

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

Product form	: Substance
Trade name	: UN1262 Isooctane AGR, ACS, Ph.Eur.
Chemical name	: 2,2,4-trimethylpentane
IUPAC name	: 2,2,4-trimethylpentane
EC Index-No.	: 601-009-00-8
EC-No.	: 208-759-1
CAS-No.	: 540-84-1
Product code	: ISCT-00A
Formula	: C8H18

1.2. Relevant identified uses of the substance or mixture and uses advised against**1.2.1. Relevant identified uses**

Main use category : Laboratory use

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

labbox labware s.l.
Migjorn, 1
P.O. Box Barcelona (SPAIN)
08338 Premia de Dalt – SPAIN
ES
T +34 937 07 79 70 - F +34 937 909 532
info@labbox.com - www.labbox.com

1.4. Emergency telephone number

Emergency number : +34 937 077 970 (For technical information_Office Hours) In case of medical emergency phone 112 or to your local emergency number.

Country	Organisation/Company	Address	Emergency number	Comment
United Kingdom	National Poisons Information Service (Belfast Centre) Royal Victoria Hospital	Grosvenor Road BT12 6BA	0344 892 0111	

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****Classification according to Regulation (EC) No. 1272/2008 [CLP]**

Flammable liquids, Category 2	H225
Aspiration hazard, Category 1	H304
Skin corrosion/irritation, Category 2	H315
Specific target organ toxicity — Single exposure, Category 3, Narcosis	H336
Hazardous to the aquatic environment — Acute Hazard, Category 1	H400
Hazardous to the aquatic environment — Chronic Hazard, Category 1	H410
Full text of H and EUH statements: see section 16	

Adverse physicochemical, human health and environmental effects

No additional information available

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according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

2.2. Label elements

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

Hazard pictograms (CLP)



Signal word (CLP)

Hazard statements (CLP)

Precautionary statements (CLP)

- : Danger
- : 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.
- : P210 - Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P240 - Ground/bond container and receiving equipment.
P273 - Avoid release to the environment.
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P331 - Do NOT induce vomiting.
P403+P235 - Store in a well-ventilated place. Keep cool.

2.3. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type : Mono-constituent

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

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

- First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. If experiencing respiratory symptoms: Call a poison center or a doctor.
- First-aid measures after skin contact : Gently wash with plenty of soap and water. If skin irritation or rash occurs: Get medical advice/attention.
- First-aid measures after eye contact : Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Consult an ophthalmologist if irritation persists.
- First-aid measures after ingestion : Rinse mouth out with water. Drink plenty of water. Do not induce vomiting. If you feel unwell, seek medical advice.

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

- Symptoms/effects after inhalation : May cause headache, nausea and irritation of respiratory tract.
- Symptoms/effects after skin contact : Irritation.
- Symptoms/effects after ingestion : Abdominal pain, nausea, nausea, vomiting.

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

Never give anything by mouth to an unconscious person.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : ABC-powder.
Unsuitable extinguishing media : Strong water jet.

5.2. Special hazards arising from the substance or mixture

Fire hazard : Highly flammable liquid and vapour.
Hazardous decomposition products in case of fire : Carbon oxides (CO, CO₂).

5.3. Advice for firefighters

Firefighting instructions : Use water spray or fog for cooling exposed containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : No flames, no sparks. Eliminate all sources of ignition.

6.1.1. For non-emergency personnel

Emergency procedures : No open flames, no sparks, and no smoking.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment.

6.2. Environmental precautions

Prevent entry to sewers and public waters.

6.3. Methods and material for containment and cleaning up

For containment : Collect spillage.
Methods for cleaning up : Take up liquid spill into absorbent material. Small quantities of liquid spill: take up in non-combustible absorbent material and shovel into container for disposal. This material and its container must be disposed of in a safe way, and as per local legislation.

6.4. Reference to other sections

See Heading 8. For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Ensure good ventilation of the work station.
Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Comply with applicable regulations.
Storage conditions : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Store in a well-ventilated place. Keep container tightly closed.
Storage area : Store away from heat. Store in a well-ventilated place.
Special rules on packaging : Keep only in original container. Store in a closed container.

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7.3. Specific end use(s)

Laboratory chemicals.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.1.1 National occupational exposure and biological limit values

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)	
USA - ACGIH - Occupational Exposure Limits	
ACGIH OEL TWA [ppm]	300 ppm

8.1.2. Recommended monitoring procedures

No additional information available

8.1.3. Air contaminants formed

No additional information available

8.1.4. DNEL and PNEC

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)	
DNEL/DMEL (Workers)	
Long-term - systemic effects, dermal	773 mg/kg bodyweight/day
Long-term - systemic effects, inhalation	2035 mg/m ³
DNEL/DMEL (General population)	
Long-term - systemic effects, oral	699 mg/kg bodyweight/day
Long-term - systemic effects, inhalation	608 mg/m ³
Long-term - systemic effects, dermal	699 mg/kg bodyweight/day

8.1.5. Control banding

No additional information available

8.2. Exposure controls

8.2.1. Appropriate engineering controls

Appropriate engineering controls:

Ensure good ventilation of the work station.

