

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

### 1.1 Product identifiers

Product name : 4'-Isobutylacetophenone

Product Number : BP557  
Brand : Sigma-Aldrich  
CAS-No. : 38861-78-8

### 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  
Skin sensitization (Category 1), H317  
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



Signal word

Warning



Hazard statement(s)	
H226	Flammable liquid and vapor.
H317	May cause an allergic skin reaction.
H411	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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P272	Contaminated work clothing should not be allowed out of the workplace.
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.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
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	: 1-[4-(2-methylpropyl)phenyl]ethan-1-one
Molecular weight	: 176.25 g/mol
CAS-No.	: 38861-78-8

Component	Classification	Concentration
<b>1-[4-(2-methylpropyl)phenyl]ethan-1-one</b>		
	Skin Irrit. 2; Skin Sens. 1B; Aquatic Acute 2; Aquatic Chronic 2; H315, H317, H401, H411	<= 100 %

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



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## 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

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## 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.

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## 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. 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.

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# **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**

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.

### **Storage stability**

Recommended storage temperature  
2 - 8 °C

### **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

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# **SECTION 8: Exposure controls/personal protection**

## **8.1 Control parameters**

### **Ingredients 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, 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.

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## 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                 | No data available      |
| f) Initial boiling point and boiling range      | 107 °C 225 °F at 3 hPa |
| g) Flash point                                  | 54.4 °C (129.9 °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) Vapor pressure                               | No data available      |



l) Vapor density	No data available
m) Density	0.96 g/cm <sup>3</sup>
Relative density	No data available
n) Water solubility	partly miscible
o) Partition coefficient: n-octanol/water	log Pow: 3.59 at 21 °C (70 °F)
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

## 9.2 Other safety information

No data available

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## 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

No data available

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Reducing agents, Strong oxidizing agents, Strong bases

### 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

LD<sub>50</sub> Oral - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 401)

Inhalation: No data available

Dermal: No data available



**Skin corrosion/irritation**

Skin - in vitro test

Result: Irritating to skin. - 0.5 h  
(OECD Test Guideline 439)

**Serious eye damage/eye irritation**

Eyes - In vitro study

Result: No eye irritation - 0.5 h  
(OECD Test Guideline 437)

**Respiratory or skin sensitization**

Maximization Test - Guinea pig

The product is a skin sensitizer, sub-category 1B.  
(OECD Test Guideline 406)

**Germ cell mutagenicity**

Test Type: Ames test

Test system: *S. 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**

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

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**SECTION 12: Ecological information****12.1 Toxicity**

Toxicity to fish	static test LC50 - <i>Cyprinodon variegatus</i> (sheepshead minnow) - 10 - 30 mg/l - 96 h
Toxicity to daphnia and other aquatic	static test EC50 - <i>Daphnia magna</i> (Water flea) - 4.92 mg/l - 48 h (OECD Test Guideline 202)

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invertebrates

static test EC50 - other microorganisms - 0.3 - 3.0 mg/l - 96 h

static test EC50 - Daphnia - 7.7 mg/l - 48 h

Toxicity to algae static test NOEC - Pseudokirchneriella subcapitata - 1.69 mg/l - 72 h  
(OECD Test Guideline 201)

static test EC50 - Pseudokirchneriella subcapitata - 5.11 mg/l - 72 h  
(OECD Test Guideline 201)

Toxicity to bacteria static test EC50 - activated sludge - 280 mg/l - 3 h  
(OECD Test Guideline 209)

## 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d  
Result: 50 - 60 % - Not readily biodegradable.  
(OECD Test Guideline 301B)

## 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

Toxic to aquatic life with long lasting effects.

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

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

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.

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## SECTION 14: Transport information

### DOT (US)

UN number: 1224 Class: 3 Packing group: III

Proper shipping name: Ketones, liquid, n.o.s.

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

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**IMDG**

UN number: 1224    Class: 3    Packing group: III    EMS-No: F-E, S-D  
Proper shipping name: KETONES, LIQUID, N.O.S.

**IATA**

UN number: 1224    Class: 3    Packing group: III  
Proper shipping name: Ketones, liquid, n.o.s.

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**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**

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

**Pennsylvania Right To Know Components**

1-[4-(2-methylpropyl)phenyl]ethan-1-one	CAS-No. 38861-78-8	Revision Date
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1-[4-(2-methylpropyl)phenyl]ethan-1-one	CAS-No. 38861-78-8	Revision Date
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**New Jersey Right To Know Components**

1-[4-(2-methylpropyl)phenyl]ethan-1-one	CAS-No. 38861-78-8	Revision Date
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**California Prop. 65 Components**

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

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**SECTION 16: Other information****Further information**

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