



Safety Data Sheet

Section 1 - Identification.....2

Section 2: Hazard Identification.....2

Section 3: Composition/information on ingredients..... 4

Section 4: First aid measures..... 5

Section 5: Firefighting measurers..... 5

Section 6: Accidental release measurers..... 6

Section 7: Handling and storage..... 7

Section 8: Exposure controls – Personal protection.....8

Section 9: Physical and chemical properties..... 9

Section 10: Stability and reactivity..... 11

Section 11: Toxicological information.....12

Section 12: Ecological information..... 14

Section 13: Disposal considerations..... 16

Section 14: Transportation information..... 17

Section 15: Regulatory information..... 18

Section 16: Other information.....19

Section 1 - Identification

1.1 Product Identifier

Product Name : Isooctane

CAS No. : 540-84-1

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

Identified uses : Reagent for analysis, Chemical production

1.3 Details of the supplier of the safety data sheet

Company : 9920 Pacific Heights Blvd
Suit 150
San Diego
California -92121

1.4 Emergency Telephone number

Emergency phone : +1 (858) 245-0283

Section 2: Hazard Identification

2.1 Classification of the substance or the mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable liquids	Category 2	H225:Highly flammable liquid and vapour.
Skin corrosion	Category 2	H315:Causes skin irritation.
Specific target organ toxicity - single exposure	Category 3	H336:May cause drowsiness or dizziness.
Aspiration hazard	Category 1	H304:May be fatal if swallowed and enters airways.
Short-term (acute) aquatic hazard	Category 1	H400:Very toxic to aquatic life.
Long-term (chronic) aquatic	Category 1	H410:Very toxic to aquatic life

hazard

with long lasting effects.

2.2 Label elements

Label according Regulation (EC) 1272/2008

Hazard Pictogram



Signal Word:
DANGER

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

Prevention

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P273	Avoid release to the environment.

Response:

P301+P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P331	Do NOT induce vomiting.

Reduced Labelling (<= 125 ml)

Hazard Pictogram



Signal Word:
DANGER

Hazard statements

H304 May be fatal if swallowed and enters airways.

Precautionary Statements

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

P331 Do NOT induce vomiting.

Supplemental Hazard Statements none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Section 3: Composition/information on ingredients

3.1 Substance

EC-No. : 208-759-1

Index-No. : 601-009-00-8

Section 4: First aid measures

4.1 Description of first aid measures

General advice

Show this safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

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

In case of eye contact

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

If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labeling (see section 2.2) and/or in section 11.

4.3 Indications 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
	Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazard arising from the substance or mixture

Specific hazards during fire fighting	: Combustible. Pay attention to flashback. Vapours are heavier than air and may spread along floors. Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.
Hazardous combustion products	: Carbon oxides

5.3 Advice for firefighters

Special protective equipment for fire-fighters	: 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. 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

Personal precautions:

Advice for non-emergency personnel: Do not breathe vapors, 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.

For personal protection see section 8.

6.2 Environment precautions

Environmental precautions : Do not let product enter drains.Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Methods for 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

For disposal considerations 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.

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.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Further information on storage conditions

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

sources of ignition.

Storage class (TRGS 510)

3, Flammable liquids

Further information on storage stability

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

Occupational Exposure Limits

Predicted No Effect Concentration (PNEC) according to Regulation (EC) No. 1907/2006

Substance name	Environmental Compartment	Value
	Not applicable	

8.2 Exposure Controls

Personal protective equipment

Eye/face protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Hand protection
Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0,4 mm
Protective index : Full contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Material	: Chloroprene
Break through time	: 120 min
Glove thickness	: 0,65 mm
Protective index	: Splash contact
Manufacturer	: KCL 720 Camapren®
Remarks	: 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Skin and body protection	: Flame retardant antistatic protective clothing.
Respiratory protection	: required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.
Recommended Filter	: Filter A (acc. to DIN 3181) for vapours of organic compounds

type:

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

Advice

Do not let product enter drains. Risk of explosion.

Section 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	: liquid (20 °C, 1.013 hPa)
Color	: Colourless

Odor	: Not data available
Melting point/range	: -107 °C
Boiling point/boiling range	: 99,2 °C (1.000 hPa)
Flammability	: Not data available
Upper explosion limit / Upper flammability limit	: Upper explosion limit 6 %(V)
Lower explosion limit / Lower flammability limit	: Lower explosion limit 1 %(V)
Flash point	: -12 °C Method: closed cup
Autoignition temperature	: 396 °C
Decomposition temperature	: Not data available
pH	: Not data available
Viscosity, dynamic	: Not data available
Viscosity, kinematic	: Not data available
Flow time	: No data available
Solubility(ies) Water solubility	: insoluble
Partition coefficient: n- octanol/water	: log Pow: 4,6 Bioaccumulation is not expected.
Vapor pressure	: 55 hPa (21 °C) 120 hPa (37,80 °C)
Relative density	: Not data available
Density	: 0,69 g/cm3 (15 °C)
Relative vapour density	: 3,94 (Air = 1.0)

9.2 Other information

Explosives	: Not classified as explosive.
Oxidizing properties	: none
Burning rate	: No data available
Evaporation rate	: No data available
Molecular weight	: 114,23 g/mol

Section 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Hazardous reactions : Violent reactions possible with:

Strong oxidizing agents

10.4 Conditions to avoid

Conditions to avoid

Warming.

