

Single Element Standard, 0.1% (1000 ppm) Sulfur in Isooctane

Revision date: 11/18/2024

Product code: AC18.05914

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1. Identification
Product identifier

Single Element Standard, 0.1% (1000 ppm) Sulfur in Isooctane

Recommended use of the chemical and restrictions on use
Use of the substance/mixture

 Reagents and laboratory chemicals
 Only for laboratory and analysis purposes.

Uses advised against

Do not use for private purposes (household).

Details of the supplier of the safety data sheet
Details of the supplier of the safety data sheet

Company name:	AnalytiChem Services, Unipessoal, Lda
Street:	Rua de Júlio Dinis 676 7º
Place:	P-4050-320 Porto
Telephone:	+351 226002917
E-mail:	info@analytichem.com
Contact person:	SDS service department
E-mail:	SDS@analytichem.com
Internet:	www.analytichem.com
Responsible Department:	SDS service department

Supplier or manufacturer details

Company name:	AnalytiChem Canada Inc.	
	Québec, CANADA	
Street:	21800 Clark Graham Ave	
Place:	CDN-H9X 4B6 Baie-D'Urfé	
Telephone:	+1 (800) 361-6820	Telefax: +1 (800) 253-5549
E-mail:	info@analytichem.com	
Contact person:	SDS service department	
E-mail:	SDS@analytichem.com	
Internet:	www.analytichem.com	
Responsible Department:	AnalytiChem:	
	EU-Belgium: AnalytiChem Belgium, Industriezone "De Arend" 2, 8210 Zedelgem, Belgium, +32 50 28 83 20	
	EU-Germany: AnalytiChem Germany, Stempelstrasse 6, 47167 Duisburg, Germany, +49 203 51 94 – 200	
	EU-Netherlands: AnalytiChem Netherlands, Communicatieweg 7, 3641 SG Mijdrecht, The Netherlands, +31 297 286848	
	UK: AnalytiChem UK, Unit 7 Launton Business Center, Murdock Road, Bicester, OX26 4XB, England, +44 1869 355 500	
	USA: AnalytiChem USA, 227 China Road, Winslow, Maine, 04901, United States, +1 800-244-8378	
	Canada: AnalytiChem Canada, 21800 Clark Graham Avenue, Baie d'Urfe, H9X 4B6, Canada, +1 514-457-0701	
	Australia: ORE Research & Exploration Pty Ltd, 37A Hosie Street, Bayswater North, 3153, Australia, +61 3 9729 0333	
Emergency phone number:	+1 703-741-5970 (CHEMTREC)	

Further Information

No data available

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2. Hazard(s) identification

Classification of the chemical

Regulation (EC) No 1272/2008

- Flam. Liq. 2; H225
- Skin Irrit. 2; H315
- STOT SE 3; H336
- Asp. Tox. 1; H304
- Aquatic Acute 1; H400
- Aquatic Chronic 1; H410

Full text of hazard statements: see SECTION 16.

Label elements

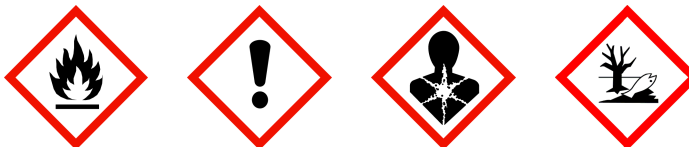
Regulation (EC) No 1272/2008

Hazard components for labelling

2,2,4-trimethylpentane

Signal word: Danger

Pictograms:



Hazard statements

- H225 Highly flammable liquid and vapor
- H304 May be fatal if swallowed and enters airways
- H315 Causes skin irritation
- H336 May cause drowsiness or dizziness
- H410 Very toxic to aquatic life with long lasting effects

Precautionary statements

- P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
- P273 Avoid release to the environment.
- P301+P310 If swallowed: Immediately call a poison center/doctor.
- P331 Do NOT induce vomiting.
- P391 Collect spillage.
- P403+P235 Store in a well-ventilated place. Keep cool.

