

Isooctane

Safety Data Sheet

according to Regulation (EU) 2015/830

Date of issue: 03/04/2017

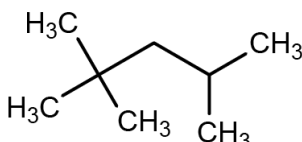
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form : Substance
Substance name : Isooctane
EC Index-No. : 601-009-00-8
EC-No. : 208-759-1
CAS-No. : 540-84-1
Type of product : Small container
Formula : C₈H₁₈
Chemical structure :



Synonyms : Octane, Octanes, 2,2,4-trimethylpentane

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

1.2.1. Relevant identified uses

Use of the substance/mixture : Certified reference material for laboratory use only
Chemical laboratory

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

ISOLAB GmbH
Bahnhofstrasse 10, D-97877
Wertheim - Germany
T +49 93 42 912 355 - F +49 93 42 912 357
prodsafe@isolab.de

1.4. Emergency telephone number

Country	Organisation/Company	Address	Emergency number	Comment
Germany	Giftnotruf der Charité CBF, Haus VIII (Wirtschaftsgebäude), UG	Hindenburgdamm 30 12203 Berlin	+49 30 19240	

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

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

Full text of hazard classes and H-statements : see section 16

Adverse physicochemical, human health and environmental effects

No additional information available

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2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



Signal word (CLP) :

Danger

Hazard statements (CLP) :

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 (CLP) :

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 - Keep container tightly closed
P240 Ground/bond container and receiving equipment.
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water.
P304+P340 - IF INHALED: remove victim to fresh air and keep at rest in a position comfortable for breathing
P331 - Do NOT induce vomiting
P403 - Store in a well-ventilated place
P235 - Keep cool

2.3. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

Name	Product identifier	%
Isooctane	(CAS-No.) 540-84-1 (EC-No.) 208-759-1 (EC Index-No.) 601-009-00-8	100

Full text of H-statements: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general

: Check the vital functions. Unconscious: maintain adequate airway and respiration. Respiratory arrest: artificial respiration or oxygen. Cardiac arrest: perform resuscitation. Victim conscious with laboured breathing: half-seated. Victim in shock: on his back with legs slightly raised. Vomiting: prevent asphyxia/aspiration pneumonia. Prevent cooling by covering the victim (no warming up). Keep watching the victim. Give psychological aid. Keep the victim calm, avoid physical strain. Depending on the victim's condition: doctor/hospital.

First-aid measures after inhalation

: Remove the victim into fresh air. Respiratory problems: consult a doctor/medical service.

First-aid measures after skin contact

: Wash immediately with lots of water. Soap may be used. Take victim to a doctor if irritation persists.

First-aid measures after eye contact

: Rinse with water. Do not apply neutralizing agents. Take victim to an ophthalmologist if irritation persists.

First-aid measures after ingestion

: Rinse mouth with water. Immediately after ingestion: give lots of water to drink. Do not induce vomiting. Ingestion of large quantities: immediately to hospital. Consult a doctor/medical service if you feel unwell. Call Poison Information Centre (www.big.be/antigif.htm).

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

Symptoms/effects after inhalation

: Central nervous system depression. Headache. Dizziness. Mental confusion. Nausea. Respiratory difficulties. EXPOSURE TO HIGH CONCENTRATIONS: Disturbances of consciousness.

Symptoms/effects after skin contact

: Tingling/irritation of the skin.

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Symptoms/effects after eye contact	: Not irritating.
Symptoms/effects after ingestion	: Nausea. Vomiting. Abdominal pain. Risk of aspiration pneumonia.
Chronic symptoms	: ON CONTINUOUS/REPEATED EXPOSURE/CONTACT: Red skin. Dry skin. Skin rash/inflammation.

