

SAFETY DATA SHEET

1. Identification

Product identifier	3-METHYL-2-CYCLOHEXENONE	
Other means of identification		
BRI Product Code	822	
FEMA number	3360	
Synonyms	2-Cyclohexen-1-one, 3-methyl- * 3-Methyl-2-cyclohexen-1-one * 3-Methylcyclohex-2-en-1-one	
Recommended use	flavors and fragrances For Manufacturing Use Only	
Recommended restrictions	Not for use in Tobacco or Nicotine delivery device applications and/or products.	
Manufacturer/Importer/Supplier/Distributor information		
Manufacturer		
Company name	Bedoukian Research	
Address	21 Finance Drive Danbury, CT 06810 United States	
Telephone	1-203-830-4000	
Website	www.bedoukian.com	
E-mail	customerservice@bedoukian.com	
Contact person	Joseph Bania	
Emergency phone number	Chemtec (North America)	1-800-424-9300
	Chemtec (International)	1-703-527-3887

2. Hazard(s) identification

Physical hazards	Flammable liquids	Category 4
Health hazards	Acute toxicity, oral	Category 4
	Serious eye damage/eye irritation	Category 2B
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	

Label elements



Signal word	Warning
Hazard statement	Combustible liquid. Harmful if swallowed. Causes eye irritation.
Precautionary statement	
Prevention	Keep away from flames and hot surfaces-No smoking. Wash thoroughly after handling. Do not eat, drink or smoke when using this product. Wear protective gloves/eye protection/face protection.
Response	If swallowed: Call a poison center/doctor if you feel unwell. If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Rinse mouth. If eye irritation persists: Get medical advice/attention. In case of fire: Use appropriate media to extinguish.
Storage	Store in a well-ventilated place. Keep cool.
Disposal	Dispose of contents/container in accordance with local/regional/national/international regulations.
Hazard(s) not otherwise classified (HNOC)	None known.
Supplemental information	None.

3. Composition/information on ingredients

Substances

Chemical name	Common name and synonyms	CAS number	%
3-METHYL-2-CYCLOHEXENONE	2-Cyclohexen-1-one, 3-methyl- 3-Methyl-2-cyclohexen-1-one 3-Methylcyclohex-2-en-1-one	1193-18-6	100

Stabilizers

Chemical name	Common name and synonyms	CAS number	%
synthetic alpha tocopherol		10191-41-0	0.1

*Designates that a specific chemical identity and/or percentage of composition has been withheld as a trade secret.

Composition comments Occupational Exposure Limits for stabilizers are listed in Section 8.

4. First-aid measures

Inhalation

Move to fresh air. Call a physician if symptoms develop or persist.

Skin contact

Wash off with soap and water. Get medical attention if irritation develops and persists.

Eye contact

Immediately flush eyes with plenty of water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention if irritation develops and persists.

Ingestion

Rinse mouth. If vomiting occurs, keep head low so that stomach content doesn't get into the lungs. Get medical advice/attention if you feel unwell.

Most important symptoms/effects, acute and delayed

Irritation of eyes. Exposed individuals may experience eye tearing, redness, and discomfort.

Indication of immediate medical attention and special treatment needed

Provide general supportive measures and treat symptomatically. Keep victim warm. Keep victim under observation. Symptoms may be delayed.

General information

Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves. Show this safety data sheet to the doctor in attendance.

5. Fire-fighting measures

Suitable extinguishing media

Water fog. Foam. Dry chemical powder. Carbon dioxide (CO₂).

Unsuitable extinguishing media

Do not use water jet as an extinguisher, as this will spread the fire.

Specific hazards arising from the chemical

The product is combustible, and heating may generate vapors which may form explosive vapor/air mixtures. During fire, gases hazardous to health may be formed.

Special protective equipment and precautions for firefighters

Self-contained breathing apparatus and full protective clothing must be worn in case of fire.

Fire fighting equipment/instructions

In case of fire and/or explosion do not breathe fumes. Move containers from fire area if you can do so without risk.

Specific methods

Use standard firefighting procedures and consider the hazards of other involved materials.

General fire hazards

Combustible liquid.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Keep unnecessary personnel away. Keep people away from and upwind of spill/leak. Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Wear appropriate protective equipment and clothing during clean-up. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. Local authorities should be advised if significant spillages cannot be contained. For personal protection, see section 8 of the SDS.

Methods and materials for containment and cleaning up

Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Keep combustibles (wood, paper, oil, etc.) away from spilled material.

Large Spills: Stop the flow of material, if this is without risk. Dike the spilled material, where this is possible. Cover with plastic sheet to prevent spreading. Use a non-combustible material like vermiculite, sand or earth to soak up the product and place into a container for later disposal. Following product recovery, flush area with water.

Small Spills: Absorb with earth, sand or other non-combustible material and transfer to containers for later disposal. Wipe up with absorbent material (e.g. cloth, fleece). Clean surface thoroughly to remove residual contamination.