Hazards not otherwise classified

No data available

3. Composition/information on ingredients

Mixtures

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Relevant ingredients

CAS No	Components			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
540-84-1	2,2,4-trimethylpentane			95 - < 100 %
	208-759-1	601-009-00-8	01-2119457965-22	
	Flam. Liq. 2, Skin Irrit. 2, STOT SE 3, Asp. Tox. 1, Aquatic Acute 1, Aquatic Chronic 1; H225 H315 H336 H304 H400 H410			

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Components	Quantity
	Specific Conc. Limits, M-factors and ATE		
540-84-1	208-759-1	2,2,4-trimethylpentane	95 - < 100 %
	inhalation: LC50 = > 33,52 mg/l (vapours); dermal: LD50 = > 2000 mg/kg; oral: LD50 = > 5000 mg/kg		

Further Information

No data available

4. First-aid measures
Description of first aid measures
General information

Remove contaminated, saturated clothing immediately.

After inhalation

Provide fresh air.

If breathing is irregular or stopped, administer artificial respiration.

Call a physician immediately.

After contact with skin

Wash immediately with: Water

Take off immediately all contaminated clothing and wash it before reuse.

In case of skin irritation, consult a physician.

After contact with eyes

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

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

In case of eye irritation consult an ophthalmologist.

After ingestion

Rinse mouth.

Observe risk of aspiration if vomiting occurs.

Call a physician immediately.

Most important symptoms and effects, both acute and delayed

Irritant

Vapors may cause drowsiness and dizziness.

Narcotic effects

Pulmonary oedema

Repeated exposure may cause skin dryness or cracking.

Prolonged or repeated skin contact may cause removal of natural fat from the skin resulting in dermatitis (skin inflammation).

Indication of any immediate medical attention and special treatment needed

No data available

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5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

- Carbon dioxide (CO₂)
- Foam
- Extinguishing powder
- Water spray jet

Unsuitable extinguishing media

- High power water jet.

Specific hazards arising from the chemical

- Combustible liquids
- Hazardous combustion products
- In case of fire may be liberated:
- Carbon dioxide (CO₂)
- Carbon monoxide
- Sulphur oxides
- Vapors are heavier than air, spread along floors and form explosive mixtures with air.
- Heating causes rise in pressure with risk of bursting.
- Beware of reignition.

Special protective equipment and precautions for fire-fighters

- In case of fire: Wear self-contained breathing apparatus.
- In case of fire and/or explosion do not breathe fumes.

Additional information

- Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.
- Move undamaged containers from immediate hazard area if it can be done safely.
- Use water spray jet to protect personnel and to cool endangered containers.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

General advice

- Keep away from sources of ignition - No smoking.
- This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).
- Take precautionary measures against static discharge.

For non-emergency personnel

- Provide adequate ventilation.
- Use personal protection equipment.
- Avoid contact with skin, eyes and clothes.
- Remove persons to safety.
- Emergency procedures
- Consult an expert
- Do not breathe dust/fume/gas/mist/vapors/spray.

For emergency responders

- Precautionary statements For emergency responders : Personal protection equipment (PPE): see section 8

Environmental precautions

- Do not allow to enter into surface water or drains.
- The vapors are heavier than air and can accumulate in high concentrations on the ground, in cavities, channels and cellars.

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Danger of explosion

Methods and material for containment and cleaning up

For containment

- Cover drains.
- Prevent spread over a wide area (e.g. by containment or oil barriers).
- Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).
- Collect in closed and suitable containers for disposal.

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

- Provide adequate ventilation.
- Do not breathe dust/fume/gas/mist/vapors/spray.
- Wear breathing apparatus if exposed to vapors/dusts/aerosols.