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

No additional information available

SECTION 5: Fire-fighting measures

5.1. Extinguishing media

Suitable extinguishing media	: Water spray. Polyvalent foam. AFFF foam. Alcohol-resistant foam. Polymer foam. BC powder. Carbon dioxide.
Unsuitable extinguishing media	: Solid water jet ineffective as extinguishing medium.

5.2. Special hazards arising from the substance or mixture

Fire hazard	: DIRECT FIRE HAZARD. Highly flammable. Gas/vapour flammable with air within explosion limits. INDIRECT FIRE HAZARD. May be ignited by sparks. Gas/vapour spreads at floor level: ignition hazard. Reactions involving a fire hazard: see "Reactivity Hazard".
Explosion hazard	: DIRECT EXPLOSION HAZARD. Gas/vapour explosive with air within explosion limits. INDIRECT EXPLOSION HAZARD. may be ignited by sparks. Reactions with explosion hazards: see "Reactivity Hazard".

5.3. Advice for firefighters

Precautionary measures fire	: Exposure to fire/heat: keep upwind. Exposure to fire/heat: have neighbourhood close doors and windows.
Firefighting instructions	: If exposed to fire cool the closed containers by spraying with water. Do not move the load if exposed to heat. Take account of environmentally hazardous firefighting water. Use water moderately and if possible collect or contain it.
Protection during firefighting	: Heat/fire exposure: compressed air/oxygen apparatus.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Protective equipment	: Gloves. Protective goggles. Head/neck protection. Protective clothing. See "Material-Handling" to select protective clothing.
Emergency procedures	: Mark the danger area. Stop engines and no smoking. No naked flames or sparks. Spark- and explosionproof appliances and lighting equipment. Wash contaminated clothes.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent soil and water pollution. Prevent spreading in sewers.

6.3. Methods and material for containment and cleaning up

For containment	: Contain leaking substance. Dam up the liquid spill. Try to reduce evaporation. Measure the concentration of the explosive gas-air mixture. Dilute/disperse combustible gas/vapour with water curtain.
Methods for cleaning up	: Take up liquid spill into a non combustible material e.g.: dry sand/earth/vermiculite kieselguhr, powdered limestone. Scoop absorbed substance into closing containers. Carefully collect the spill/leftovers. Clean contaminated surfaces with a soap solution. Take collected spill to manufacturer/competent authority. Wash clothing and equipment after handling.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling	: Comply with the legal requirements. Remove contaminated clothing immediately. Clean contaminated clothing. Do not discharge the waste into the drain. Insufficient ventilation: take precautions against electrostatic charges. Insufficient ventilation: use spark-/explosionproof appliances and lighting system. Keep away from naked flames/heat. Insufficient ventilation: keep naked flames/sparks away. Observe normal hygiene standards. Keep container tightly closed. Measure the concentration in the air regularly. Work under local exhaust/ventilation.
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7.2. Conditions for safe storage, including any incompatibilities

Heat and ignition sources	: KEEP SUBSTANCE AWAY FROM: heat sources. ignition sources.
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Information on mixed storage	: KEEP SUBSTANCE AWAY FROM: oxidizing agents.
Storage area	: Store in a cool area. Ventilation at floor level. Fireproof storeroom. Unauthorized persons are not admitted. Meet the legal requirements.
Special rules on packaging	: SPECIAL REQUIREMENTS: closing. clean. correctly labelled. meet the legal requirements. Secure fragile packagings in solid containers.
Packaging materials	: SUITABLE MATERIAL: glass. tin. MATERIAL TO AVOID: No data available.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Isooctane (540-84-1)		
Austria	Local name	2,2,4-Trimethylpentan
Austria	MAK (mg/m ³)	1400 mg/m ³
Austria	MAK (ppm)	300 ppm
Austria	MAK Short time value (mg/m ³)	5600 mg/m ³
Austria	MAK Short time value (ppm)	1200 ppm
Finland	Local name	2,2,4-Trimetyylipentaani
Finland	HTP-arvo (8h) (mg/m ³)	1400 mg/m ³
Finland	HTP-arvo (8h) (ppm)	300 ppm
Finland	HTP-arvo (15 min)	1800 mg/m ³
Finland	HTP-arvo (15 min) (ppm)	380 ppm
USA - ACGIH	ACGIH TWA (ppm)	300 ppm (Octane, all isomers; USA; Time-weighted average exposure limit 8 h; TLV - Adopted Value)

