SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: Hexane, mixture of isomers

Product Number: 178918

Brand: SIGALD

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 Inc.

3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765

Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

- Flammable liquids (Category 2), H225
- Skin irritation (Category 2), H315
- Reproductive toxicity (Category 2), H361
- Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
- Specific target organ toxicity - repeated exposure, Inhalation (Category 2), H373
- Aspiration hazard (Category 1), H304
- Short-term (acute) aquatic hazard (Category 2), H401
- Long-term (chronic) aquatic hazard (Category 2), H411

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

2.2 GHS Label elements, including precautionary statements

Pictogram:

SIGALD - 178918
Signal word: Danger

Hazard statement(s):
- H225: Highly flammable liquid and vapor.
- H304: May be fatal if swallowed and enters airways.
- H315: Causes skin irritation.
- H336: May cause drowsiness or dizziness.
- H361: Suspected of damaging fertility or the unborn child.
- H373: May cause damage to organs through prolonged or repeated exposure if inhaled.
- H411: Toxic to aquatic life with long lasting effects.

Precautionary statement(s):
- P201: Obtain special instructions before use.
- P202: Do not handle until all safety precautions have been read and understood.
- P210: Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
- P233: Keep container tightly closed.
- P240: Ground/bond container and receiving equipment.
- P241: Use explosion-proof electrical/ ventilating/ lighting/ equipment.
- P242: Use only non-sparking tools.
- P243: Take precautionary measures against static discharge.
- P260: Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
- P264: Wash skin thoroughly after handling.
- P271: Use only outdoors or in a well-ventilated area.
- P273: Avoid release to the environment.
- P280: Wear protective gloves/ protective clothing/ eye protection/ face protection.
- 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/ shower.
- P304 + P340 + P312: IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
- P305 + P313: IF exposed or concerned: Get medical advice/ attention.
- P331: Do NOT induce vomiting.
- P332 + P313: If skin irritation occurs: Get medical advice/ attention.
- P362: Take off contaminated clothing and wash before reuse.
- P370 + P378: In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- P391: Collect spillage.
- P403 + P233: Store in a well-ventilated place. Keep container tightly closed.
- P403 + P235: Store in a well-ventilated place. Keep cool.
- P405: Store locked up.
- P501: Dispose of contents/ container to an approved waste disposal plant.

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms: Hexanes
Isohexane

SIGALD - 178918
Molecular weight : 86.18 g/mol

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-Hexane</td>
<td>Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H361, H336, H373, H304, H401, H411</td>
<td>&gt;= 50 - &lt; 70 %</td>
</tr>
<tr>
<td>Hexanes, isomers</td>
<td>Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; Asp. Tox. 1; Aquatic Chronic 2; H225, H315, H361, H336, H304, H411</td>
<td>&gt;= 20 - &lt; 30 %</td>
</tr>
<tr>
<td>methylcyclopentane</td>
<td>Flam. Liq. 2; Asp. Tox. 1; H225, H304</td>
<td>&gt;= 10 - &lt; 20 %</td>
</tr>
<tr>
<td>2-Methylpentane</td>
<td>Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H361, H336, H304, H401, H411</td>
<td>&gt;= 1 - &lt; 5 %</td>
</tr>
<tr>
<td>3-methylpentane</td>
<td>Flam. Liq. 2; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H319, H336, H304, H401, H411</td>
<td>&gt;= 1 - &lt; 5 %</td>
</tr>
</tbody>
</table>

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

**SECTION 4: First aid measures**

### 4.1 Description of first-aid measures

**General advice**
Consult a physician. Show this material 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
Do NOT induce vomiting. 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Dry powder Dry sand

Unsuitable extinguishing media
Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Combustible.

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.
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
Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).
6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion
Use explosion-proof equipment. Advice on protection against fire and explosion
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
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.

Moisture sensitive.

Storage class
Storage class (TRGS 510): 3: Flammable liquids

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

Ingredients with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-Hexane</td>
<td>110-54-3</td>
<td>TWA</td>
<td>50 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

Remarks Danger of cutaneous absorption

TWA 50 ppm 180 mg/m³ USA. NIOSH Recommended Exposure Limits

TWA 500 ppm 1,800 mg/m³ USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants

PEL 50 ppm 180 mg/m³ California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Skin
<table>
<thead>
<tr>
<th>Hexanes, isomers 92112-69-1</th>
<th>TWA</th>
<th>500 ppm</th>
<th>USA. ACGIH Threshold Limit Values (TLV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>STEL</td>
<td>1,000 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td>TWA</td>
<td>500 ppm 1,800 mg/m3</td>
<td>USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td>STEL</td>
<td>1,000 ppm 3,600 mg/m3</td>
<td>USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td>TWA</td>
<td>100 ppm 350 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>510 ppm 1,800 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td>PEL</td>
<td>500 ppm 1,800 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td>STEL</td>
<td>1,000 ppm 3,600 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td>2-Methylpentane 107-83-5</td>
<td>TWA</td>
<td>500 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td>STEL</td>
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</tr>
<tr>
<td></td>
<td>STEL</td>
<td>1,000 ppm 3,600 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td>3-methylpentane 96-14-0</td>
<td>TWA</td>
<td>500 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
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<tr>
<td></td>
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</tr>
</tbody>
</table>
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada.

### Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Biological Exposure Indices (BEI)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-Hexane</td>
<td>110-54-3</td>
<td>2,5-Hexanedione</td>
<td>0.5 mg/l</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

### 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.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 480 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 480 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.
Body Protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., 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.