Never return spills to original containers for re-use. For waste disposal, see section 13 of the SDS. Avoid discharge into drains, water courses or onto the ground.

Environmental precautions

7. Handling and storage

Precautions for safe handling

Keep away from open flames, hot surfaces and sources of ignition. Do not taste or swallow. Avoid contact with eyes. When using, do not eat, drink or smoke. Provide adequate ventilation. Wear appropriate personal protective equipment. Wash hands thoroughly after handling. Observe good industrial hygiene practices.

Conditions for safe storage, including any incompatibilities

Keep away from heat, sparks and open flame. Store in a cool, dry place out of direct sunlight. Store in original tightly closed container. Store in a well-ventilated place. Keep in an area equipped with sprinklers. Store away from incompatible materials (see Section 10 of the SDS). Recommended Packaging: Glass, Plastic, Aluminum or Phenolic Lined Steel. Store tightly sealed under inert gas in a cool, well-ventilated area.

8. Exposure controls/personal protection

Occupational exposure limits

No exposure limits noted for ingredient(s).

Biological limit values

No biological exposure limits noted for the ingredient(s).

Appropriate engineering controls

Good general ventilation (typically 10 air changes per hour) should be used. Ventilation rates should be matched to conditions. If applicable, use process enclosures, local exhaust ventilation, or other engineering controls to maintain airborne levels below recommended exposure limits. If exposure limits have not been established, maintain airborne levels to an acceptable level. Provide eyewash station.

Individual protection measures, such as personal protective equipment

Eye/face protection

Face shield is recommended. Wear safety glasses with side shields (or goggles).

Skin protection

Hand protection

Wear appropriate chemical resistant gloves. Suitable gloves can be recommended by the glove supplier.

Other

Wear suitable protective clothing.

Respiratory protection

If engineering controls do not maintain airborne concentrations below recommended exposure limits (where applicable) or to an acceptable level (in countries where exposure limits have not been established), an approved respirator must be worn.

Thermal hazards

Wear appropriate thermal protective clothing, when necessary.

General hygiene considerations

When using do not smoke. Keep away from food and drink. Always observe good personal hygiene measures, such as washing after handling the material and before eating, drinking, and/or smoking. Routinely wash work clothing and protective equipment to remove contaminants.

9. Physical and chemical properties

Appearance

Physical state

Liquid.

Color

colorless to yellow

Odor

powerful nutty, caramel-like odor

Odor threshold

Not available.

pH

Not available.

Melting point/freezing point

-5.8 °F (-21 °C)

Initial boiling point and boiling range

393.8 °F (201 °C) Literature reference.

Flash point

165 °F (74 °C) Closed Cup

Evaporation rate

Not available.

Flammability (solid, gas)	Not applicable.
Upper/lower flammability or explosive limits	
Flammability limit - lower (%)	Not available.
Flammability limit - upper (%)	Not available.
Explosive limit - lower (%)	Not available.
Explosive limit - upper (%)	Not available.
Vapor pressure	0.34 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Vapor density	3.8 Relative to air; air = 1
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	1.75 US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Auto-ignition temperature	Not available.
Decomposition temperature	Not available.
Viscosity	Not available.
Other information	
Density	0.962 - 0.972 g/cm3
Explosive properties	Not explosive.
Flammability class	Combustible IIIA estimated
Molecular formula	C7H10O
Molecular weight	110.16
Oxidizing properties	Not oxidizing.
Specific gravity	0.962 - 0.972 at 25°C

10. Stability and reactivity

Reactivity	The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability	Material is stable under normal conditions.
Possibility of hazardous reactions	Hazardous polymerization does not occur.
Conditions to avoid	Avoid heat, sparks, open flames and other ignition sources. Avoid temperatures exceeding the flash point. Contact with incompatible materials.
Incompatible materials	Strong oxidizing agents.
Hazardous decomposition products	No hazardous decomposition products are known.

11. Toxicological information

Information on likely routes of exposure

Inhalation	No adverse effects due to inhalation are expected.
Skin contact	No adverse effects due to skin contact are expected.
Eye contact	Causes eye irritation.
Ingestion	Harmful if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics Irritation of eyes. Exposed individuals may experience eye tearing, redness, and discomfort.

Information on toxicological effects

Acute toxicity Harmful if swallowed.

Product	Species	Test Results
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3-METHYL-2-CYCLOHEXENONE (CAS 1193-18-6)

Acute

Inhalation

Liquid

LC0	Rat	> 19.7 mg/l, 1 hr No mortality noted. Literature reference
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Oral

Vapor

LD50	Mouse	1600 mg/kg Literature reference
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* Estimates for product may be based on additional component data not shown.

Skin corrosion/irritation Prolonged skin contact may cause temporary irritation.