8.2. Exposure controls

Materials for protective clothing:

GIVE EXCELLENT RESISTANCE: No data available. GIVE GOOD RESISTANCE: nitrile rubber. viton. PVA. GIVE LESS RESISTANCE: neoprene. GIVE POOR RESISTANCE: butyl rubber. natural rubber. PVC

Hand protection:

Gloves

Eye protection:

Safety glasses

Skin and body protection:

Head/neck protection. Protective clothing

Respiratory protection:

Wear gas mask with filter type A if conc. in air > exposure limit

Device	Filter type	Condition	Standard
Gas mask	Type A - High-boiling (>65 °C) organic compounds	If conc. in air > exposure limit	



SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Liquid.
Molecular mass	: 114.23 g/mol
Colour	: Colourless.

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Odour	: Almost odourless. Petroleum-like odour.
Odour threshold	: No data available
pH	: Neutral
Relative evaporation rate (butylacetate=1)	: > 1
Melting point	: -107 °C
Freezing point	: No data available
Boiling point	: 99 °C (1013 hPa)
Flash point	: -12 °C
Auto-ignition temperature	: 415 °C
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapour pressure	: 51 hPa (20 °C)
Relative vapour density at 20 °C	: 3.9
Relative density	: 0.69
Relative density of saturated gas/air mixture	: 1.15
Density	: 690 kg/m ³
Solubility	: Insoluble in water. Substance floats in water. Soluble in ethanol. Soluble in ether. Soluble in acetone. Soluble in oils/fats. Soluble in tetrachloromethane. Soluble in chloroform. Soluble in toluene. Soluble in xylene. Soluble in heptane. Soluble in carbondisulfide. Soluble in dimethylformamide. Water: 0.56 mg/l (25°C) Ethanol: soluble Ether: soluble Acetone: soluble
Log Pow	: 4.08 - 5.18 (Calculated; KOWWIN)
Viscosity, kinematic	: No data available
Viscosity, dynamic	: 0.0005 Pa.s
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: 1.1 - 6.0 vol % 45 - 290 g/m ³

9.2. Other information

Minimum ignition energy	: 1.4 mJ
Specific conductivity	: < 10000 pS/m
Saturation concentration	: 244 g/m ³
VOC content	: 100 %
Other properties	: Gas/vapour heavier than air at 20°C. Clear. Volatile. Substance has neutral reaction. May generate electrostatic charges.

SECTION 10: Stability and reactivity

10.1. Reactivity

Upon combustion: CO and CO₂ are formed. Reacts exothermically with (strong) oxidizers: (increased) risk of fire/explosion.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

No additional information available

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

No additional information available

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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Isooctane (540-84-1)	
LD50 oral rat	> 2500 mg/kg bodyweight (Rat; Acute Oral Toxicity; IUCLID)
LD50 dermal rabbit	> 2000 mg/kg bodyweight (Rabbit; Experimental value; OECD 402: Acute Dermal Toxicity)
LC50 inhalation rat (mg/l)	> 33.52 mg/l/4h (Rat; Experimental value)

Skin corrosion/irritation : Causes skin irritation.
Serious eye damage/irritation : Not classified
Respiratory or skin sensitisation : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
STOT-single exposure : May cause drowsiness or dizziness.
STOT-repeated exposure : Not classified
Aspiration hazard : May be fatal if swallowed and enters airways.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Dangerous for the environment.
Ecology - air : Not classified as dangerous for the ozone layer (Regulation (EC) No 1005/2009). TA-Luft Klasse 5.2.5/l.
Ecology - water : Ground water pollutant. Harmful to fishes. Very toxic to invertebrates (Daphnia). Toxic to algae. Harmful to bacteria.