Reference to other sections

- Safe handling: see section 7
- Personal protection equipment (PPE): see section 8
- Disposal: see section 13

7. Handling and storage

Precautions for safe handling

Advice on safe handling

- Read label before use. Handle and open container with care.
- When using do not eat, drink, smoke, sniff. Keep container tightly closed.
- Use personal protection equipment. Use extractor hood (laboratory).
- Provide adequate ventilation. Do not breathe vapor.

Advice on protection against fire and explosion

Take precautionary measures against static discharge. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Advice on general occupational hygiene

- Keep away from food, drink and animal feedingstuffs.
- The choice of body protection depends on the concentration and quantity of hazardous substances. The chemical resistance of the protective agents should be clarified with their suppliers.

Further information on handling

- Take off immediately all contaminated clothing and wash it before reuse.
- Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. If handled uncovered, arrangements with local exhaust ventilation have to be used.

Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

- Keep in a cool, well-ventilated place.
- Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Hints on joint storage

National regulations

Further information on storage conditions

- Keep container tightly closed and dry.
- Keep cool. Protect from sunlight.

Specific end use(s)

- Laboratory chemicals
- Only for laboratory and analysis purposes.

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8. Exposure controls/personal protection
Control parameters
Exposure limits

CAS No	Substance	ppm	mg/m ³	Category	Origin
-	Octane: all isomers	300	1401	TWA (8 h)	ACGIH-2025

DNEL/DMEL values

CAS No	Substance	Exposure route	Effect	Value
540-84-1	2,2,4-trimethylpentane			
Worker DNEL, long-term		inhalation	systemic	2035 mg/m ³
Worker DNEL, long-term		dermal	systemic	773 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	608 mg/m ³
Consumer DNEL, long-term		dermal	systemic	699 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	699 mg/kg bw/day

Exposure controls
Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment.

If handled uncovered, arrangements with local exhaust ventilation have to be used.

Individual protection measures, such as personal protective equipment
Eye/face protection

goggles

Face protection umbrella

Hand protection

Tested protective gloves must be worn

The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances.

For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

Skin protection

Take off immediately all contaminated clothing and wash it before reuse.

Wear fire resistant or flame retardant clothing.

Wash hands and face before breaks and after work and take a shower if necessary.

Draw up and observe skin protection programme.

Respiratory protection

Wear breathing apparatus if exposed to vapors/dusts/aerosols.

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. A respiratory protection program that meets OSHA's 29 CFR 1910.134 requirements must be followed whenever workplace conditions warrant a respirator's use.

Thermal hazards

No data available

Environmental exposure controls

Do not allow to enter into surface water or drains.

Due to danger of explosion, prevent leakage of vapors into cellars, flues and ditches.

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Danger of explosion

9. Physical and chemical properties
Information on basic physical and chemical properties

Physical state:	Liquid
Color:	colorless
Odor:	like: Gasoline
Odour threshold:	No data available
Melting point/freezing point:	-107 (-161 °F) °C
Boiling point or initial boiling point and boiling range:	99 (210 °F) °C
Flammability:	No data available
Lower explosion limits:	1 vol. %
Upper explosion limits:	6 vol. %
Flash point:	-12 (10 °F) °C
Auto-ignition temperature:	No data available
Decomposition temperature:	No data available
pH-Value:	No data available
Viscosity / kinematic:	No data available
Water solubility:	No data available
Solubility in other solvents	No data available
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	No data available
Dispersion stability:	No data available
Vapor pressure:	55 (70 °F) hPa
(at 21 °C)	
Vapor pressure:	120 (100.04 °F) hPa
(at 37.8 °C)	
Density:	0.6877 g/cm ³
Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available
Particle characteristics:	No data available

Other information
Information with regard to physical hazard classes
Explosive properties

Vapors are heavier than air, spread along floors and form explosive mixtures with air.

