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

1.1 Product identifiers
Product name : Isobutylbenzene
Product Number : 113166
Brand : Aldrich
CAS-No. : 538-93-2

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 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 3), H226
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (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)
H226  Flammable liquid and vapor.
H410  Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)
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.
P273  Avoid release to the environment.
P280  Wear protective gloves/ eye protection/ face protection.
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 dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391  Collect spillage.
P403 + P235  Store in a well-ventilated place. Keep cool.
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

3.1  Substances
Synonyms : 2-Methyl-1-phenylpropane
Formula : C_{10}H_{14}
Molecular weight : 134.22 g/mol
CAS-No. : 538-93-2
EC-No. : 208-706-2

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isobutylbenzene</td>
<td>Flam. Liq. 3; Aquatic Acute 1; Aquatic Chronic 1; H226, H400, H410 M-Factor - Aquatic Acute: 1</td>
<td>&lt;= 100 %</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**
Show this material safety data sheet to the doctor in attendance.

**If inhaled**
After inhalation: fresh air.

**In case of skin contact**
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

**In case of eye contact**
After eye contact: rinse out with plenty of water. Remove contact lenses.

**If swallowed**
After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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**
Carbon dioxide (CO2) Foam Dry powder

**Unsuitable extinguishing media**
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
In the event of fire, wear self-contained breathing apparatus.

5.4 Further information
Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Change contaminated clothing. Wash hands after working with substance. 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. Keep away from heat and sources of ignition.

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
Contains no substances with occupational exposure limit values.

8.2 Exposure controls
Appropriate engineering controls
Change contaminated clothing. Wash hands after working with substance.
**Personal protective equipment**

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

**Skin protection**
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact
Material: Viton®
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 10 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains. Risk of explosion.

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**SECTION 9: Physical and chemical properties**

9.1 Information on basic physical and chemical properties

a) Appearance
Form: clear, liquid
Color: colorless

b) Odor
No data available
c) Odor Threshold: No data available

d) pH: No data available

e) Melting point/freezing point: Melting point/range: -51 °C (-60 °F) - lit.

f) Initial boiling point and boiling range: 170 °C 338 °F at 981 hPa - lit.

g) Flash point: 48.1 °C (118.6 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9

h) Evaporation rate: No data available

i) Flammability (solid, gas): No data available

j) Upper/lower flammability or explosive limits: Upper explosion limit: 6 % (V)

k) Vapor pressure: 1.8 hPa at 20 °C (68 °F) - OECD Test Guideline 104

l) Vapor density: No data available

m) Density: 0.853 g/mL at 25 °C (77 °F) - lit.

n) Relative density: No data available

o) Water solubility: 0.012 g/l at 20 °C (68 °F) - OECD Test Guideline 105

p) Partition coefficient: n-octanol/water: No data available

q) Autoignition temperature: No data available

r) Decomposition temperature: No data available

s) Viscosity: No data available

t) Explosive properties: No data available

u) Oxidizing properties: No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions

Strong oxidizing agents
Violent reactions possible with:

**10.4 Conditions to avoid**
Heating.

**10.5 Incompatible materials**
No data available

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

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**SECTION 11: Toxicological information**

**11.1 Information on toxicological effects**

**Acute toxicity**
LO50 Oral - Rat - female - > 2,000 mg/kg
(OECD Test Guideline 423)
Inhalation: No data available
Dermal: No data available
No data available

**Skin corrosion/irritation**
Skin - human skin
Result: No skin irritation
(OECD Test Guideline 431)

**Serious eye damage/eye irritation**
Eyes - In vitro study
Result: No eye irritation
(OECD Test Guideline 492)

**Respiratory or skin sensitization**
Direct Peptide Reactivity Assay (DPRA) - Humans
Result: Not a skin sensitizer.
(OECD Test Guideline 442C)

**Germ cell mutagenicity**
Test Type: reverse mutation assay
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

**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

RTECS: DA3550000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

### SECTION 12: Ecological information

12.1 Toxicity
No data available

- **Toxicity to daphnia and other aquatic invertebrates**
  Immobilization EC50 - Daphnia magna (Water flea) - 0.6 mg/l - 45 h (OECD Test Guideline 202)

- **Toxicity to algae**
  Growth inhibition EC50 - Pseudokirchneriella subcapitata (green algae) - 0.42 mg/l - 72 h (OECD Test Guideline 201)
  Growth inhibition NOEC - Pseudokirchneriella subcapitata (green algae) - 0.26 mg/l - 72 h (OECD Test Guideline 201)

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 Endocrine disrupting properties
No data available

12.7 Other adverse effects
Discharge into the environment must be avoided.
SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)
UN number: 2709  Class: 3  Packing group: III
Proper shipping name: Butyl benzenes
Reportable Quantity (RQ):
Marine pollutant: yes  Poison Inhalation Hazard: No

IMDG
UN number: 2709  Class: 3  Packing group: III  EMS-No: F-E, S-D
Proper shipping name: BUTYLBENZENES
Marine pollutant: yes
Marine pollutant: yes

IATA
UN number: 2709  Class: 3  Packing group: III
Proper shipping name: Butylbenzenes

SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

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
Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

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Pennsylvania Right To Know Components

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Further information
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.