Isooctane (540-84-1)	
EC50 Daphnia 1	0.4 mg/l (EC50; Other; 48 h; Daphnia magna; Static system; Fresh water; Read-across)
Threshold limit algae 1	2.943 mg/l (EC50; Other; 72 h; Pseudokirchneriella subcapitata; Fresh water)

12.2. Persistence and degradability

Isooctane (540-84-1)	
Persistence and degradability	Not readily biodegradable in water. Non degradable in the soil.
ThOD	3.5 g O ₂ /g substance

12.3. Bioaccumulative potential

Isooctane (540-84-1)	
BCF fish 2	231 (BCF)
Log Pow	4.08 - 5.18 (Calculated; KOWWIN)

12.4. Mobility in soil

Isooctane (540-84-1)	
Log Koc	log Koc, SRC PCKOCWIN v2.0; 2.58; Calculated value; Koc; SRC PCKOCWIN v2.0; 240.3; Calculated value

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

No additional information available

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SECTION 13: Disposal considerations

13.1. Waste treatment methods

- Product/Packaging disposal recommendations : Remove waste in accordance with local and/or national regulations. Hazardous waste shall not be mixed together with other waste. Different types of hazardous waste shall not be mixed together if this may entail a risk of pollution or create problems for the further management of the waste. Hazardous waste shall be managed responsibly. All entities that store, transport or handle hazardous waste shall take the necessary measures to prevent risks of pollution or damage to people or animals. Recycle by distillation. Remove to an authorized waste incinerator for solvents with energy recovery. Do not discharge into surface water.
- Additional information : LWCA (the Netherlands): KGA category 03. Hazardous waste according to Directive 2008/98/EC.
- European List of Waste (LoW) code : 07 01 04* - other organic solvents, washing liquids and mother liquors

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

ADR	IMDG	IATA	ADN	RID
14.1. UN number				
1262	1262	1262	1262	1262
14.2. UN proper shipping name				
OCTANES	OCTANES	Octanes	OCTANES	OCTANES
Transport document description				
UN 1262 OCTANES, 3, II, (D/E), ENVIRONMENTALLY HAZARDOUS	UN 1262 OCTANES, 3, II, MARINE POLLUTANT/ENVIRONMENTALLY HAZARDOUS	UN 1262 Octanes, 3, II, ENVIRONMENTALLY HAZARDOUS	UN 1262 OCTANES, 3, II, ENVIRONMENTALLY HAZARDOUS	UN 1262 OCTANES, 3, II, ENVIRONMENTALLY HAZARDOUS
14.3. Transport hazard class(es)				
3	3	3	3	3
				
14.4. Packing group				
II	II	II	II	II
14.5. Environmental hazards				
Dangerous for the environment : Yes	Dangerous for the environment : Yes Marine pollutant : Yes	Dangerous for the environment : Yes	Dangerous for the environment : Yes	Dangerous for the environment : Yes
No supplementary information available				

14.6. Special precautions for user

- Overland transport

- Classification code (ADR) : F1
- Limited quantities (ADR) : 11
- Excepted quantities (ADR) : E2
- Packing instructions (ADR) : P001, IBC02, R001
- Mixed packing provisions (ADR) : MP19
- Portable tank and bulk container instructions (ADR) : T4
- Portable tank and bulk container special provisions (ADR) : TP1
- Tank code (ADR) : LGBF
- Vehicle for tank carriage : FL
- Transport category (ADR) : 2
- Special provisions for carriage - Operation (ADR) : S2, S20
- Hazard identification number (Kemler No.) : 33

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Orange plates :

