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

1.1 Product identifiers

Product name: Vanillylacetone

Product Number: W312401
Brand: Aldrich
CAS-No.: 122-48-5

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

Not a hazardous substance or mixture.

2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

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

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms: Zingerone

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada.

Formula: \( \text{C}_{11}\text{H}_{14}\text{O}_3 \)
Molecular weight: 194.23 g/mol
CAS-No.: 122-48-5
EC-No.: 204-548-3

No components need to be disclosed according to the applicable regulations.

**SECTION 4: First aid measures**

**4.1 Description of first-aid measures**

*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*
Water Foam Carbon dioxide (CO2) 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 on intense heating.
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**
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: Avoid inhalation of dusts. 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.

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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 **Reference to other sections**
For disposal see section 13.

**SECTION 7: Handling and storage**

7.1 **Precautions for safe handling**
For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**

*Storage conditions*
Tightly closed. Dry.

*Storage stability*
Recommended storage temperature
2 - 8 °C

*Storage class*
Storage class (TRGS 510): 11: Combustible Solids

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**
Handle with impervious gloves.

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: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

**Respiratory protection**
Recommended Filter type: Filter type P1

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.

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.

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**SECTION 9: Physical and chemical properties**

9.1 **Information on basic physical and chemical properties**

| a) Appearance | Form: solid |
| 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 | 141 °C 286 °F at 0.7 hPa - lit. |
and boiling range

g) Flash point 113 °C (235 °F) - closed cup
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 1.14 g/mL at 25 °C (77 °F) - lit.
   Relative density No data available
n) Water solubility No data available
o) Partition coefficient: n-octanol/water No data available
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

SECTION 10: Stability and reactivity

10.1 Reactivity
Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

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

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
Strong heating.
10.5 **Incompatible materials**  
Strong oxidizing agents

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**  
Acute toxicity estimate Oral - 2,580 mg/kg  
(Calculation method)
LD50 Oral - Rat - 2,580 mg/kg
Inhalation: No data available
LD50 Dermal - Rabbit - > 5,000 mg/kg
No data available

**Skin corrosion/irritation**  
Skin - Rabbit
Result: Mild skin irritation - 24 h

**Serious eye damage/eye irritation**  
Remarks: 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
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: EL8900000

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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

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
No data available

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

**DOT (US)**
Not dangerous goods

**IMDG**
Not dangerous goods

**IATA**

Aldrich - W312401
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
No SARA Hazards

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

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

Pennsylvania Right To Know Components

<table>
<thead>
<tr>
<th>4-(4-Hydroxy-3-methoxyphenyl)butan-2-one</th>
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<th>Revision Date</th>
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New Jersey Right To Know Components

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SECTION 16: Other information

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.

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