8.2.2. Personal protection equipment

Personal protective equipment:

EN 374.

Personal protective equipment symbol(s):



8.2.2.1. Eye and face protection

Eye protection:

Safety glasses

8.2.2.2. Skin protection

Hand protection:

protective gloves

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8.2.2.3. Respiratory protection

Respiratory protection:

Wear appropriate mask

8.2.2.4. Thermal hazards

No additional information available

8.2.3. Environmental exposure controls

No additional information available

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Colour	: Colourless.
Appearance	: Liquid.
Molecular mass	: 114,23 g/mol
Odour	: gasoline-like.
Odour threshold	: Not available
Melting point	: -107 °C
Freezing point	: Not available
Boiling point	: 99,2 °C Atm. press.: 100 kPa Decomposition: 'no'
Flammability	: Not available
Explosive limits	: Not available
Lower explosion limit	: 1,1 vol %
Upper explosion limit	: 6 vol %
Flash point	: -12 °C
Auto-ignition temperature	: 415 °C
Decomposition temperature	: Not available
pH	: Not available
Viscosity, kinematic	: 0,723 mm ² /s
Viscosity, dynamic	: 0,5 mPa·s (20 °C)
Solubility	: insoluble in water. Soluble in ethanol. Soluble in ether. Soluble in acetone. Soluble in oils/fats. Soluble in tetrachloroethane. Soluble in chloroform. Soluble in toluene. Soluble in heptane. Soluble in dimethylformamide. Water: < 0,001 g/100ml
Partition coefficient n-octanol/water (Log Kow)	: Not available
Partition coefficient n-octanol/water (Log Pow)	: 4,08 – 5,18
Vapour pressure	: 2,8 kPa Temp.: 20 °C
Vapour pressure at 50 °C	: 195 hPa
Density	: 0,69 g/cm ³ Type: 'density' Temp.: 15 °C
Relative density	: Not available
Relative vapour density at 20 °C	: 3,9
Relative density of saturated gas/air mixture	: 1,2
Particle characteristics	: Not applicable

9.2. Other information

9.2.1. Information with regard to physical hazard classes

No additional information available

9.2.2. Other safety characteristics

Minimum ignition energy	: 1,4 mJ
Specific conductivity	: < 10000 pS/m
VOC content	: 100 %

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

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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

SECTION 11: Toxicological information

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

Acute toxicity (oral) : Not classified
Acute toxicity (dermal) : Not classified
Acute toxicity (inhalation) : Not classified

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)

LD50 oral rat	> 5000 mg/kg bodyweight Animal: rat, Guideline: OECD Guideline 401 (Acute Oral Toxicity), Guideline: EPA OPPTS 870.1100 (Acute Oral Toxicity)
LD50 dermal rabbit	> 2000 mg/kg bodyweight Animal: rabbit, Guideline: OECD Guideline 402 (Acute Dermal Toxicity), Guideline: EPA OPPTS 870.1200 (Acute Dermal Toxicity)
LC50 inhalation rat (mg/l)	> 33,52 mg/l air Animal: rat, Guideline: OECD Guideline 403 (Acute Inhalation Toxicity), Guideline: EPA OPPTS 870.1300 (Acute inhalation toxicity)

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

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)

NOAEC (inhalation, rat, vapour, 90 days)	24,3 mg/l air Animal: rat, Guideline: OECD Guideline 413 (Subchronic Inhalation Toxicity: 90-Day Study)
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Aspiration hazard : May be fatal if swallowed and enters airways.

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)

Viscosity, kinematic	0,723 mm ² /s
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11.2. Information on other hazards

No additional information available

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SECTION 12: Ecological information

12.1. Toxicity

Hazardous to the aquatic environment, short-term (acute) : Very toxic to aquatic life.

Hazardous to the aquatic environment, long-term (chronic) : Very toxic to aquatic life with long lasting effects.

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)

LC50 - Fish [1]	0,11 mg/l Test organisms (species): Oncorhynchus mykiss (previous name: Salmo gairdneri)
EC50 - Daphnia [1]	0,4 mg/l Test organisms (species): Daphnia magna
LOEC (chronic)	0,32 mg/l Test organisms (species): Daphnia magna Duration: '21 d'
NOEC (chronic)	0,17 mg/l Test organisms (species): Daphnia magna Duration: '21 d'

12.2. Persistence and degradability

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)

ThOD	3,5 g O ₂ /g substance
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12.3. Bioaccumulative potential

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)

BCF - Fish [1]	231
Partition coefficient n-octanol/water (Log Pow)	4,08 – 5,18

12.4. Mobility in soil

UN1262 Isooctane AGR, ACS, Ph.Eur. (540-84-1)