SECTION 9: Physical and chemical properties
9.1 Information on basic physical and chemical properties

a) Appearance Form: liquid
b) Odor No data available
c) Odor Threshold No data available
d) pH No data available
e) Melting point/freezing point Melting point/range: -95 °C (-139 °F)
f) Initial boiling point and boiling range 68 - 70 °C 154 - 158 °F at 1,013 hPa
g) Flash point -23 °C (-9 °F)
h) Evaporation rate No data available
i) Flammability (solid, gas) No data available
j) Upper/lower flammability or explosive limits Upper explosion limit: 7.5 % (V)
Lower explosion limit: 1.1 % (V)
k) Vapor pressure No data available
l) Vapor density No data available
m) Density 0.672 g/cm³
Relative density No data available
n) Water solubility No data available
o) Partition coefficient: n-octanol/water No data available
p) Autoignition temperature 225 °C (437 °F)
q) Decomposition temperature No data available
r) Viscosity No data available
9.2 **Other safety information**
No data available

### SECTION 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**
Vapors may form explosive mixture with air.

10.4 **Conditions to avoid**
Heat, flames and sparks.

10.5 **Incompatible materials**
Oxidizing agents, Strong oxidizing agents

10.6 **Hazardous decomposition products**
In the event of fire: see section 5

### SECTION 11: Toxicological information

11.1 **Information on toxicological effects**

**Mixture**

**Acute toxicity**
Oral: No data available
Inhalation: No data available
Dermal: No data available

Acute toxicity estimate Dermal - 3,846 mg/kg
(Calculation method)
No data available

**Skin corrosion/irritation**
No data available

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
No data available

**Carcinogenicity**
IARC: No ingredient 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 ingredient 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

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information

Prolonged or repeated contact with skin may cause: defatting, Dermatitis, Contact with eyes can cause: Redness, Blurred vision, Provokes tears., Effects due to ingestion may include: Gastrointestinal discomfort, Central nervous system depression, Lung irritation, chest pain, pulmonary edema
Liver - Irregularities - Based on Human Evidence

Components

n-Hexane

Acute toxicity
LD50 Oral - Rat - male and female - 16,000 mg/kg (OECD Test Guideline 401)
LC50 Inhalation - Rat - 4 h - 172 mg/l
Remarks: (RTECS)
LD50 Dermal - Rabbit - male - > 2,000 mg/kg (OECD Test Guideline 402)
Remarks: (ECHA)

Skin corrosion/irritation
Skin - Rabbit
Result: Skin irritation - 24 h (OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation - 72 h (OECD Test Guideline 405)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: negative (OECD Test Guideline 429)

Germ cell mutagenicity
No data available
Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Species: Mouse - male
Result: negative
Remarks: (ECHA)

**Carcinogenicity**

No data available

**Reproductive toxicity**
Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. Suspected human reproductive toxicant Suspected of damaging fertility.

**Specific target organ toxicity - single exposure**
May cause drowsiness or dizziness. - Central nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Specific target organ toxicity - repeated exposure**
Inhalation - May cause damage to organs through prolonged or repeated exposure. - Nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Aspiration hazard**
May be fatal if swallowed and enters airways. Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

**Hexanes, isomers**

**Acute toxicity**
Oral: No data available
Inhalation: No data available
Dermal: No data available

**Skin corrosion/irritation**
Causes skin irritation. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
No data available

**Carcinogenicity**
No data available

**Reproductive toxicity**
Suspected of damaging fertility.

**Specific target organ toxicity - single exposure**
May cause drowsiness or dizziness.
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
The value is given in analogy to the following substances: 2-Methylpentane

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
May be fatal if swallowed and enters airways.

**methylcyclopentane**

**Acute toxicity**
Oral: No data available
Inhalation: No data available
Dermal: No data available

**Skin corrosion/irritation**
No data available

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
No data available

**Carcinogenicity**
No data available

**Reproductive toxicity**
No data available

**Specific target organ toxicity - single exposure**
No data available

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

**2-Methylpentane**

**Acute toxicity**
Oral: No data available
Inhalation: No data available
Dermal: No data available
No data available

**Skin corrosion/irritation**
No data available

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
No data available
3-methylpentane

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitization
Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
May be fatal if swallowed and enters airways.

SECTION 12: Ecological information

12.1 Toxicity

Mixture
No data available
12.2 Persistence and degradability
No data available

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.
Toxic to aquatic life with long lasting effects.

Components

n-Hexane
Toxicity to fish
LC50 - Pimephales promelas (fathead minnow) - 2.5 mg/l - 96 h
Remarks: (ECOTOX Database)

Toxicity to daphnia and other aquatic invertebrates
EC50 - Daphnia magna (Water flea) - 2.1 mg/l - 48 h
Remarks: (Lit.)

Hexanes, isomers
No data available

methylcyclopentane
No data available

2-Methylpentane
No data available

3-methylpentane
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Contact a licensed professional waste disposal service to dispose of this material. Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable.

Contaminated packaging
Dispose of as unused product.
SECTION 14: Transport information

**DOT (US)**
- UN number: 1208  Class: 3  Packing group: II
- Proper shipping name: Hexanes
- Reportable Quantity (RQ):
- Poison Inhalation Hazard: No

**IMDG**
- UN number: 1208  Class: 3  Packing group: II
- Proper shipping name: HEXANES
- Marine pollutant: yes
- Marine pollutant: yes

**IATA**
- UN number: 1208  Class: 3  Packing group: II
- Proper shipping name: Hexanes

SECTION 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**
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-Hexane</td>
<td>110-54-3</td>
<td>2020-07-14</td>
</tr>
</tbody>
</table>

**SARA 311/312 Hazards**
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information

**Further information**
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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.