

SECTION 1: Identification

1.1. Product identifier

Product name	: NEOHEXENE
Product code	: ENEN3030
Product form	: Substance
Physical state	: Liquid
Formula	: C6H12
Synonyms	: 3,3-DIMETHYL-1-BUTENE
Chemical family	: HYDROCARBON

1.2. Recommended use of the chemical and restrictions on use

Recommended use	: Chemical intermediate For research and industrial use only
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1.3. Details of the supplier of the safety data sheet

GELEST, INC.
11 East Steel Road
Morrisville, PA 19067
USA
T 215-547-1015 - F 215-547-2484 - (M-F): 8:00 AM - 5:30 PM EST
info@gelest.com - www.gelest.com

1.4. Emergency telephone number

Emergency number	: CHEMTREC: 1-800-424-9300 (USA); +1 703-527-3887 (International)
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SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS-US classification

Flammable liquids Category 2	H225
Hazardous to the aquatic environment - Acute Hazard Category 2	H401
Full text of H statements : see section 16	

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :



GHS02

Signal word (GHS-US)	: Danger
Hazard statements (GHS-US)	: H225 - Highly flammable liquid and vapor H401 - Toxic to aquatic life
Precautionary statements (GHS-US)	: P280 - Wear protective gloves/protective clothing/eye protection/face protection P210 - Keep away from heat, open flames, sparks. - No smoking P233 - Keep container tightly closed P240 - Ground/Bond container and receiving equipment P241 - Use explosion-proof electrical equipment P242 - Use only non-sparking tools P243 - Take precautionary measures against static discharge P273 - Avoid release to the environment P303+P361+P353 - If on skin (or hair): take off immediately all contaminated clothing. rinse skin with water/shower P370+P378 - In case of fire: Use water spray or fog, foam, carbon dioxide, dry chemical to extinguish P403+P235 - Keep in a cool place P501 - Dispose of contents/container to licensed waste disposal facility

2.3. Hazards not otherwise classified (HNOC)

No additional information available

2.4. Unknown acute toxicity (GHS US)

No data available

NEOHEXENE

Safety Data Sheet

SECTION 3: Composition/Information on ingredients

3.1. Substances

Substance type : Multi-constituent
Name : NEOHEXENE
CAS No : 558-37-2

Name	Product identifier	%	GHS-US classification
Neohexene	(CAS No) 558-37-2	95 - 100	Flam. Liq. 2, H225 Aquatic Acute 2, H401
2,3-Dimethylbutene	(CAS No) 563-78-0	0 - 3	Flam. Liq. 2, H225

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

3.2. Mixtures

Not applicable

4.1. Description of first aid measures

First-aid measures general : Remove contaminated clothing and shoes. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). If possible show this sheet; if not available show packaging or label.

First-aid measures after inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If you feel unwell, seek medical advice.

First-aid measures after skin contact : Wash with plenty of soap and water. Get medical advice/attention.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.

First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Get medical advice/attention.

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

Symptoms/injuries after inhalation : May cause irritation to the respiratory tract. May be harmful if inhaled.

Symptoms/injuries after skin contact : May cause mild skin irritation. May be harmful in contact with skin.

Symptoms/injuries after eye contact : May cause eye irritation.

Symptoms/injuries after ingestion : May be harmful if swallowed.

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

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Water spray. Water fog. Foam. Carbon dioxide. Dry chemical.

Unsuitable extinguishing media : None known.

5.2. Special hazards arising from the substance or mixture

Fire hazard : Highly flammable liquid and vapor. Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.

Explosion hazard : May form flammable/explosive vapor-air mixture.

5.3. Advice for firefighters

Firefighting instructions : Exercise caution when fighting any chemical fire. Use water spray or fog for cooling exposed containers.

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection. Avoid all eye and skin contact and do not breathe vapor and mist.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Eliminate every possible source of ignition. Use special care to avoid static electric charges.

6.1.1. For non-emergency personnel

Protective equipment : Wear protective equipment as described in Section 8.

Emergency procedures : Evacuate unnecessary personnel.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Equip cleanup crew with proper protection. For further information refer to section 8: "Exposure controls/personal protection".

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

NEOHEXENE

Safety Data Sheet

6.3. Methods and material for containment and cleaning up

For containment	: Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams.
Methods for cleaning up	: Clean up any spills as soon as possible, using an absorbent material to collect it. Use only non-sparking tools.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed	: Handle empty containers with care because residual vapors are flammable. Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
Precautions for safe handling	: Avoid all eye and skin contact and do not breathe vapor and mist. Ground/bond container and receiving equipment. Provide good ventilation in process area to prevent accumulation of vapors. Take precautionary measures against static discharge. Use only non-sparking tools.
Hygiene measures	: Wash contaminated clothing before reuse. 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	: Proper grounding procedures to avoid static electricity should be followed. Use explosion-proof electrical equipment.
Storage conditions	: Keep container tightly closed. Keep in a cool place.
Incompatible materials	: Oxidizing agent.
Storage area	: Store in a well-ventilated place. Store away from heat.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls	: Provide local exhaust or general room ventilation.
Personal protective equipment	: Avoid all unnecessary exposure. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.
Hand protection	: Neoprene or nitrile rubber gloves.
Eye protection	: Chemical goggles. Contact lenses should not be worn.
Skin and body protection	: Wear suitable protective clothing.
Respiratory protection	: Where exposure through inhalation may occur from use, respiratory protection equipment is recommended. NIOSH-certified organic vapor (black cartridge) respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Clear liquid.
Molecular mass	: 84.16 g/mol
Color	: No data available
Odor	: Mild. Sweet.
Odor threshold	: No data available
Refractive index	: 1.376
pH	: No data available
Relative evaporation rate (butyl acetate=1)	: > 1
Melting point	: -115 °C
Freezing point	: No data available
Boiling point	: 41 °C
Flash point	: -32 °C
Auto-ignition temperature	: 357 °C
Decomposition temperature	: No data available
Flammability (solid, gas)	: Highly flammable liquid and vapor
Vapor pressure	: No data available
Relative vapor density at 20 °C	: > 1

NEOHEXENE

Safety Data Sheet

Relative density	: 0.653
VOC content	: 100 %
Solubility	: Insoluble in water.
Log Pow	: No data available
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Explosion limits	: 1.2 - 9 vol % (lower; upper)

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Heat. Open flame. Sparks.