Organic Carbon Normalized Adsorption Coefficient (Log Koc)	2,38
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12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Endocrine disrupting properties

No additional information available

12.7. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste treatment methods : Must follow special treatment according to local regulation.
European List of Waste (LoW) code : 15 01 10* - packaging containing residues of or contaminated by dangerous substances
07 01 04* - other organic solvents, washing liquids and mother liquors

SECTION 14: Transport information

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

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14.1. UN number or ID number

UN-No. (ADR) : UN 1262
UN-No. (IMDG) : UN 1262
UN-No. (IATA) : UN 1262
UN-No. (ADN) : UN 1262
UN-No. (RID) : UN 1262

14.2. UN proper shipping name

Proper Shipping Name (ADR) : OCTANES
Proper Shipping Name (IMDG) : OCTANES
Proper Shipping Name (IATA) : Octanes
Proper Shipping Name (ADN) : OCTANES
Proper Shipping Name (RID) : OCTANES
Transport document description (ADR) : UN 1262 OCTANES, 3, II, (D/E), ENVIRONMENTALLY HAZARDOUS
Transport document description (IMDG) : UN 1262 OCTANES, 3, II, MARINE POLLUTANT/ENVIRONMENTALLY HAZARDOUS
Transport document description (IATA) : UN 1262 Octanes, 3, II, ENVIRONMENTALLY HAZARDOUS
Transport document description (ADN) : UN 1262 OCTANES, 3, II, ENVIRONMENTALLY HAZARDOUS
Transport document description (RID) : UN 1262 OCTANES, 3, II, ENVIRONMENTALLY HAZARDOUS

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR) : 3
Danger labels (ADR) : 3



IMDG

Transport hazard class(es) (IMDG) : 3
Danger labels (IMDG) : 3



IATA

Transport hazard class(es) (IATA) : 3
Danger labels (IATA) : 3



ADN

Transport hazard class(es) (ADN) : 3
Danger labels (ADN) : 3



RID

Transport hazard class(es) (RID) : 3
Danger labels (RID) : 3

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14.4. Packing group



Packing group (ADR)	: II
Packing group (IMDG)	: II
Packing group (IATA)	: II
Packing group (ADN)	: II
Packing group (RID)	: II

14.5. Environmental hazards

Dangerous for the environment	: Yes
Marine pollutant	: Yes
Other information	: No supplementary information available

14.6. Special precautions for user

Overland transport

Classification code (ADR)	: F1
Limited quantities (ADR)	: 1I
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
Orange plates	:  
Tunnel restriction code (ADR)	: D/E
EAC code	: 3YE

Transport by sea

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% ISOCTANE: flashpoint-12°C c.c. n-OCTANE: flashpoint 13°C c.c. Immiscible with water.

Air transport

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

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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

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

14.7. Maritime transport in bulk according to IMO instruments

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

REACH Annex XVII (Restriction List)

EU restriction list (REACH Annex XVII)	
Reference code	Applicable on
3.	UN1262 Isooctane AGR, ACS, Ph.Eur.
40.	UN1262 Isooctane AGR, ACS, Ph.Eur.

REACH Annex XIV (Authorisation List)

UN1262 Isooctane AGR, ACS, Ph.Eur. is not on the REACH Annex XIV List

REACH Candidate List (SVHC)

UN1262 Isooctane AGR, ACS, Ph.Eur. is not on the REACH Candidate List

PIC Regulation (Prior Informed Consent)

UN1262 Isooctane AGR, ACS, Ph.Eur. is not subject to Regulation (EU) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of hazardous chemicals.

POP Regulation (Persistent Organic Pollutants)

UN1262 Isooctane AGR, ACS, Ph.Eur. is not subject to Regulation (EU) No 2019/1021 of the European Parliament and of the Council of 20 June 2019 on persistent organic pollutants

Ozone Regulation (1005/2009)

Isooctane is not subject to REGULATION (EU) No 1005/2009 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 September 2009 on substances that deplete the ozone layer.

VOC Directive (2004/42)

VOC content : 100 %

UN1262 Isooctane AGR, ACS, Ph.Eur.

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according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

Explosives Precursors Regulation (2019/1148)

Contains no substance subject to Regulation (EU) 2019/1148 of the European Parliament and of the Council of 20 June 2019 on the marketing and use of explosives precursors.

Drug Precursors Regulation (273/2004)

Contains no substance subject to Regulation (EC) 273/2004 of the European Parliament and of the Council of 11 February 2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances.

15.1.2. National regulations

Germany

Water hazard class (WGK) : WGK 2, Significantly hazardous to water (KBwS-Beschluss; ID No. 479).
Hazardous Incident Ordinance (12. BImSchV) : Is not subject of the Hazardous Incident Ordinance (12. BImSchV)

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
Danish National Regulations : 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

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

Safety Data Sheet (SDS), EU

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.