Irritation Corrosion - Skin

3-METHYL-2-CYCLOHEXENONE

100 % Buehler, Preliminary irritation study as part of a skin sensitization assay. Vehicle acetone, 10, 25, 50, 75% tested. 50% was selected for the challenge phase of the sensitization study. At 75% there was 1/4 guinea pigs with a mild erythema (0.5) after 24 hours, that was still present at 48 hours.
Result: Irritation noted.
Species: Guinea pig
Organ: Skin
Notes: BRI study

Serious eye damage/eye irritation Causes eye irritation.

Irritation Corrosion - Eye

3-METHYL-2-CYCLOHEXENONE

100 %, 6 animals tested. Conjunctival irritation, but no effects on the iris or cornea were noted. All effects decreased in severity after 24 hours and no effects were observed 1 week after treatment.
Result: Irritation noted.
Species: Rabbit
Organ: Eye
Notes: Literature reference

Respiratory or skin sensitization

Respiratory sensitization Not a respiratory sensitizer.

Skin sensitization This product is not expected to cause skin sensitization.

Skin sensitization

3-METHYL-2-CYCLOHEXENONE

USEPA OPPTS 870.2600, Induction at 100%, challenge 50% in acetone.
Result: Not sensitizing.
Species: Guinea pig
Organ: Skin
Notes: BRI study

Germ cell mutagenicity No data available to indicate product or any components present at greater than 0.1% are mutagenic or genotoxic.

Germ cell mutagenicity: Ames test

3-METHYL-2-CYCLOHEXENONE

quantitative forward mutation assay, Strain TM 677 with and without metabolic activation. Doses 0.31 - 5.0 mg/mL. Vehicle DMSO.
Result: exhibited no significant activity
Species: Salmonella typhimurium
Notes: Literature reference

Carcinogenicity This product is not considered to be a carcinogen by IARC, ACGIH, NTP, or OSHA.

IARC Monographs. Overall Evaluation of Carcinogenicity

Not listed.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity	This product is not expected to cause reproductive or developmental effects.
Specific target organ toxicity - single exposure	Not classified.
Specific target organ toxicity - repeated exposure	Not classified.
Aspiration hazard	Not an aspiration hazard.

12. Ecological information

Ecotoxicity	The product is not classified as environmentally hazardous. However, this does not exclude the possibility that large or frequent spills can have a harmful or damaging effect on the environment.
Persistence and degradability	No data is available on the degradability of this product.
Bioaccumulative potential	

Partition coefficient n-octanol / water (log Kow)

3-METHYL-2-CYCLOHEXENONE

1.75, US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

Mobility in soil	No data available.
Other adverse effects	No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations

Disposal instructions	Collect and reclaim or dispose in sealed containers at licensed waste disposal site. Dispose of contents/container in accordance with local/regional/national/international regulations.
Local disposal regulations	Dispose in accordance with all applicable regulations.
Hazardous waste code	The waste code should be assigned in discussion between the user, the producer and the waste disposal company.
Waste from residues / unused products	Dispose of in accordance with local regulations. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).
Contaminated packaging	Since emptied containers may retain product residue, follow label warnings even after container is emptied. Empty containers should be taken to an approved waste handling site for recycling or disposal.

14. Transport information

DOT	Not regulated as dangerous goods.
IATA	Not regulated as dangerous goods.
IMDG	Not regulated as dangerous goods.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not established.

15. Regulatory information

US federal regulations	This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.
TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)	Not regulated.
CERCLA Hazardous Substance List (40 CFR 302.4)	Not listed.
SARA 304 Emergency release notification	Not regulated.
OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)	Not regulated.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

Hazard categories Immediate Hazard - Yes
Delayed Hazard - No
Fire Hazard - Yes
Pressure Hazard - No
Reactivity Hazard - No

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous chemical Yes

SARA 313 (TRI reporting)
Not regulated.

Other federal regulations

Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act (SDWA) Not regulated.

US state regulations

US. California Controlled Substances. CA Department of Justice (California Health and Safety Code Section 11100)

Not listed.

US. Massachusetts RTK - Substance List

Not regulated.

US. New Jersey Worker and Community Right-to-Know Act

Not listed.

US. Pennsylvania Worker and Community Right-to-Know Law

Not listed.

US. Rhode Island RTK

Not regulated.

US. California Proposition 65

California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins.

International Inventories

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	Yes
Canada	Domestic Substances List (DSL)	Yes
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	No
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	Yes
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	No
Korea	Existing Chemicals List (ECL)	Yes
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	No
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	Yes

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)

A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision

Issue date 05-26-2015
Revision date 03-09-2017
Version # 02

Disclaimer

Bedoukian Research cannot anticipate all conditions under which this information and its product, or the products of other manufacturers in combination with its product, may be used. It is the user's responsibility to ensure safe conditions for handling, storage and disposal of the product, and to assume liability for loss, injury, damage or expense due to improper use. The information in the sheet was written based on the best knowledge and experience currently available.

Revision information

This document has undergone significant changes and should be reviewed in its entirety.

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