

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 1 of 11

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

1.1. Product identifier

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

REACH Registration Number: 01-2119457965-22-XXXX
CAS No: 540-84-1
Index No: 601-009-00-8
EC No: 208-759-1

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

Use of the substance/mixture

Laboratory chemicals

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name: AnalytiChem GmbH
Street: Stempelstraße 6
Place: D-47167 Duisburg
Telephone: 0203/5194-0
E-mail: info@analytichem.de
Contact person: Abteilung Produktsicherheit
E-mail: produktsicherheit@analytichem.de
Internet: www.analytichem.de
Responsible Department: Abteilung Produktsicherheit
Telefax: 0203/5194-290
Telephone: 0203/5194-107/117

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

No data available

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

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.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Danger

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 2 of 11

Pictograms:



Hazard statements

H225	Highly flammable liquid and vapour.
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, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P240	Ground and bond container and receiving equipment.
P273	Avoid release to the environment.
P301+P330+P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302+P352	IF ON SKIN: Wash with plenty of soap and water.
P403+P233	Store in a well-ventilated place. Keep container tightly closed.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula:	C ₈ H ₁₈
Molecular weight:	114.23 g/mol

Hazardous components

CAS No	Chemical name	Quantity		
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
540-84-1	2,2,4-trimethylpentane			100 %
	208-759-1	601-009-00-8	01-2119457965-22-XXXX	
	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	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
540-84-1	208-759-1	2,2,4-trimethylpentane	100 %
	inhalation: LC ₅₀ = > 33,52 mg/l (vapours); dermal: LD ₅₀ = > 2000 mg/kg; oral: LD ₅₀ = > 5000 mg/kg		

Further Information

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 = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

No data available

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 3 of 11

After inhalation

Provide fresh air.
Call a physician immediately.

After contact with skin

Wash immediately with: Water
Take off immediately all contaminated clothing and wash it before reuse.

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.

After ingestion

Observe risk of aspiration if vomiting occurs.
Call a physician immediately.

4.2. Most important symptoms and effects, both acute and delayed

Irritant
Vapours may cause drowsiness and dizziness.
Narcotic effects
Pulmonary oedema

4.3. Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂)
Foam
Extinguishing powder

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible liquids
Hazardous combustion products
In case of fire may be liberated: Carbon dioxide (CO₂) Carbon monoxide
Vapours 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.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.
In case of fire and/or explosion do not breathe fumes.
Avoid contact with skin, eyes and clothes.

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.

SECTION 6: Accidental release measures

6.1. 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,

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 4 of 11

and pagers which have not been certified as intrinsically safe).

Take action to prevent static discharges.

For non-emergency personnel

Provide adequate ventilation.

Use personal protection equipment.

Avoid contact with skin, eyes and clothes.

Remove persons to safety.

Emergency procedures

Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.

Danger of explosion

6.3. 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).

Collect in closed and suitable containers for disposal.

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

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/vapours/spray.

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

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

SECTION 7: Handling and storage

7.1. 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 vapour.

Advice on protection against fire and explosion

Take action to prevent static discharges. 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.

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.

7.2. Conditions for safe storage, including any incompatibilities

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 5 of 11

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.

Further information on storage conditions

Keep container tightly closed and dry.
Keep cool. Protect from sunlight.
storage temperature +5°C - +30°C

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

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

8.2. 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

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact
Trade name/designation KCL 730 Camatril® Velours
Suitable material: NBR (Nitrile rubber) 0,4 mm
Wearing time with permanent contact: > 480 min

By short-term hand contact
Trade name/designation KCL 741 Dermatril® L
Suitable material: NBR (Nitrile rubber) 0,11 mm
Wearing time with occasional contact (splashes): > 60 min

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).

