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

1.1 Product identifiers

<table>
<thead>
<tr>
<th>Product name</th>
<th>Acetylacetone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product Number</td>
<td>P7754</td>
</tr>
<tr>
<td>Brand</td>
<td>SIGALD</td>
</tr>
<tr>
<td>Index-No.</td>
<td>606-029-00-0</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>123-54-6</td>
</tr>
</tbody>
</table>

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
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Short-term (acute) aquatic hazard (Category 3), H402

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 : Danger
Hazard statement(s)
H226 Flammable liquid and vapor.
H302 Harmful if swallowed.
H311 + H331 Toxic in contact with skin or if inhaled.
H402 Harmful to aquatic life.

Precautionary statement(s)
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233 Keep container tightly closed.
P240 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.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P311 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
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.
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

3.1 Substances
Synonyms: 2,4-Pentanediol

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetylacetone</td>
<td>Flam. Liq. 3; Acute Tox. 4; Acute Tox. 3; Aquatic Acute 3; H226, H302,</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

SIGALD - P7754
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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

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

If swallowed
After swallowing: immediately make victim drink water (two glasses at most). 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
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
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.
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. Avoid substance contact. 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 carefully 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 safe handling**  
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

**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**  
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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. Keep locked up or in an area accessible only to qualified or authorized persons.

**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>Acetylacetone</td>
<td>123-54-6</td>
<td>TWA</td>
<td>25 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td>Remarks</td>
<td></td>
<td></td>
<td></td>
<td>Danger of cutaneous absorption</td>
</tr>
</tbody>
</table>

Derived No Effect Level (DNEL)

<table>
<thead>
<tr>
<th>Application Area</th>
<th>Routes of exposure</th>
<th>Health effect</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Workers</td>
<td>Skin contact</td>
<td>Long-term systemic effects</td>
<td>12mg/kg BW/d</td>
</tr>
<tr>
<td>Workers</td>
<td>Inhalation</td>
<td>Long-term systemic effects</td>
<td>84 mg/m3</td>
</tr>
</tbody>
</table>

Predicted No Effect Concentration (PNEC)

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil</td>
<td>0.01582 mg/kg</td>
</tr>
<tr>
<td>Sea water</td>
<td>0.0026 mg/l</td>
</tr>
<tr>
<td>Fresh water</td>
<td>0.026 mg/l</td>
</tr>
<tr>
<td>Sewage treatment plant</td>
<td>1.32 mg/l</td>
</tr>
<tr>
<td>Fresh water sediment</td>
<td>0.155 mg/kg</td>
</tr>
<tr>
<td>Sea sediment</td>
<td>0.0155 mg/kg</td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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
required

Body Protection
Flame retardant antistatic protective clothing.

Respiratory protection
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.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: liquid
   Color: colorless

b) Odor
   ester-like

c) Odor Threshold
   No data available

d) pH
   No data available

e) Melting point/freezing point
   Melting point/range: -23 °C (-9 °F) - lit.

f) Initial boiling point and boiling range
   140.4 °C 284.7 °F - lit.

g) Flash point

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   Upper explosion limit: 11.4 % (V)
   Lower explosion limit: 1.7 % (V)

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

l) Vapor density
   No data available

m) Density
   0.975 g/cm3 at 25 °C (77 °F) - lit.
   Relative density
   0.9720 °C - Regulation (EC) No. 440/2008, Annex, A.3

n) Water solubility
   ca.153.8 g/l at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.6 - completely soluble

o) Partition coefficient: n-octanol/water
   log Pow: ca.0.68 at 40 °C (104 °F) - OECD Test Guideline 117 - Bioaccumulation is not expected.

p) Autoignition temperature
   No data available

q) Decomposition temperature
   Distillable in an undecomposed state at normal pressure.