33
1262

Tunnel restriction code (ADR) : D/E
EAC code : 3YE

- Transport by sea

Transport regulations (IMDG) : Subject
Limited quantities (IMDG) : 1 L
Excepted quantities (IMDG) : E2
Packing instructions (IMDG) : P001
IBC packing instructions (IMDG) : IBC02
Tank instructions (IMDG) : T4
Tank special provisions (IMDG) : TP1
EmS-No. (Fire) : F-E
EmS-No. (Spillage) : S-E
Stowage category (IMDG) : B
Properties and observations (IMDG) : Colourless liquids. Explosive limits: 1% to 6.5% ISOOCTANE: flashpoint-12°C c.c. n-OCTANE: flashpoint 13°C c.c. Immiscible with water.
MFAG-No : 128

- Air transport

Transport regulations (IATA) : Subject to the provisions
PCA Excepted quantities (IATA) : E2
PCA Limited quantities (IATA) : Y341
PCA limited quantity max net quantity (IATA) : 1L
PCA packing instructions (IATA) : 353
PCA max net quantity (IATA) : 5L
CAO packing instructions (IATA) : 364
CAO max net quantity (IATA) : 60L
ERG code (IATA) : 3H

- Inland waterway transport

Classification code (ADN) : F1
Limited quantities (ADN) : 1 L
Excepted quantities (ADN) : E2
Carriage permitted (ADN) : T
Equipment required (ADN) : PP, EX, A
Ventilation (ADN) : VE01
Number of blue cones/lights (ADN) : 1

- Rail transport

Transport regulations (RID) : Subject
Classification code (RID) : F1
Limited quantities (RID) : 1L
Excepted quantities (RID) : E2
Packing instructions (RID) : P001, IBC02, R001
Mixed packing provisions (RID) : MP19
Portable tank and bulk container instructions (RID) : T4
Portable tank and bulk container special provisions (RID) : TP1
Tank codes for RID tanks (RID) : LGBF
Transport category (RID) : 2
Colis express (express parcels) (RID) : CE7
Hazard identification number (RID) : 33

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14.7. Transport in bulk according to Annex II of Marpol and the IBC Code

Not applicable

SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

No REACH Annex XVII restrictions

Isooctane is not on the REACH Candidate List

Isooctane is not on the REACH Annex XIV List

VOC content : 100 %

15.1.2. National regulations

Germany

VwVwS Annex reference : Water hazard class (WGK) 2, hazard to waters (KBwS-Beschluss; ID No. 479)

WGK remark : Classification water polluting in compliance with Verwaltungsvorschrift wassergefährdender Stoffe (VwVwS) of 27 July 2005 (Anhang 2)

12th Ordinance Implementing the Federal Immission Control Act - 12.BImSchV : Is not subject of the 12. BImSchV (Hazardous Incident Ordinance)

Netherlands

SZW-lijst van kankerverwekkende stoffen : The substance is not listed

SZW-lijst van mutagene stoffen : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Borstvoeding : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Vruchtbaarheid : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Ontwikkeling : The substance is not listed

Denmark

Classification remarks : Emergency management guidelines for the storage of flammable liquids must be followed

Recommendations Danish Regulation : Young people below the age of 18 years are not allowed to use the product

15.2. Chemical safety assessment

No additional information available

SECTION 16: Other information

Abbreviations and acronyms:

ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE	Acute Toxicity Estimate
BCF	Bioconcentration factor
CLP	Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008
EC50	Median effective concentration
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods
LC50	Median lethal concentration
LD50	Median lethal dose
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals Regulation (EC) No 1907/2006
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail

Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Full text of H- and EUH-statements:

Aquatic Acute 1	Hazardous to the aquatic environment — Acute Hazard, Category 1
Aquatic Chronic 1	Hazardous to the aquatic environment — Chronic Hazard, Category 1

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Asp. Tox. 1	Aspiration hazard, Category 1
Flam. Liq. 2	Flammable liquids, Category 2
Skin Irrit. 2	Skin corrosion/irritation, Category 2
STOT SE 3	Specific target organ toxicity — Single exposure, Category 3, Narcosis
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

SDS ISOLAB

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product