10.5 Incompatible materials

Materials to avoid : various plastics

10.6 Hazardous decomposition products

In the event of fire: see section 5

Section 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - > 5.000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 33,52 mg/l - vapour

(OECD Test Guideline 403)

Symptoms: mucosal irritations

LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

(OECD Test Guideline 404)

Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximisation Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: TA98

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: human lymphoblastoid cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative

Test Type: unscheduled DNA synthesis assay
Species: Rat
Cell type: Liver cells
Application Route: Oral
Method: OECD Test Guideline 486
Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

Section 12: Ecological information

12.1 Toxicity

Components:

isooctane:

Toxicity to fish	: LC50 (Oncorhynchus mykiss (rainbow trout)): 0,11 mg/l End point: mortality Exposure time: 96 h Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): 0,4 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Remarks: (in analogy to similar products) (ECHA) The value is given in analogy to the following substances: 2,3,4-Trimethylpentane
M-Factor (Acute aquatic toxicity)	: 1
Toxicity to microorganisms	: EC0 (Pseudomonas putida): 10.000 mg/l Remarks: (IUCLID)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : EC50: 0,23 mg/l
Exposure time: 21 d
Species: Daphnia magna (Water flea)
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 211
GLP: yes

M-Factor (Chronic aquatic toxicity) : 1

12.2 Persistence and degradability

Components:

isooctane:

Biodegradability : Test Type: aerobic
Inoculum: activated sludge
Concentration: 49 mg/l
Result: Inherently biodegradable.
Biodegradation: 51,3 %
Exposure time: 28 d
Method: OECD Test Guideline 301F

12.3 Bioaccumulated potential

Components:

isooctane:

Bioaccumulation : Bioconcentration factor (BCF): 231
Partition coefficient: n-octanol/water : log Pow: 4,6
Remarks: Bioaccumulation is not expected.

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

Product:

Assessment:-This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Components:

isooctane:

Assessment : Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

12.6 Endocrine disrupting properties

Product:

Assessment:-The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

Components:

isooctane:

Additional ecological
information

: Biological effects:

Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities.

Discharge into the environment must be avoided.

Section 13: Disposal considerations

13.1 Waste treatment methods

Product : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Section 14: Transportation information

14.1 UN Number or ID number

ADR	UN 1262
IMDG	UN 1262
IATA	UN 1262

14.2 UN proper shipping name

ADR	OCTANES
IMDG	OCTANES
IATA	OCTANES

14.3 Transport hazard class(es)

Class

ADR	3
IMDG	3
IATA	3

Subsidiary risks

ADR	-
IMDG	-
IATA	-

14.4 Packaging group

ADR

Packing group	II
Classification Code	F1
Hazard Identification Number	33
Labels	3
Tunnel restriction code	(D/E)

IMDG

Packing group	II
Labels	3
EmS Code	F-E, S-E

IATA (Cargo)

Packing instruction (cargo aircraft)	364
Packing instruction (LQ)	Y341
Packing group	II
Labels	Class 3 - Flammable liquids

IATA_P (Passenger)

Packing instruction (passenger aircraft)	353
Packing instruction (LQ)	Y341
Packing group	II
Labels	Class 3 - Flammable liquids

14.5 Environmental hazards

ADR

Environmentally hazardous	yes
---------------------------	-----

IMDG

Marine pollutant	yes
------------------	-----

14.6 Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

Section 15: Regulatory information

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

REACH - Restrictions on the manufacture, placing on : Conditions of restriction for the

the market and use of certain dangerous substances, mixtures and articles (Annex XVII)

following entries should be considered:

Number on list 3

Number on list 40

Number on list 75: If you intend to use this product as tattoo ink, please contact your vendor.

REACH - Candidate List of Substances of Very High Concern for Authorisation (Article 59) : Not applicable

Regulation (EU) No 2024/590 on substances that deplete the ozone layer : Not applicable

Regulation (EU) 2019/1021 on persistent organic pollutants (recast) : Not applicable

REACH - List of substances subject to authorisation (Annex XIV) : Not applicable

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

E1 ENVIRONMENTAL HAZARDS

15.2 Chemical safety assessment

A Chemical Safety Assessment has been carried out for this substance.

Section 16: Other information

Full text of H-Statements

H336

May cause drowsiness or dizziness.

Further information

The information and recommendations in this SDS are to the best of our knowledge, information and belief accurate at the time of publication. Although utmost care is been taken in composition of this text, Highpuris LLC cannot be held responsible for any damage resulting from any possible error in this publication.