Sustained combustibility: Sustained combustibility

Self-ignition temperature

Solid: No data available

Gas: No data available

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate: No data available

Solvent separation test: No data available

Solvent content: 100%

Solid content: 0%

Sublimation point: No data available

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Softening point: No data available
 Pour point: No data available
 Viscosity / dynamic: No data available
 Flow time: No data available

Further Information

No data available

10. Stability and reactivity

Reactivity

Vapours may form explosive mixtures with air.

Chemical stability

The product is stable under storage at normal ambient temperatures.

Possibility of hazardous reactions

Oxidising agent

Conditions to avoid

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

Incompatible materials

Plastic articles

Hazardous decomposition products

in case of fire, see:
 SECTION 5: Fire fighting measures

Further information

No data available

11. Toxicological information

Information on toxicological effects

Toxicokinetics, metabolism and distribution

There are no data available on the mixture itself.

Acute toxicity

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

ATEmix calculated

ATE (oral) > 2000 mg/kg; ATE (dermal) > 2000 mg/kg; ATE (inhalation vapour) > 20 mg/l; ATE (inhalation dust/mist) > 5 mg/l

CAS No	Components				
	Exposure route	Dose	Species	Source	Method
540-84-1	2,2,4-trimethylpentane				
	oral	LD50 > 5000 mg/kg	Rat	Study report (1982)	OECD Guideline 401
	dermal	LD50 > 2000 mg/kg	Rabbit	Study report (1982)	OECD Guideline 402
	inhalation (4 h) vapour	LC50 > 33,52 mg/l	Rat	Study report (1982)	OECD Guideline 403

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Irritation and corrosivity

Skin corrosion/irritation: Causes skin irritation

Serious eye damage/eye irritation: Based on available data, the classification criteria are not met.

Prolonged or repeated skin contact may cause removal of natural fat from the skin resulting in dermatitis (skin inflammation).

Sensitizing effects

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

Carcinogenic/mutagenic/toxic effects for reproduction

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

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

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

Specific target organ toxicity (STOT) - single exposure

May cause drowsiness or dizziness (2,2,4-trimethylpentane)

Organs affected: central nervous system

Specific target organ toxicity (STOT) - repeated exposure

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

Aspiration hazard

May be fatal if swallowed and enters airways

Route(s) of Entry

There are no data available on the mixture itself.

Specific effects in experiment on an animal

There are no data available on the mixture itself.

Additional information on tests

There are no data available on the mixture itself.

Practical experience

There are no data available on the mixture itself.

Information on other hazards

Endocrine disrupting properties

This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

Other information

There are no data available on the mixture itself.

Further information

Irritant

Vapors may cause drowsiness and dizziness.

Narcotic effects

Pulmonary oedema

Repeated exposure may cause skin dryness or cracking.

Prolonged or repeated skin contact may cause removal of natural fat from the skin resulting in dermatitis (skin inflammation).

12. Ecological information

Ecotoxicity

Very toxic to aquatic life

Very toxic to aquatic life with long lasting effects

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CAS No	Components					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
540-84-1	2,2,4-trimethylpentane					
	Acute fish toxicity	LC50 0,11 mg/l	96 h	Oncorhynchus mykiss	SIDS Initial Assessment Report For SIAM	OECD Guideline 203
	Acute algae toxicity	ErC50 mg/l 2,943	72 h	Pseudokirchneriella subcapitata	CONCAWE, Brussels, Belgium (2010)	The aquatic toxicity was estimated by a
	Acute crustacea toxicity	EC50 0,4 mg/l	48 h	Daphnia magna	Publication (1986)	other: As described in: The evaluation o
	Fish toxicity	NOEC mg/l 0,82	28 d	Oncorhynchus mykiss	CONCAWE, Brussels, Belgium (2010)	The aquatic toxicity was estimated by a
	Crustacea toxicity	NOEC 1 mg/l	21 d	Daphnia magna	SIDS Initial Assessment Report For SIAM	OECD Guideline 211

Persistence and degradability

There are no data available on the mixture itself.

