

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 05.12.2018

Version 7.5

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

1.1 Product identifier

Catalogue No.	808076
Product name	Thioacetic acid 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.	507-09-5

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).
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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.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 2, H225
Acute toxicity, Category 3, Oral, H301
Acute toxicity, Category 4, Inhalation, H332
Serious eye damage, Category 1, H318
Skin sensitisation, Category 1, H317

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

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Catalogue No.
Product name

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.

H301 Toxic if swallowed.

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

H332 Harmful if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P240 Ground/bond container and receiving equipment.

P280 Wear protective gloves.

P280 Wear eye protection.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue rinsing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/physician.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H301 Toxic if swallowed.

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P280 Wear protective gloves.

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P280 Wear eye protection.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

CAS-No. 507-09-5

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CH ₃ COSH	C ₂ H ₄ OS (Hill)
EC-No.	208-063-8	
Molar mass	76,12 g/mol	

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

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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thioacetic acid (>= 80 % - <= 100 %)

507-09-5 *)

Flammable liquid, Category 2, H225
Acute toxicity, Category 3, H301
Acute toxicity, Category 4, H332
Serious eye damage, Category 1, H318
Skin sensitisation, Category 1, H317

*) 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.

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. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately 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. Immediately call in ophthalmologist. Remove contact lenses.

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If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

4.2 Most important symptoms and effects, both acute and delayed

Irritation and corrosion, Allergic reactions, Cough, Shortness of breath
Risk of serious damage to eyes.

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

Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

Water, Foam

5.2 Special hazards arising from the substance or mixture

Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at ambient temperatures.

May not get in touch with:

Water

Caution! in contact with water product releases:

hydrogen sulphide

Pay attention to flashback.

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

Fire may cause evolution of:

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

Remove container from danger zone and cool with water. 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: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

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Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. 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

Tightly fitting safety goggles

Hand protection

full contact:

Glove material: butyl-rubber
Glove thickness: 0,7 mm
Break through time: > 480 min

splash contact:

Glove material: natural latex
Glove thickness: 0,6 mm
Break through time: > 30 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 898 Butoject® (full contact), KCL 706 Lapren® (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

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

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Product name	Thioacetic acid for synthesis

Form	liquid
Colour	colourless to light yellow
Odour	stinging
Odour Threshold	No information available.
pH	1,8 at 100 g/l 20 °C Hydrolysis
Melting point	-17 °C Method: DIN 53181
Boiling point/boiling range	86 °C at 1.013 hPa
Flash point	18 °C Method: c.c.
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 20 °C
Relative vapour density	2,6
Density	1,07 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	27 g/l at 15 °C (slow decomposition)
Partition coefficient: n-octanol/water	No information available.
Auto-ignition temperature	No information available.
Decomposition temperature	> 93 °C

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Viscosity, dynamic	6,3 mPa.s at 20 °C
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Explosive properties	Not classified as explosive.
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Oxidizing properties	none
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9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapours may form explosive mixture with air.

10.2 Chemical stability

sensitive to moisture

Sensitivity to light

Sensitive to air.

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Metals, Strong bases

Exothermic reaction with:

strong reducing agents

Risk of ignition or formation of inflammable gases or vapours with:

Strong oxidizing agents, hydrogen sulphide

Release of:

sulphur dioxide

can decompose violently in contact with:, Water

Release of:

hydrogen sulphide

10.4 Conditions to avoid

Warming.

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: 200 - 350 mg/kg

OECD Test Guideline 401

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach., Risk of aspiration upon vomiting., Pulmonary failure possible after aspiration of vomit.
absorption

Acute inhalation toxicity

Acute toxicity estimate: 11,1 mg/l; vapour

Expert judgement

Symptoms: Possible damages:, Irritation symptoms in the respiratory tract., Inhalation may lead to the formation of oedemas in the respiratory tract.
absorption

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: No irritation

OECD Test Guideline 404

Eye irritation

Rabbit

Result: Irreversible effects on the eye

OECD Test Guideline 405

Causes serious eye damage.

Sensitisation

Maximisation Test Guinea pig

Result: positive

Method: OECD Test Guideline 406

May cause an allergic skin reaction.

Germ cell mutagenicity

Genotoxicity in vitro

Mutagenicity (mammal cell test): chromosome aberration.

Human lymphocytes

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.

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

Possible effect after contact with substance:

Damage to:

Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates

static test EC50 Daphnia magna (Water flea): 2,1 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

12.2 Persistence and degradability

Biodegradability

84 %; 28 d

OECD Test Guideline 301D

(ECHA)

Readily biodegradable

12.3 Bioaccumulative potential

No information available.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

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

12.6 Other adverse effects

Discharge into the environment must be avoided.

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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 UN number	UN 2436
14.2 Proper shipping name	THIOACETIC ACID
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 2436
14.2 Proper shipping name	THIOACETIC ACID
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

14.1 UN number	UN 2436
14.2 Proper shipping name	THIOACETIC ACID
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-E S-D

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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

Major Accident Hazard	SEVESO III
Legislation	FLAMMABLE LIQUIDS
	P5c
	Quantity 1: 5.000 t
	Quantity 2: 50.000 t

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

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 not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).
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National legislation

Storage class	3
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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.

H225	Highly flammable liquid and vapour.
H301	Toxic if swallowed.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H332	Harmful if inhaled.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.
H301 Toxic if swallowed.
H317 May cause an allergic skin reaction.
H318 Causes serious eye damage.
H332 Harmful if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P240 Ground/bond container and receiving equipment.
P280 Wear eye protection.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.
Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/physician.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

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.

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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.