Category 4, H302

Reproductive toxicity, Category 1B, H360D

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

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air. Call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, Cough, Shortness of breath, Nausea, Vomiting, Headache

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Foam, Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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5.2 Special hazards arising from the substance or mixture

Combustible.

Forms explosive mixtures with air on intense heating.

Vapours are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

nitrogen oxides, Sulphur oxides

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Work under hood. Do not inhale substance/mixture.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

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

Engineering measures

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Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

protective clothing

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Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 3 (acc. to DIN 3181) for solid and liquid particles of toxic and very toxic substances

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	solid
Colour	white
Odour	weakly aromatic
Odour Threshold	No information available.
pH	No information available.
Melting point	199 °C Method: OECD Test Guideline 102
Boiling point/boiling range	ca. 240 °C at 1.010 hPa Method: OECD Test Guideline 103
Flash point	253 °C

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Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	< 1 hPa at 25 °C Method: OECD Test Guideline 104
Relative vapour density	No information available.
Density	1,4 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	ca.8 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 0,67 (20 °C) OECD Test Guideline 107 Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	240 °C
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.

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Oxidizing properties	none
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9.2 Other data

Bulk density	750 - 900 kg/m ³
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SECTION 10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, Strong acids

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See section 5.

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 710 mg/kg

(External MSDS)

LD50 Rat: 1.832 mg/kg

Acute inhalation toxicity

Symptoms: Possible damages:, May cause irritation of respiratory tract.

Acute dermal toxicity

LD50 Rat: 2.000 mg/kg

OECD Test Guideline 402

Skin irritation

Rabbit

Result: No skin irritation

OECD Test Guideline 404

Eye irritation

Rabbit

Result: No eye irritation

OECD Test Guideline 405

Sensitisation

Open epicutaneous test Mouse

Result: negative

(ECHA)

Germ cell mutagenicity

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Genotoxicity in vivo

Chromosome aberration test

Mouse

male

Intraperitoneal injection

Red blood cells (erythrocytes)

Result: negative

(ECHA)

unscheduled DNA synthesis assay

Mouse

male

Oral

Liver cells

Result: negative

(ECHA)

Genotoxicity in vitro

In vitro mammalian cell gene mutation test

Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 476

Mutagenicity (mammal cell test): chromosome aberration.

Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 473

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

Carcinogenicity

This information is not available.

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Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

CMR effects

Teratogenicity:

May damage the unborn child.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

After absorption:

Headache, Nausea, Vomiting

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

semi-static test LC50 *Poecilia reticulata* (guppy): 7.500 mg/l; 96 h

Analytical monitoring: yes

OECD Test Guideline 203

static test LC50 *Oncorhynchus mykiss* (rainbow trout): > 5.020 mg/l; 96 h
(ECOTOX Database)

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Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 26,4 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

Toxicity to algae

IC50 chlorella pyrenoidosa: 6.600 mg/l; 96 h

(ECOTOX Database)

static test EC50 Pseudokirchneriella subcapitata (green algae): > 100 mg/l; 72 h

OECD Test Guideline 201

Toxicity to bacteria

static test EC50 activated sludge: > 100 mg/l; 3 h

OECD Test Guideline 209

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

semi-static test NOEC Daphnia magna (Water flea): 3,2 mg/l; 21 d

OECD Test Guideline 211

12.2 Persistence and degradability

Biodegradability

0 %; 28 d; aerobic

OECD Test Guideline 301F

Not biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0,67 (20 °C)

OECD Test Guideline 107

Bioaccumulation is not expected.

12.4 Mobility in soil

Distribution among environmental compartments

log Koc: 6,5

(calculated) (HSDB)

12.5 Results of PBT and vPvB assessment

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PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 - 14.6	Not classified as dangerous in the meaning of transport regulations.
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Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 - 14.6	Not classified as dangerous in the meaning of transport regulations.
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Sea transport (IMDG)

14.1 - 14.6	Not classified as dangerous in the meaning of transport regulations.
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14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

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

EU regulations

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Major Accident Hazard	SEVESO III
Legislation	Not applicable

Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
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Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
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Substances of very high concern (SVHC)	This product does contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 59 above the respective regulatory concentration limit of > 0.1 % (w/w).
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Contains: Imidazolidine-2-thione

National legislation

Storage class	6.1C
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15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

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SECTION 16. Other information

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

H302	Harmful if swallowed.
H360D	May damage the unborn child.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H302 Harmful if swallowed.
H360 May damage fertility or the unborn child.

Precautionary statements

Prevention

P201 Obtain special instructions before use.

Response

P308 + P313 IF exposed or concerned: Get medical advice/ attention.

Further information

Restricted to professional users.

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Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.