Bioaccumulative potential

There are no data available on the mixture itself.

Partition coefficient n-octanol/water

CAS No	Components	Log Pow
540-84-1	2,2,4-trimethylpentane	4,08

BCF

CAS No	Components	BCF	Species	Source
540-84-1	2,2,4-trimethylpentane	231	calculated	Other company data (

Mobility in soil

There are no data available on the mixture itself.

Results of PBT and vPvB assessment

The substances in the mixture do not meet the PBT/vPvB criteria according to REACH, annex XIII.

Endocrine disrupting properties

This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

Other adverse effects

Do not allow to enter into surface water or drains.

Avoid release to the environment.

Further information

No data available

13. Disposal considerations
Waste treatment methods
Disposal recommendations

Send to a physico-chemical treatment facility under observation of official regulations .

Do not allow to enter into surface water or drains.

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.

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Contaminated packaging

Handle contaminated packages in the same way as the substance itself.

14. Transport information

Land transport (ADR/RID)

UN number or ID number: UN 1262
UN proper shipping name: OCTANES
Transport hazard class(es): 3
Packing group: II
Hazard label: 3
Classification Code: F1
Limited quantity: 1 L
Excepted quantity: E2
Transport category: 2
Hazard No: 33
Tunnel restriction code: D/E

Inland waterways transport (ADN)

UN number or ID number: UN 1262
UN proper shipping name: OCTANES
Transport hazard class(es): 3
Packing group: II
Hazard label: 3
Classification Code: F1
Limited quantity: 1 L
Excepted quantity: E2

Marine transport (IMDG)

UN number or ID number: UN 1262
UN proper shipping name: OCTANES
Transport hazard class(es): 3
Packing group: II
Hazard label: 3
Marine pollutant: P
Special Provisions: -
Limited quantity: 1 L
Excepted quantity: E2
EmS: F-E, S-E

Air transport (ICAO-TI/IATA-DGR)

UN number or ID number: UN 1262
UN proper shipping name: OCTANES
Transport hazard class(es): 3
Packing group: II
Hazard label: 3
Limited quantity Passenger: 1 L
Passenger LQ: Y341
Excepted quantity: E2
IATA-packing instructions - Passenger: 353
IATA-max. quantity - Passenger: 5 L
IATA-packing instructions - Cargo: 364
IATA-max. quantity - Cargo: 60 L

Environmental hazards

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ENVIRONMENTALLY HAZARDOUS: Yes
 Danger releasing substance: octane

15. Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40, Entry 75

Information according to Directive 2012/18/EU (SEVESO III): E1 Hazardous to the Aquatic Environment

Additional information:

P5c

National regulatory information

16. Other information

Abbreviations and acronyms

- Flam. Liq. 2: Flammable liquids
- Asp. Tox. 1: Aspiration hazard
- Skin Irrit. 2: Skin irritation
- STOT SE 3: Specific target organ toxicity single exposure
- Aquatic Acute 1: Acute aquatic hazard
- Aquatic Chronic 1: Chronic aquatic hazard

Classification for mixtures and used evaluation method according to regulation (EC) No 1272/2008

Classification	Classification procedure
Flam. Liq. 2; H225	On basis of test data
Skin Irrit. 2; H315	Calculation method
STOT SE 3; H336	Calculation method
Asp. Tox. 1; H304	Calculation method
Aquatic Acute 1; H400	Calculation method
Aquatic Chronic 1; H410	Calculation method

Relevant H statements (full text)

- H225 Highly flammable liquid and vapor
- H304 May be fatal if swallowed and enters airways
- H315 Causes skin irritation
- H336 May cause drowsiness or dizziness
- H400 Very toxic to aquatic life
- H410 Very toxic to aquatic life with long lasting effects

Other data

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material. The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations. Provide appropriate information, instructions and training to users.

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(The data for the relevant ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)