

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 7-Acetyl-1,2,3,4,5,6,7,8-octahydro-1,1,6,7-tetramethylnaphthalene, mixture of isomers

Product Number : 38375
Brand : Sigma-Aldrich

CAS-No. : 54464-57-2

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin irritation (Category 2), H315

Skin sensitisation (Category 1), H317

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Warning

Hazard statement(s)

H315

Causes skin irritation.

H317

May cause an allergic skin reaction.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P261

Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.

P264

Wash skin thoroughly after handling.

P272

Contaminated work clothing should not be allowed out of the workplace.

P273

Avoid release to the environment.

P280

Wear protective gloves.

P302 + P352

IF ON SKIN: Wash with plenty of soap and water.

P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P391	Collect spillage.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : ISO E® alpha + beta+ gamma
 Iso E Super
 2-Acetyl-2,3,8,8-tetramethyloctalin
 1-(1,2,3,4,5,6,7,8-Octahydro-2,3,8,8-tetramethyl-2-naphthalenyl)ethanone

Formula : C16H26O
 CAS-No. : 54464-57-2

Hazardous components

Component	Classification	Concentration
Reaction Mass of 1-(1,2,3,4,5,6,7,8-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one and 1-(1,2,3,4,6,7,8,8a-octahydro-2,3,8,8-tetramethyl-2- naphthyl)ethan-1-one and 1-(1,2,3,5,6,7,8,8a-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1- one		
	Skin Irrit. 2; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1; H315, H317, H410	90 - 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.
For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature 2 - 8 °C

Moisture sensitive. Store under argon.

Storage class (TRGS 510): 10: Combustible liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

Hazardous components without workplace control parameters

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES**9.1 Information on basic physical and chemical properties**

a) Appearance	Form: liquid Colour: light yellow
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/freezing point: < -20 °C (< -4 °F)
f) Initial boiling point and boiling range	290.4 °C (554.7 °F) at 1,013.25 hPa (760.00 mmHg)
g) Flash point	134 °C (273 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	0.233 hPa (0.175 mmHg) at 23 °C (73 °F)
l) Vapour density	No data available
m) Relative density	0.996 g/cm ³ at 25 °C (77 °F)
n) Water solubility	2.68 g/l at 20 °C (68 °F) at > 6.59 - < 6.69 hPa (> 4.94 - < 5.02 mmHg) - slightly soluble
o) Partition coefficient: n-octanol/water	log Pow: 5.65 at 30 °C (86 °F)
p) Auto-ignition temperature	260 °C (500 °F) at 1,021 - 1,025 hPa (766 - 769 mmHg)
q) Decomposition temperature	No data available
r) Viscosity	32.61 mm ² /s at 20 °C (68 °F) -
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY**10.1 Reactivity**

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION**11.1 Information on toxicological effects****Acute toxicity**

LD50 Oral - Rat - > 5,000 mg/kg

Inhalation: No data available

LD50 Dermal - Rat - > 5,000 mg/kg

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

in vivo assay - Mouse

Result: May cause sensitisation by skin contact.

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: Not available

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish semi-static test NOEC - Danio rerio (zebra fish) - 0.16 mg/l - 30 d

12.2 Persistence and degradability

Biodegradability Result: - Not rapidly biodegradable

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life with long lasting effects.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

UN number: 3082

Class: 9

Packing group: III

EMS-No: F-A, S-F

Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Reaction Mass of 1-(1,2,3,4,5,6,7,8-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one and 1-(1,2,3,4,6,7,8,8a-octahydro-2,3,8,8-tetramethyl-2- naphthyl)ethan-1-one and 1-(1,2,3,5,6,7,8,8a-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1- one)
Marine pollutant:yes

IATA

UN number: 3082

Class: 9

Packing group: III

Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Reaction Mass of 1-(1,2,3,4,5,6,7,8-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one and 1-(1,2,3,4,6,7,8,8a-octahydro-2,3,8,8-tetramethyl-2- naphthyl)ethan-1-one and 1-(1,2,3,5,6,7,8,8a-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1- one)

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Reaction Mass of 1-(1,2,3,4,5,6,7,8-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one and 1- (1,2,3,4,6,7,8,8a-octahydro-2,3,8,8-tetramethyl-2- naphthyl)ethan-1-one and 1-(1,2,3,5,6,7,8,8a-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1- one	54464-57-2	

	CAS-No.	Revision Date
Reaction Mass of 1-(1,2,3,4,5,6,7,8-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one and 1- (1,2,3,4,6,7,8,8a-octahydro-2,3,8,8-tetramethyl-2- naphthyl)ethan-1-one and 1-(1,2,3,5,6,7,8,8a-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1- one	54464-57-2	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Reaction Mass of 1-(1,2,3,4,5,6,7,8-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one and 1- (1,2,3,4,6,7,8,8a-octahydro-2,3,8,8-tetramethyl-2- naphthyl)ethan-1-one and 1-(1,2,3,5,6,7,8,8a-octahydro- 2,3,8,8-tetramethyl-2-naphthyl)ethan-1- one	54464-57-2	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.
Skin Irrit.	Skin irritation

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	1
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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