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 6 of 11

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 vapours/dusts/aerosols.
- Filtering device with filter or ventilator filtering device of type: A

Environmental exposure controls

- Do not allow to enter into surface water or drains.
- Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.
- Danger of explosion

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid
Colour:	colourless
Odour:	like: Gasoline
Odour threshold:	No data available
Melting point/freezing point:	-107 °C
Boiling point or initial boiling point and boiling range:	99 °C
Flammability:	No data available
Lower explosion limits:	1 vol. %
Upper explosion limits:	6 vol. %
Flash point:	-12 °C
Auto-ignition temperature:	418 °C
Decomposition temperature:	No data available
pH-Value:	No data available
Viscosity / kinematic:	No data available
Water solubility: (at 25 °C)	0,56 g/L
Solubility in other solvents	No data available
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	log Pow: 4,09
Dispersion stability:	No data available
Vapour pressure: (at 20 °C)	51 hPa
Vapour pressure:	No data available
Density:	0,69 g/cm ³
Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available
Particle characteristics:	No data available

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

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

Sustaining combustion: Sustaining combustion

Self-ignition temperature

Solid: No data available

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 7 of 11

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:	No data available
Sublimation point:	No data available
Softening point:	No data available
Pour point:	No data available
Viscosity / dynamic: (at 20 °C)	0,5 mPa·s
Flow time:	No data available

Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Vapours may form explosive mixtures with air.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Oxidising agent

10.4. Conditions to avoid

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

10.5. Incompatible materials

Plastic articles

10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

Further information

No data available

SECTION 11: Toxicological information

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

Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

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

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 8 of 11

CAS No	Chemical name				
	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

Irritation and corrosivity

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).

Sensitising effects

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

Carcinogenic/mutagenic/toxic effects for reproduction

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

STOT-single exposure

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

Organs affected: central nervous system

STOT-repeated exposure

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

Aspiration hazard

May be fatal if swallowed and enters airways.

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards

Endocrine disrupting properties

No data available

Other information

No data available

Further information

Irritant

Vapours may cause drowsiness and dizziness.

Narcotic effects

Pulmonary oedema

SECTION 12: Ecological information

12.1. Toxicity

Very toxic to aquatic life.

Very toxic to aquatic life with long lasting effects.

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 9 of 11

CAS No	Chemical name						
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method	
540-84-1	2,2,4-trimethylpentane						
	Acute fish toxicity	LC50 mg/l	0,11	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

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

Bioaccumulative potential

Partition coefficient n-octanol/water

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

BCF

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

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6. Endocrine disrupting properties

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

12.7. Other adverse effects

Do not allow to enter into surface water or drains.

Avoid release to the environment.

Further information

No data available

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

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

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

Do not empty into drains.

Contaminated packaging

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

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 10 of 11

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number or ID number:	UN 1262
14.2. UN proper shipping name:	OCTANES
14.3. Transport hazard class(es):	3
14.4. 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)

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

Marine transport (IMDG)

14.1. UN number or ID number:	UN 1262
14.2. UN proper shipping name:	OCTANES
14.3. Transport hazard class(es):	3
14.4. 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)

14.1. UN number or ID number:	UN 1262
14.2. UN proper shipping name:	OCTANES
14.3. Transport hazard class(es):	3
14.4. 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

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS:	Yes
Danger releasing substance:	octane

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctane > 99 % (2,2,4-Trimethylpentane) pure

Revision date: 03.08.2023

Product code: 16477

Page 11 of 11

SECTION 15: Regulatory information

15.1. 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 2012/18/EU
(SEVESO III):

E1 Hazardous to the Aquatic Environment

Additional information:

P5c

National regulatory information

Employment restrictions:

Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).

Water hazard class (D):

2 - obviously hazardous to water

15.2. Chemical safety assessment

For this substance a chemical safety assessment is not required.

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 12.

Abbreviations and acronyms

Flam. Liq: Flammable liquid

Asp. Tox: Aspiration hazard

Skin Irrit: Skin irritation

STOT SE: Specific target organ toxicity - single exposure

Aquatic Acute: Acute aquatic hazard

Aquatic Chronic: Chronic aquatic hazard

Relevant H and EUH statements (number and full text)

H225 Highly flammable liquid and vapour.

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.

Further Information

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.