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   none

9.2 Other safety information

Surface tension
   72 mN/m at 1g/l at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.5
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
Violent reactions possible with:
- Acids
- Bases
- Amines
- Aldehydes
- Anhydrides
- Oxidizing agents
- Hydrogen fluoride
- Halogenated compounds
- Cyanides
- Isocyanates
- Alkalines
- Bases
Risk of ignition or formation of inflammable gases or vapours with:
- Hydrides
- Nitrides
- Alkali metals

10.4 Conditions to avoid
Heating.

10.5 Incompatible materials
- Mild steel, Zinc, Copper, Nickel, various alloys

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

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
- LD50 Oral - Rat - female - 570 mg/kg
- Remarks: (ECHA)
- LC50 Inhalation - Rat - male and female - 4 h - 5.0305 mg/l - vapor

(OECD Test Guideline 403)
- Symptoms: mucosal irritations, Cough
- LD50 Dermal - Rabbit - female - 790 mg/kg
- Remarks: (ECHA)
- No data available

Skin corrosion/irritation
- Skin - Rabbit
- Result: No skin irritation - 4 h
- Remarks: (ECHA)
Serious eye damage/eye irritation
Eyes - Rabbit
Result: slight irritation
Remarks: (ECHA)

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

Germ cell mutagenicity
Laboratory experiments have shown mutagenic effects.
Test Type: Mutagenicity (mammal cell test): chromosome aberration.
Test system: Chinese hamster ovary cells
Metabolic activation: without metabolic activation
Method: OECD Test Guideline 473
Result: positive
Test Type: sister chromatid exchange assay
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 479
Result: positive
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

Test Type: Micronucleus test
Species: Mouse
Cell type: Bone marrow
Application Route: inhalation (vapor)
Method: US-EPA
Result: negative

Test Type: comet assay
Species: Rat
Cell type: Liver cells
Application Route: Oral
Result: negative
Remarks: (ECHA)

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
Ingestion of excessive amounts by pregnant animals resulted in maternal and fetal 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
Repeated dose toxicity - Rabbit - male and female - Dermal - 9 Days - NOAEL (No observed adverse effect level) - 244 mg/kg - LOAEL (Lowest observed adverse effect level) - 975 mg/kg
Remarks: (ECHA)

RTECS: SA1925000
Inhalation may provoke the following symptoms: Dizziness, Suffocation
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Systemic effects:

Dizziness
Headache
Shortness of breath
respiratory arrest
Unconsciousness

Damage to:

Liver
Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish
flow-through test LC50 - Pimephales promelas (fathead minnow) - 104 mg/l - 96 h
(OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates
- static test EC50 - Daphnia magna (Water flea) - 25.9 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae
- static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 83.22 mg/l - 72 h (OECD Test Guideline 201)

Toxicity to bacteria
- static test EC50 - activated sludge - 107.6 mg/l - 3 h (OECD Test Guideline 209)

Toxicity to fish (Chronic toxicity)
- flow-through test NOEC - Pimephales promelas (fathead minnow) - 10 mg/l - 34 d (OECD Test Guideline 210)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)
- semi-static test NOEC - Daphnia magna (Water flea) - 18 mg/l - 21 d (OECD Test Guideline 211)

12.2 Persistence and degradability

Biodegradability
- aerobic - Exposure time 28 d
  Result: 83 - 100 % - Readily biodegradable.
  (OECD Test Guideline 301C)

Ratio BOD/ThBOD
- 5.6 %
  Remarks: (Lit.)

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. 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)
- UN number: 2310
- Class: 3 (6.1)
- Packing group: III

SIGALD - P7754
Proper shipping name: Pentane-2,4-dione
Reportable Quantity (RQ): Poison Inhalation Hazard: No

**IMDG**
UN number: 2310  Class: 3 (6.1)  Packing group: III  EMS-No: F-E, S-D
Proper shipping name: PENTANE-2,4-DIONE

**IATA**
UN number: 2310  Class: 3 (6.1)  Packing group: III
Proper shipping name: Pentane-2,4-dione

**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, Chronic Health Hazard

**Massachusetts Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetylacetone</td>
<td>123-54-6</td>
<td>1993-04-24</td>
</tr>
</tbody>
</table>

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetylacetone</td>
<td>123-54-6</td>
<td>1993-04-24</td>
</tr>
</tbody>
</table>

**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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