10.5. Incompatible materials

Oxidizing agent.

10.6. Hazardous decomposition products

Organic acid vapors.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Neohexene (558-37-2)	
LD50 oral rat	> 5000 mg/kg RTECS Number: EM5105000
LD50 oral rabbit	3000 mg/kg
LC50 inhalation rat (ppm)	> 51000 ppm/4h

Skin corrosion/irritation : Not classified

Serious eye damage/irritation : Not classified

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

None of the components in this product at concentrations >0.1% are listed by IARC, NTP, OSHA or ACGIH as a carcinogen

Reproductive toxicity : Not classified

Specific target organ toxicity – single exposure : Not classified

Specific target organ toxicity – repeated exposure : Not classified

Aspiration hazard : Not classified

Symptoms/injuries after inhalation : May cause irritation to the respiratory tract. May be harmful if inhaled.

Symptoms/injuries after skin contact : May cause mild skin irritation. May be harmful in contact with skin.

Symptoms/injuries after eye contact : May cause eye irritation.

Symptoms/injuries after ingestion : May be harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Toxic to aquatic life.

NEOHEXENE

Safety Data Sheet

Neohexene (558-37-2)

ErC50 (algae) : 5.02 mg/l (selenastrum capricornutum)

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Effect on ozone layer : No additional information available
Effect on the global warming : No known effects from this product.
GWPmix comment : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Sewage disposal recommendations : Do not dispose of waste into sewer.
Waste disposal recommendations : Incinerate. Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to licensed waste disposal facility.
Additional information : Handle empty containers with care because residual vapors are flammable.
Ecology - waste materials : Avoid release to the environment.

SECTION 14: Transport information

14.1. UN number

UN-No.(DOT) : 2288
DOT NA no. : UN2288

14.2. UN proper shipping name

Transport document description : UN2288 Isohexenes, 3, II
Proper Shipping Name (DOT) : Isohexenes
Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120
Packing group (DOT) : II - Medium Danger
Hazard labels (DOT) : 3 - Flammable liquid



DOT Packaging Non Bulk (49 CFR 173.xxx) : 202
DOT Packaging Bulk (49 CFR 173.xxx) : 242
DOT Packaging Exceptions (49 CFR 173.xxx) : 150

14.3. Additional information

Emergency Response Guide (ERG) Number : 128
Other information : No supplementary information available.

Transport by sea

DOT Vessel Stowage Location : E - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length, but is prohibited from carriage on passenger vessels in which the limiting number of passengers is exceeded

Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 5 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 60 L

SECTION 15: Regulatory information

15.1. US Federal regulations

NEOHEXENE

Safety Data Sheet

Neohexene (558-37-2)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

2,3-Dimethylbutene (563-78-0)

Not listed on the United States TSCA (Toxic Substances Control Act) inventory

15.2. International regulations

CANADA

Neohexene (558-37-2)

Listed on the Canadian NDSL (Non-Domestic Substances List)

EU-Regulations

Neohexene (558-37-2)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

2,3-Dimethylbutene (563-78-0)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

National regulations

Neohexene (558-37-2)

Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
Listed on the Japanese ISHL (Industrial Safety and Health Law)
Listed on the Korean ECL (Existing Chemicals List)
Listed on NZIoC (New Zealand Inventory of Chemicals)

2,3-Dimethylbutene (563-78-0)

Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Listed on the Korean ECL (Existing Chemicals List)

15.3. US State regulations

No additional information available

SECTION 16: Other information

Full text of H-phrases::

H225	Highly flammable liquid and vapor
H401	Toxic to aquatic life

Abbreviations and acronyms

: Abbreviations: ND: Not Determined, No Data; NA: Not Applicable; LD: Lethal Dose; LC: Lethal Concentration; ATE: Acute Toxicity Estimates; H: hour; °: °C unless otherwise stated; mm: millimeters Hg, torr; PEL: permissible exposure level; TWA: time weighted average; TLV: threshold limit value; TG: Test Guideline; NIOSH: National Institute for Occupational Safety and Health; IARC: International Agency for Research on Cancer; NTP: National Toxicology Program; HMIS: Hazardous Material Information System; CAS No.: Chemical Abstract Service Registration Number; EC No.: European Commission Registration Number; EC Index No.: European Commission Index Number; OECD: The Organisation for Economic Co-operation and Development; GHS: The Globally Harmonized System of Classification and Labelling.

HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur
Flammability : 4 Severe Hazard - Flammable gases, or very volatile flammable liquids with flash points below 73 F, and boiling points below 100 F. Materials may ignite spontaneously with air. (Class IA)
Physical : 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

Prepared by safety and environmental affairs.

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SDS US (GHS HazCom 2012) - Custom

According to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

NEOHEXENE

Safety Data Sheet

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